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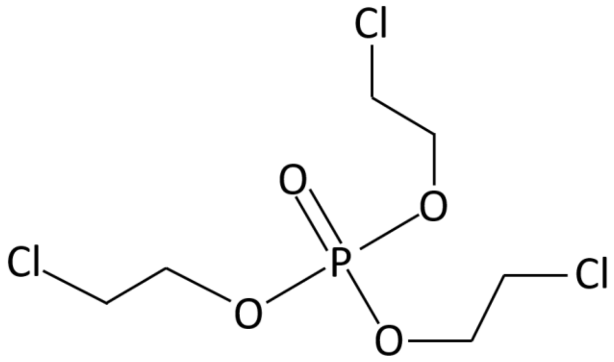
Office of Chemical Safety and
Pollution Prevention

Risk Evaluation for Tris(2-chloroethyl) Phosphate (TCEP)

Supplemental Information File:

Supplemental Information on Environmental Release and Occupational Exposure Assessment

CASRN: 115-96-8



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ABBREVIATIONS AND ACRONYMS

AC	Acute exposure concentration
ACC	American Chemistry Council
AC_{CT}	Acute exposure concentration (central tendency)
ACGIH	American Conference of Governmental Industrial Hygienists
AC_{HE}	Acute exposure concentration (high-end)
AD	Acute retained dose
ADC	Average daily concentration
ADC_{CT}	Average daily concentration (central tendency)
ADC_{HE}	Average daily concentration (high-end)
$ADC_{subchronic}$	Subchronic average daily concentration
AD_{CT}	Acute retained dose (central tendency)
ADD	Average daily dose
ADD_{CT}	Average daily dose (central tendency)
ADD_{HE}	Average daily dose (high-end)
AD_{HE}	Acute retained dose (high-end)
AIHA	American Industrial Hygiene Association
APDR	Acute potential dermal dose rate
APF	Assigned protection factor
AT_{acute}	Acute averaging time
AT_{C}	Averaging time for cancer risk
AT_{SC}	Averaging time for subchronic exposure
AWD	Annual working days
BLS	Bureau of Labor Statistics
BR	Breathing rate ratio
BW	Body weight
C	Contaminant concentration in air
CDR	Chemical Data Reporting (Rule)
CEB	Chemical Engineering Branch
CEC	Commission for Environmental Cooperation
CEHD	Chemical Exposure Health Database
CEPE	European Council of the Paint, Printing Ink, and Artist’s Colours Industry
CFR	Code of Federal Regulations
CPS	Current population survey
CPSC	Consumer Product Safety Commission
CT	Central tendency
$Cv_{activity}$	Exposure activity volumetric concentration
$Days_{application}$	Days of application
$D_{container\_lab\_analysis}$	Diameter of laboratory analysis containers
DD	Dermal daily dose
DMR	Discharge Monitoring Report
$D_{opening}$	Diameter of opening
$D_{opening\_blending}$	Diameter of opening for blending/process operations
$D_{opening\_cont\text{-}cleaning}$	Diameter of opening for container cleaning
$D_{opening\_curing}$	Diameter of opening for curing
$D_{opening\_equip\text{-}cleaning}$	Diameter of opening for equipment cleaning

$D_{\text{opening\_filter-changeout}}$	Diameter of opening for filter changeout
$D_{\text{opening\_sampling}}$	Diameter of opening for sampling
DUR	Site daily use rate
ECETOC TRA	European Centre for Ecotoxicology and Toxicology of Chemicals’ Targeted Risk Assessment tool (model)
ED	Exposure duration
EF	Exposure frequency
EF_{SC}	Subchronic exposure frequency
EF_{yearly}	Number of exposure days
ELG	Effluent Limitation Guidelines
EPA	Environmental Protection Agency
ESD	Emission Scenario Document
ETIMEOFF	Months when not working (CPS data)
f	Fractional number of working days per year a worker works
$F_{\text{activity\_loss}}$	Loss fraction for activity
$F_{\text{correction\_factor}}$	Vapor pressure correction factor
F_{exposure}	Fraction of operating days with worker exposure
$F_{\text{loss\_can}}$	Loss fraction for cans/small containers
$F_{\text{loss\_cont}}$	Container loss fraction
$F_{\text{loss\_cont-residue}}$	Loss fraction for containers
$F_{\text{loss\_drum}}$	Loss fraction for drum containers
$F_{\text{loss\_equipment}}$	Loss fraction for equipment cleaning
$F_{\text{loss\_filter}}$	Loss fraction for filter changeout
$F_{\text{loss\_off-spec}}$	Loss fraction for off-specification wastes
$F_{\text{loss\_smallcont}}$	Loss fraction for small containers
FR	Federal Register
$F_{\text{saturation\_loading}}$	Saturation factor loading
$F_{\text{saturation\_unloading}}$	Saturation factor unloading
$F_{\text{TCEP\_import}}$	Import concentration
$F_{\text{TCEP\_prod}}$	Product concentration
G	Vapor generation rate
G_{activity}	Vapor generation rate for an activity
GS	Generic Scenario
h	Exposure durations
HAP	Hazardous Air Pollutant
HE	High-end
HVLP	High volume low pressure
IFC	Industrial Function Category
IL	Illinois
IOM	Institute of Occupational Medicine
k	Mixing Factor
LADC	Lifetime average daily concentration
$LADC_{CT}$	Lifetime average daily concentration (central tendency)
$LADC_{HE}$	Lifetime average daily concentration (high-end)
LADD	Lifetime average daily dose
$LADD_{CT}$	Lifetime average daily dose (central tendency)

$\mathrm{LADD}_{\mathrm{HE}}$	Lifetime average daily dose (high-end)
LOD	Limit of detection
LT	Lifetime Years for cancer risk
m_{batch}	Batch size
$\mathrm{MW}_{\mathrm{TCEP}}$	Molecular weight
NAICS	North American Industry Classification System
$N_{\mathrm{batch\_yr}}$	Annual number of batches
$N_{\mathrm{cont\_yr}}$	Annual number of import containers
NEI	National Emissions Inventory
NESHAP	National Emissions Standards of Hazardous Air Pollutants
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
NIOSH	National Institute of Occupational Safety and Health
$N_{\mathrm{prodcont\_yr}}$	Annual number of product containers
N_{s}	Number of sites
NY	New York
OAQPS	Office of Air Quality Planning and Standards (EPA)
OARS	Occupational Alliance for Risk Science
OD	Operating days
OECD	Organisation for Economic Co-Operation and Development
OEL	Occupational exposure limit
OES	Occupational exposure scenario
$\mathrm{OH}_{\mathrm{batch}}$	Hours per batch
OH_{C}	Operating hours for equipment cleaning
$\mathrm{OH}_{\mathrm{curing}}$	Time for drying/curing
$\mathrm{OH}_{\mathrm{equip\_cleaning}}$	Hours per equipment cleaning
$\mathrm{OH}_{\mathrm{rp}}$	Operating hours for release points
$\mathrm{OH}_{\mathrm{sampling}}$	Hours per analysis sampling
OIS	Occupational Safety and Health Information System
ONU	Occupational non-user
OPPT	Office of Pollution Prevention and Toxics
OSHA	Occupational Safety and Health Administration
OVS	OSHA Versatile Sampler
P	Pressure
P_atm	Pressure (atm)
P_torr	Pressure (torr)
PAPR	Power Air-Purifying Respirator
PBZ	Personal Breathing Zone
PEI	PEI Associates, Inc.
PEL	Permissible exposure limit
PF	Protection factor
POTW	Publicly owned treatment work
PPE	Personal protective equipment
PV	Production volume
PV_lb	Production volume assessed
$\mathrm{PV}_{\mathrm{site}}$	Facility Production Rate
Q	Ventilation Rate

$Q_{product}$	Facility Production Rate
$Q_{stock\_site\_day}$	Daily throughput of stock solutions
R	Universal gas constant
$RATE_{air\_speed}$	Air speed
$RATE_{fill}$	Fill rate of container
$RATE_{fill\_drum}$	Fill rate of drum
$RATE_{fill\_drum/small}$	Fill rate of small drum
$RATE_{fill\_small}$	Fill rate of small container
$RATE_{fill\_smallcont}$	Fill rate of small container
RD	Release days
REL	Recommended exposure limits
$Release\_Year_{activity}$	TCEP released for activity per site-year
$Release\_Year_{RP}$	TCEP released for release point
$\rho_{product}$	Product density
ρ_{TCEP}	TCEP density
RP_7	Filter changeout
RP_9	Product sampling
RP_{11}	Equipment cleaning
RQ	Reportable quantity
SADC	Subchronic average daily concentration
$SADC_{CT}$	Subchronic average daily concentration (central tendency)
$SADC_{HE}$	Subchronic average daily concentration (high-end)
SAR	Supplied-air respirator
SCBA	Self-contained breathing apparatus
SCD	Days for subchronic duration
SCDC	Subchronic average daily concentrations
$SCDD_{CT}$	Subchronic average daily doses (central tendency)
$SCDD_{HE}$	Subchronic average daily doses (high-end)
SDS	Safety data sheet
SIC	Standard Industrial Classification
SIPP	Survey of Income and Program Participation
SpERC	Specific Environmental Release Category
SRRP	Source Reduction Research Partnership
SUSB	Statistics of U.S. Businesses
T	Temperature
TAGE	Worker age in SIPP
TCEP	Tris(2-chloroethyl) phosphate
TDS	Technical data sheet
TE	Transfer efficiency
$Time_{activity}$	Operating time for activity
$TIME_{operating\_days}$	Operating days
$TIME_{RP}$	Operating time for a release point
TJBIND1	Employed individual works (SIPP data)
TLV	Threshold limit value
TMAKMNYR	First year worked (SIPP Data)
TOC	Total organic carbon

TRI	Toxics Release Inventory
TSCA	Toxic Substances Control Act
TWA	Time-weighted average
V_{batch}	Batch volume
V_{fill_cont}	Small container volume
V_{import_cont}	Import container volume
Vm_{TCEP}	Molar volume of TCEP
VOC	Volatile organic compound
VP	TCEP vapor pressure
V_{prod_cont}	Small container volume
W	Workers
WEEL	Workplace Environmental Exposure Level
WoSE	Weight of scientific evidence
WWT	Wastewater treatment
WY	Working years per lifetime

EXECUTIVE SUMMARY

TSCA section 6(b)(4) requires the U.S. Environmental Protection Agency (EPA) to establish a risk evaluation process. In performing risk evaluations for existing chemicals, EPA is directed to "determine whether a chemical substance presents an unreasonable risk of injury to health or the environment, without consideration of costs or other non-risk factors, including an unreasonable risk to a potentially exposed or susceptible subpopulation identified as relevant to the risk evaluation by the Administrator under the conditions of use." In December of 2019, EPA published a list of 22 chemical substances that are the subject of the Agency's chemical risk evaluations (84 FR 71924, December 20, 2019), as required by TSCA section 6(b)(2)(A). TCEP was one of these chemicals.

TCEP, also known as 2-chloroethanol phosphate, tri(beta-chloroethyl) phosphate, phosphoric acid tris(2-chloroethyl) ester, and tris(chloroethyl)phosphate, is a colorless volatile liquid primarily used as an additive flame retardant in paint and coating manufacturing, polymers including polyester resin, and articles, for use in aerospace equipment and products; it is also used as a laboratory chemical. In the past, TCEP was primarily incorporated into rigid foams used for roofing insulation with minor uses for other building and construction materials such as wood resin composites. Other past, minor, uses of TCEP were for fabric and textiles and foam seating and bedding products. Some of these products may still be present in consumers' homes and commercial infrastructure. TCEP is not subject to federal regulations and reporting requirements, but it is listed on California's Proposition 65. TCEP was only recently added to the Toxics Release Inventory (TRI) but will not have any reporting until 2024.

Focus of the Supplemental Report on Environmental Release and Occupational Exposure Assessment
During scoping, EPA considered all known TSCA uses for TCEP. The most recently available data from the 2016 Chemical Data Reporting (CDR) indicated approximately 39,682 pounds were either manufactured or imported in the United States in 2015 (U.S. EPA, 2019). There were no reporters for manufacturing or importing TCEP into the United States for the 2020 CDR (U.S. EPA, 2020a). The largest uses of TCEP are as a flame retardant in paint and coating manufacturing, polymers including polyester resin, and articles, such as aerospace equipment and products. Secondary uses of TCEP includes incorporating TCEP into fabric and textiles, foam seating and bedding products, and as a laboratory chemical. In the past, TCEP was incorporated into building and construction materials, such as roofing insulation and wood resin composites.

Exposures to workers, consumers, general populations, and ecological species may occur from industrial, commercial, and consumer uses of TCEP and releases to air, water, or land. Workers and occupational non-users (ONUs) may be exposed to TCEP during conditions of use such as the recycling of electronics. Exposure to the general population and ecological species may occur from industrial releases related to the manufacture, import, processing, distribution, and use of TCEP. This supplemental report provides the details of the assessment of the environmental releases and occupational exposures from each condition of use (COU) of TCEP.

Approach for Environmental Releases and Occupational Exposures in this Risk Evaluation
EPA evaluated environmental releases of TCEP to air, water, and land from the conditions of use assessed in this risk evaluation. EPA used release data from literature sources where available and used modeling approaches where release data were not available.

EPA evaluated acute, subchronic, and chronic exposures to workers and ONUs in association with TCEP conditions of use. EPA used inhalation monitoring data from literature sources where available and exposure models where monitoring data were not available or were deemed insufficient for capturing actual exposure within the COU. EPA also used modeling approaches to estimate dermal exposures to workers.

Uncertainties of this Risk Evaluation

There are a number of uncertainties associated with the monitoring and modeling approaches used to assess TCEP environmental releases and occupational exposures. For example, the lack of TCEP facility production volume data and use of throughput estimates based on CDR reporting thresholds may not be representative of the total production volume of TCEP used in the United States. EPA also used generic EPA models and default input parameter values when data when site-specific data was not available. In addition, site-specific differences in use practices and engineering controls exist, but are largely unknown, this represents another source of variability that EPA could not quantify in the assessment.

Environmental and Exposure Pathways Considered in this Risk Evaluation

EPA assessed environmental releases to air, water, and land to estimate exposures to the general population and ecological species for TCEP conditions of use outlined under *Focus of the Supplemental Report on Environmental Release and Occupational Exposure Assessment* on page 17. The environmental release estimates developed by EPA are used to estimate the presence of TCEP in the environment and biota and evaluate the environmental hazards. The release estimates were used to model exposure to the general population and ecological species where environmental monitoring data were not available.

EPA assessed risks for acute, subchronic, and chronic exposure scenarios in workers (those directly handling TCEP) and ONUs (workers not directly involved with the use of TCEP) for TCEP conditions of use outlined under *Focus of the Supplemental Report on Environmental Release and Occupational Exposure Assessment* on page 17. EPA assumed that workers and ONUs would be individuals of both sexes (age 16 years and older, including pregnant workers) based upon occupational work permits, although exposures to younger workers in occupational settings cannot be ruled out. An objective of the monitored and modeled inhalation data was to provide separate exposure level estimates for workers and ONUs. Dermal exposures were considered for workers but not ONUs.

1 INTRODUCTION

1.1 Overview

TSCA section 6(b)(4) requires the EPA to establish a risk evaluation process. In performing risk evaluations for existing chemicals, EPA is directed to "determine whether a chemical substance presents an unreasonable risk of injury to health or the environment, without consideration of costs or other non-risk factors, including an unreasonable risk to a potentially exposed or susceptible subpopulation identified as relevant to the risk evaluation by the Administrator under the conditions of use." In December of 2019, EPA published a list of 22 chemical substances that are the subject of the Agency's initial chemical risk evaluations (84 FR 71924, December 20, 2019), as required by TSCA section 6(b)(2)(A). Tris(2-chloroethyl) phosphate (TCEP) was one of these chemicals.

TCEP, also known as 2-chloroethanol phosphate, tri(beta-chloroethyl) phosphate, phosphoric acid tris(2-chloroethyl) ester, and tris(chloroethyl)phosphate, is a colorless volatile liquid that is used primarily as a flame retardant in various applications, such as coatings, resins, plastic articles, and a laboratory chemical in some instances. All uses are subject to federal and state regulations and reporting requirements. TCEP is not a Toxics Release Inventory (TRI)-reportable substance; however, it is on the Toxic Substances Control Act (TSCA) Inventory and reported under the CDR rule.

1.2 Scope

EPA assessed environmental releases and occupational exposures for conditions of use as described in Table 2-2 of the *Final Scope of the Risk Evaluation for Tris(2-chloroethyl) phosphate (TCEP) CASRN 115-96-8* (U.S. EPA, 2020c). To estimate environmental releases and occupational exposures, EPA first developed Occupational Exposure Scenarios (OESs) related to the conditions of use of TCEP. An OES is based on a set of facts, assumptions, and inferences that describe how releases and exposures takes place within an occupational condition of use. How releases/exposures take place may be similar across multiple COUs, or there may be several ways in which releases/exposures takes place for a given COU. Table 1-1 shows mapping between the conditions of use in Table 2-2 of the Scope Document to the OES assessed in this report.

In general, EPA mapped OESs to COUs using professional judgment based on available data and information. Several of the COU categories and subcategories were grouped and assessed together in a single OES due to similarities in the processes or lack of data to differentiate between them. This grouping minimized repetitive assessments. In other cases, conditions of use subcategories were further delineated into multiple OES based on expected differences in process equipment and associated releases/exposure potentials between facilities. EPA assessed environmental releases and occupational exposures for the following TCEP OES:

1. Import – Repackaging
2. Incorporation into Paints and Coatings
3. Use in Paints and Coatings
4. Incorporation into Resins
5. Incorporation into Articles
6. Use and Installation of Articles
7. Recycling
8. Waste Handling, Disposal and Treatment
9. Distribution in Commerce

10. Use of Laboratory Chemicals

EPA was informed by the Auto Alliance that it is possible that TCEP-containing articles, replacement parts, and paints could be in use in the automotive industry, however, no data regarding product(s), operating site(s), etc was provided. In the absence of reasonably available data to refine our modelling, EPA expects modelled environmental releases and occupational exposures to be similar to the OES's already previously assessed for other industry sectors on a per generic site basis. Specifically, this means that that the recently added industrial use of paints and coatings would be similar to the commercial use of paints and coatings and that the recently modified COUs of incorporation into article and installation of article would be similar regardless of whether or not it is being done for aircraft or automobiles.

Table 1-1. Crosswalk of Subcategories of Use Listed in the Final Scope Document to OESs Assessed in the Risk Evaluation

Life Cycle Stage	Category	Subcategory	OES
Manufacturing[a]	Import	Import	Import – Repackaging; see Section 3.1
Processing	Incorporation into formulation, mixture or reaction product	Flame retardant in: Paint and coating manufacturing	Incorporation into Paints and Coatings; see Section 3.2
	Incorporation into formulation, mixture or reaction product	Polymers used in aerospace equipment and products and automotive articles and replacement parts containing TCEP	Incorporation into Resins; see Section 3.4
	Incorporation into article	Aerospace equipment and products and automotive articles and replacement parts containing TCEP	Incorporation into Articles; see Section 3.5
	Recycling	Recycling	Recycling; see Section 3.7
Distribution in commerce	Distribution in commerce	Distribution in commerce	Distribution in Commerce; see Section 3.9
Industrial Use	Paints and coatings	Paints and coatings	Use in Paints and Coatings; see Section 3.3
	Other use	Aerospace equipment and products and automotive articles and replacement parts containing TCEP	Use and Installation of Articles; see Section 3.6
Commercial Use	Other use	Aerospace equipment and products	
Commercial Use	Paints and coatings	Paints and coatings	Use in Paints and Coatings; see Section 3.3
	Other use	*e.g.*, Laboratory chemicals	Use in Laboratory Chemicals; see Section 3.10

Life Cycle Stage	Category	Subcategory	OES
	Furnishing, cleaning, treatment/care products	Fabric and textile products	Waste Handling, Disposal, and Treatment; see Section 3.8
	Construction, paint, electrical, and metal products	Building/construction materials – insulation	
	Furnishing, cleaning, treatment/care products	Foam Seating and Bedding Products	
	Construction, paint, electrical, and metal products	Building/construction materials – wood and engineered wood products – wood resin composites	
Consumer Use	Paints and coatings	Paints and coatings	Not included in the supplemental report.
	Furnishing, cleaning, treatment/care products	Fabric and textile products	
	Construction, paint, electrical, and metal products	Building/construction materials – insulation	
	Furnishing, cleaning, treatment/care products	Foam Seating and Bedding Products	
	Construction, paint, electrical, and metal products	Building/construction materials –wood and engineered wood products – wood resin composites	
Disposal	Disposal	Disposal	Waste Handling, Disposal, and Treatment; see Section 3.8

[a] The repackaging scenario covers only those sites that purchase TCEP or TCEP-containing products from domestic and/or foreign suppliers and repackage the TCEP from bulk containers into smaller containers for resale. Sites that import and directly process/use TCEP are assessed in the relevant OES. Sites that import and either directly ship to a customer site for processing or use or warehouse the imported TCEP and then ship to customers without repackaging are assumed to have no exposures or releases and only the processing/use of TCEP at the customer sites are assessed in the relevant OES.

[b] Each of the COU of TCEP may generate waste streams of the chemical that are collected and transported to third-party sites for disposal, treatment, or recycling. Industrial sites that treat, dispose, or directly discharge onsite wastes that they themselves generate are assessed in each COU assessment. This section only assesses wastes of TCEP that are generated during a COU and sent to a third-party site for treatment, disposal, or recycling.

EPA’s assessment of releases includes quantifying annual and daily releases of TCEP to air, water, and land. Releases to air include both fugitive and stack air emissions and emissions resulting from on-site waste treatment equipment, such as incinerators. For purposes of this report, releases to water include both direct discharges to surface water and indirect discharges to publicly owned treatment works (POTWs) or non-POTW wastewater treatment (WWT). It should be noted that for purposes of risk evaluation, discharges to POTW and non-POTW WWT are not evaluated the same as discharges to surface water. EPA considers removal efficiencies of POTWs and WWT and environmental fate and transport properties when evaluating risks from indirect discharges. Releases to land include any disposal of liquid or solids wastes containing TCEP into landfills, land treatment, surface impoundments, or other land applications. The purpose of this supplemental report is only to quantify releases; therefore, downstream environmental fate and transport factors used to estimate exposures to the general population and ecological species are not discussed. The details on how these factors were considered when determining risk are described in the *Risk Evaluation for Tris(2-chloroethyl) Phosphate (TCEP) CASRN 115-96-8* (U.S. EPA, 2024) (hereinafter referred to as the “TCEP Risk Evaluation”).

For workplace exposures, EPA considered exposures to both workers who directly handle TCEP and ONUs who do not directly handle TCEP but may be exposed to vapors or mists that enter their breathing zone while working in locations in close proximity to where TCEP is being used. EPA evaluated inhalation exposures to both workers and ONUs and dermal exposures to workers.

2 COMPONENTS OF AN OCCUPATIONAL EXPOSURE AND RELEASE ASSESSMENT

The occupational exposure and environmental release assessment of each COU comprises the following components:

- **Process Description:** A description of the OES, including the function of the chemical in the OES; physical forms and weight fractions of the chemical throughout the process; the total production volume associated with the OES; per site throughputs/use rates of the chemical; operating schedules; and process vessels, equipment, and tools used during the COU.
- **Estimates of Number of Facilities:** An estimate of the number of sites that use TCEP for the given OES.
- **Environmental Release Points:** A description of each of the potential sources of environmental releases in the process and their expected media of release for the given OES.
- **Environmental Release Assessment Results:** Estimates of chemical released into each environmental media (surface water, POTW, non-POTW WWT, fugitive air, stack air, and each type of land disposal).
- **Worker Activities:** A descriptions of the worker activities, including an assessment for potential points of worker and ONU exposure.
- **Number of Workers and ONUs:** An estimate of the number of workers and ONUs potentially exposed to the chemical for the given OES.
- **Occupational Inhalation Exposure Results:** Central tendency and high-end estimates of inhalation exposure to workers and ONUs. See Section 2.4.3 for a discussion of EPA’s statistical analysis approach for assessing inhalation exposure.
- **Occupational Dermal Exposure Results:** Central tendency and high-end estimates of dermal exposure to workers. See Section 2.4.4 for a discussion of EPA’s approach for assessing dermal exposure.

2.1 Approach and Methodology for Process Descriptions

EPA performed a literature search to find descriptions of processes involved in each OES. Where data were available to do so, EPA included the following information in each process description:

- Total production volume associated with the OES,
- Name and location of sites the OES occurs,
- Facility operating schedules (*e.g.*, year-round, five days/week, batch process, continuous process, multiple shifts),

- Key process steps,
- Physical form and weight fraction of the chemical throughout the process steps,
- Information on receiving and shipping containers, and
- Ultimate destination of chemical leaving the facility.

Where TCEP-specific process descriptions were unclear or not available, EPA referenced generic process descriptions from literature, including relevant Emission Scenario Documents (ESD) or Generic Scenarios (GS). Process descriptions for each OES can be found in Section 3.

2.2 Approach and Methodology for Estimating Number of Facilities

To estimate the number of facilities within each OES, EPA used a combination of bottom-up analyses of EPA reporting programs and top-down analyses of U.S. economic data and industry-specific data. Generally, EPA used the following steps to develop facility estimates:

1. Identify or "map" each facility reporting for TCEP in the 2016 and 2020 CDR (U.S. EPA, 2019, 2020a) to an OES. The full details of the methodology for mapping facilities from EPA reporting programs is described in Appendix A. In brief, mapping consists of using facility reported industry sectors (typically reported as either North American Industry Classification System (NAICS) or Standard Industrial Classification (SIC) codes), and chemical activity, processing, and use information to assign the most likely OES to each facility.
2. Based on the reporting thresholds and requirements of each dataset, evaluate whether the data in the reporting programs is expected to cover most or all of the facilities within the OES. If so, no further action was required, and EPA assessed the total number of facilities in the OES as equal to the count of facilities mapped to the OES from each dataset. If not, EPA proceeded to Step 3.
3. Supplement the available reporting data with U.S. economic and market data using the following method:
    a. Identify the NAICS codes for the industry sectors associated with the OES.
    b. Estimate total number of facilities using the U.S. Census' Statistics of U.S. Businesses (SUSB) data on total establishments by 6-digit NAICS.
    c. Use market penetration data to estimate the percentage of establishments likely to be using TCEP instead of other chemicals.
    d. Combine the data generated in Steps 3a through 3c to produce an estimate of the number of facilities using TCEP in each 6-digit NAICS code and sum across all applicable NAICS codes for the OES to arrive at a total estimate of the number of facilities within the OES. Typically, EPA assumed this estimate encompasses the facilities identified in Step 1; therefore, EPA assessed the total number of facilities for the OES as the total generated from this analysis.
4. If market penetration data required for Step 3c are not available, use generic industry data from GSs, ESDs, and other literature sources on typical throughputs/use rates, operating schedules, and the TCEP production volume used within the OES to estimate the number of facilities. In cases where EPA identified a range of operating data in the literature for an OES, EPA used stochastic modeling to provide a range of estimates for the number of facilities within an OES. EPA provided the details of the approaches, equations, and input parameters used in stochastic modeling in the relevant OES sections throughout this report.

2.3 Environmental Releases Approach and Methodology

Releases to the environment are a component of potential exposure and may be derived from reported data that are obtained through direct measurement via monitoring, calculations based on empirical data, and/or assumptions and models. For each OES, EPA attempted to provide annual releases, high-end and central tendency daily releases, and the number of release days per year for each media of release (air, water, and land).

EPA used the following hierarchy in selecting data and approaches for assessing environmental releases:

1. Monitoring and measured data:
    a. Releases calculated from site-specific concentration in medium and flow rate data
    b. Releases calculated from mass balances or emission factor methods using site-specific measured data
2. Modeling approaches:
    a. Surrogate release data
    b. Fundamental modeling approaches
    c. Statistical regression modeling approaches
3. Release limits:
    a. Company-specific limits
    b. Regulatory limits (*e.g.*, National Emission Standards for Hazardous Air Pollutants [NESHAPs] or effluent limitations/requirements

EPA's preference was to rely on facility-specific release data reported in TRI, Discharge Monitoring Report (DMR), and the National Emissions Inventory (NEI), where available. However, TCEP is not a TRI reportable substance, a water pollutant monitored in non-POTW facility DMRs, or a Hazardous Air Pollutant (HAP) reported in NEI. Therefore, EPA primarily relied on data from literature, relevant ESDs or GSs, existing EPA models, and/or relevant regulatory limits to estimate releases. EPA's general approach to estimating releases from these sources is described in Sections 2.3.1 through 2.3.5. Specific details related to the use of release data or models for each OES can be found in Section 3.

The final release results may be described as a point estimate (*i.e.*, a single descriptor or statistic, such as central tendency or high-end) or a full distribution. EPA considered three general approaches for estimating the final release result:

1. **Deterministic calculations:** EPA used combinations of point estimates of each input parameter to estimate a central tendency and high-end for each final release result. EPA documented the method and rationale for selecting parametric combinations to be representative of central tendency and high-end in the relevant OES subsections in Section 3.
2. **Probabilistic (stochastic) calculations:** EPA used a Monte Carlo simulation using the full distribution of each input parameter to calculate a full distribution of the final release results and selecting the 50th and 95th percentiles of this resulting distribution as the central tendency and high-end, respectively.
3. **Combination of deterministic and probabilistic calculations:** EPA had full distributions for some parameters but point estimates of the remaining parameters. For example, EPA used a Monte Carlo simulation to estimate annual throughputs and emission factors, but only had point estimates of release frequency and production volume. In this case, EPA documented the approach and rationale for combining point estimates with distribution results for estimating central tendency and high-end results in the relevant OES subsections in Section 3.

2.3.1 Identifying Release Points

EPA performed a literature search to identify process operations that could potentially result in releases of TCEP to air, water, or land from each OES. For each OES, EPA identified the release points and the associated media of release. Where TCEP-specific release points were unclear or not available, EPA referenced relevant ESDs or GSs. Descriptions of release points for each OES can be found in Section 3.

2.3.2 Estimating Release Days per Year

EPA typically assumed the number of release days per year from any release point will be equal to the number of operating days at the facility unless information is available to indicate otherwise. To estimate the number of operating days, EPA used the following hierarchy:

1. **Facility-specific data:** EPA used facility-specific operating days per year data if available. If facility-specific data was not available for one facility of interest but was available for other facilities within the same OES, EPA estimated the operating days per year using one of the following approaches:
    a. If other facilities have known or estimated average daily use rates, EPA calculated the days per year as:

$$\text{Days Per Year} = \frac{\text{Estimated Annual Use Rate for the Facility (kg/yr)}}{\text{Average Daily Use Rate from Facilities with Available Data (kg/day)}}$$

    b. If facilities with days per year data do not have known or estimate average daily use rates, EPA used the average number of days per year from the facilities with such data available.
2. **Industry-specific data:** EPA used industry-specific data available from GSs, ESDs, trade publications, or other relevant literature.
3. **Manufacture of large-production volume (PV) commodity chemicals:** For the manufacture of the large-PV commodity chemicals, EPA used a value of 350 days per year. This assumes the plant runs seven days per week and 50 weeks per year (with two weeks down for turnaround) and assumes that the plant is always producing the chemical.
4. **Manufacture of lower-PV specialty chemicals:** For the manufacture of lower-PV specialty chemicals, it is unlikely the chemical is being manufactured continuously throughout the year. Therefore, EPA used a value of 250 days per year. This assumes the plant manufactures the chemical five days per week and 50 weeks per year (with two weeks down for turnaround).
5. **Processing as reactant (intermediate use) in the manufacture of commodity chemicals:** Similar to #3, EPA assumed the manufacture of commodity chemicals occurs 350 days per year such that the use of a chemicals as a reactant to manufacture a commodity chemical would also occur 350 days per year.
6. **Processing as reactant (intermediate use) in the manufacture of specialty chemicals:** Similar to #4, the manufacture of specialty chemicals is not likely to occur continuously throughout the year. Therefore, EPA used a value of 250 days per year.
7. **Other Chemical Plant OES (*e.g.*, processing into formulation and use of industrial processing aids):** For these OES, EPA assumed that the chemical of interest is not always in use at the facility, even if the facility operates 24/7. Therefore, in general, EPA used a value of 300 days/year based on the “SpERC fact sheet – Formulation & (re)packing of substances and mixtures – Industrial (Solvent-borne)” which uses a default of 300 days per year for the chemical industry (ESIG, 2012). However, in instances where the OES uses a low volume of the chemical of interest, EPA used 250 days per year as a lower estimate.
8. **POTWs:** Although EPA expects POTWs to operate continuously over 365 days per year, the discharge frequency of the chemical of interest from a POTW will be dependent on the discharge

patterns of the chemical from the upstream facilities discharging to the POTW. However, there can be multiple upstream facilities (possibly with different OES) discharging to the same POTW and information to determine when the discharges from each facility occur on the same day or separate days is typically not available. Therefore, EPA could not determine an exact number of days per year the chemical of interest is discharged from the POTW and used a value of 365 days per year.

9. **All Other OES:** Regardless of what the facility operating schedule is, other OES are unlikely to use the chemical of interest every day. Therefore, EPA used a value of 250 days per year for these OES.

2.3.3 Estimating Releases from Models

Where releases were expected for an OES but TRI, DMR, and/or NEI data were not available or where EPA determined they did not capture the entirety of environmental releases for an OES, EPA utilized models to estimate environmental releases. Outputs from models may be the result of deterministic calculations, stochastic calculations, or a combination of both deterministic and stochastic calculations. For each OES with modeled releases, EPA followed these steps to estimate releases:

1. Identify release points from process and associated release media,
2. Identify or develop model equations for estimating releases from each release points,
3. Identify model input parameter values from relevant literature sources,
4. If a range of input values is available for an input parameter, determine the associated distribution of input values,
5. Calculate annual and daily release volumes for each release point using input values and model equations, and
6. Aggregate release volumes by release media and report total releases to each media from each facility.

For release models that utilized stochastic calculations, EPA performed a Monte Carlo simulation using the Palisade's @RISK software[1] with 100,000 iterations and the Latin Hypercube sampling method. Detailed descriptions of the model approaches used for each OES, model equations, input parameter values and associated distributions are provided in Section 3 and Appendix E.

2.3.4 Estimating Releases Using Literature Data

Where available, EPA used data identified from literature sources to estimate releases. Literature data may include directly measured release data or information useful for release modeling. Therefore, EPA's approach to literature data differs depending on the type of literature data available. For example, if facility-specific release data is available, EPA may use that data directly to estimate releases for that facility. If facility-specific data is available for only a subset of the facilities within an OES, EPA may also build a distribution of the available data and estimate releases from facilities within the OES using central tendency and high-end values from the distribution. If facility-specific data is not available, but industry- or chemical-specific emission factors are available, EPA may use those directly to calculate releases for an OES or incorporate the emission factors into release models to develop a distribution of potential releases for the OES. Detailed descriptions of how various literature data was incorporated into release estimates for each OES are described in Section 3.

2.3.5 Estimating Releases from Regulatory Limits

If EPA did not have data or models to estimate environmental releases from an OES, EPA relied on

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[1] See Palisade's @RISK software for additional information.

relevant regulatory limits, where available. Relevant regulatory limits may include Effluent Limitation Guidelines (ELGs) and NESHAPs. ELGs are national regulatory standards set forth by EPA for wastewater discharges to surface water and municipal sewage treatment plants. NESHAPs stationary source standards for HAPs. Both ELGs and NESHAPs are typically issued for specific industries and may have chemical-specific or generic limits (*e.g.*, limits on total organic carbon [TOC] or volatile organic compounds [VOCs]). When utilizing regulatory limits, EPA gave preference to chemical-specific limits and assumed facilities subject to the limit operate at the limit throughout the year. EPA then assessed annual and daily releases at the regulatory limit.

2.4 Occupational Exposure Approach and Methodology

For workplace exposures, EPA considered exposures to both workers who directly handle TCEP and ONUs who do not directly handle TCEP but may be exposed to vapors, particulates, or mists that enter their breathing zone while working in locations in close proximity to where TCEP is being used. EPA evaluated inhalation exposures to both workers and ONUs and dermal exposures to workers.

EPA provided occupational inhalation and dermal exposure results representative of *central tendency* conditions and *high-end* conditions. A central tendency is assumed to be representative of occupational exposures in the center of the distribution for a given COU. For risk evaluations, EPA uses the 50th percentile (median), mean (arithmetic or geometric), mode, or midpoint values of a distribution as representative of the central tendency scenario. EPA's preference is to provide the 50th percentile of the distribution. However, if the full distribution is not known, EPA may assume that the mean, mode, or midpoint of the distribution represents the central tendency depending on the statistics available for the distribution.

A high-end is assumed to be representative of occupational exposures that occur at probabilities above the 90th percentile but below the exposure of the individual with the highest exposure (U.S. EPA, 1992a). For risk evaluation, EPA provided high-end results at the 95th percentile. If the 95th percentile is not available, EPA used a different percentile greater than or equal to the 90th percentile but less than or equal to the 99.9th percentile, depending on the statistics available for the distribution. If the full distribution is not known and the preferred statistics are not available, EPA estimated a maximum or bounding estimate in lieu of the high-end.

For each OES, EPA attempted to provide high-end and central tendency full-shift time-weighted averages (TWAs) (typically as 8-hr TWAs) inhalation exposure concentrations and high-end and central tendency acute potential dermal dose rates (APDR). EPA follows the following hierarchy in selecting data and approaches for assessing occupational exposures:

1. Monitoring data:
    a. Personal and directly applicable
    b. Area and directly applicable
    c. Personal and potentially applicable or similar
    d. Area and potentially applicable or similar
2. Modeling approaches:
    a. Surrogate monitoring data
    b. Fundamental modeling approaches
    c. Statistical regression modeling approaches
3. Occupational exposure limits:
    a. Company-specific occupational exposure limits (OELs) (for site-specific exposure

assessments, *e.g.*, there is only one manufacturer who provides to EPA their internal OEL but does not provide monitoring data)

b. Occupational Safety and Health Administration (OSHA) Permissible Exposure Limits (PEL)

c. Voluntary limits (American Conference of Governmental Industrial Hygienists [ACGIH] Threshold Limit Values [TLV], National Institute for Occupational Safety and Health [NIOSH] Recommended Exposure Limits [REL], Occupational Alliance for Risk Science (OARS) workplace environmental exposure level (WEEL) [formerly by American Industrial Hygiene Association (AIHA)])

EPA used the estimated high-end and central tendency full-shift TWA inhalation exposure concentrations and APDR to calculate exposure metrics required for risk evaluation. Exposure metrics for inhalation exposures include acute concentrations (AC), subchronic average daily concentrations (SCDC), average daily concentrations (ADC), and lifetime average daily concentrations (LADC). The approach for estimating each inhalation exposure metric is described in Section 2.4.3. Exposure metrics for dermal exposures include dermal daily dose (DD), average daily dose (ADD), subchronic ADD, and chronic ADD. The approach to estimating each dermal exposure metric is described in Section 2.4.4.

2.4.1 Identifying Worker Activities

EPA performed a literature search to identify worker activities that could potentially result in occupational exposures. Where worker activities were unclear or not available, EPA referenced relevant ESDs or GSs. Worker activities for each COU can be found in Section 3.

2.4.2 Estimating Number of Workers and Occupational Non-Users

Where available, EPA used CDR data to provide a basis to estimate the number of workers and ONUs. EPA supplemented the available CDR data with U.S. economic data using the following method:

1. Identify the NAICS codes for the industry sectors associated with these uses.
2. Estimate total employment by industry/occupation combination using the Bureau of Labor Statistics' Occupational Employment Statistics data (BLS Data).
3. Refine the Occupational Employment Statistics estimates where they are not sufficiently granular by using the SUSB Data on total employment by 6-digit NAICS.
4. Use market penetration data to estimate the percentage of employees likely to be using TCEP instead of other chemicals.
5. Where market penetration data are not available, use the estimated workers/ONUs per site in the 6-digit NAICS code and multiply by the number of sites estimated from CDR, TRI, DMR and/or NEI. In DMR data, sites report SIC codes rather than NAICS codes; therefore, EPA mapped each reported SIC code to a NAICS code for use in this analysis.
6. Combine the data generated in Steps 1 through 5 to produce an estimate of the number of employees using TCEP in each industry/occupation combination and sum these to arrive at a total estimate of the number of employees with exposure within the COU.

2.4.3 Estimating Inhalation Exposures

2.4.3.1 Inhalation Monitoring Data

EPA reviewed workplace inhalation monitoring data collected by government agencies such as OSHA and NIOSH, monitoring data found in published literature (*i.e.*, personal exposure monitoring data and area monitoring data), and monitoring data submitted via public comments. Studies were evaluated using the evaluation strategies laid out in the *Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances* (U.S. EPA, 2021) (hereinafter referred to as the "2021 Draft Systematic Review Protocol").

Exposures are calculated from the monitoring datasets provided in the sources depending on the size of the dataset. For datasets with six or more data points, central tendency and high-end exposures were estimated using the 50th percentile and 95th percentile. For datasets with three to five data points, central tendency exposure was calculated using the 50th percentile and the maximum was presented as the high-end exposure estimate. For datasets with two data points, the midpoint was presented as a midpoint value and the higher of the two values was presented as a higher value. Finally, data sets with only one data point presented the single exposure value. For datasets including exposure data that were reported as below the limit of detection (LOD), EPA estimated the exposure concentrations for these data, following EPA's *Guidelines for Statistical Analysis of Occupational Exposure Data* (U.S. EPA, 1994) which recommends using the $\frac{LOD}{\sqrt{2}}$ if the geometric standard deviation of the data is less than 3.0 and $\frac{LOD}{2}$ if the geometric standard deviation is 3.0 or greater.

A key source of monitoring data is samples collected by OSHA during facility inspections. OSHA inspection data are compiled in the Occupational Safety and Health Information System (OIS) for internal use. Air sampling data records from inspections are entered into the OSHA Chemical Exposure Health Database (CEHD) that can be accessed on the agency website (https://www.osha.gov/opengov/healthsamples.html). The database includes personal breathing zone (PBZ) monitoring data, area monitoring data, bulk samples, wipe samples, and serum samples. The collected samples are used for comparing to OSHA's PEL. OSHA's CEHD website indicates that they do not: perform routine inspections at every business that uses toxic/hazardous chemicals, completely characterize all exposures for all employees every day, or always obtain a sample for an entire shift. Rather, OSHA performs targeted inspections of certain industries based on national and regional emphasis programs, often attempts to evaluate worst case chemical exposure scenarios, and develop "snapshots" of chemical exposures and assess their significance (*e.g.*, comparing measured concentrations to PELs). However, there is no OSHA data available for TCEP. Specific details related to the use of monitoring data for each COU can be found in Section 3.

2.4.3.2 Inhalation Exposure Modeling

Where inhalation exposures are expected for an OES but monitoring data were not available or where EPA determined monitoring data did not sufficiently capture the exposures for an OES, EPA attempted to utilize models to estimate inhalation exposures. Outputs from models may be the result of deterministic calculations, stochastic calculations, or a combination of both deterministic and stochastic calculations. For each OES with modeled inhalation exposures, EPA followed these steps to estimate exposures:

1. Identify worker activities/sources of exposures from process.
2. Identify or develop model equations for estimating exposures from each source.
3. Identify model input parameter values from relevant literature sources, including activity durations associated with sources of exposures.
4. If a range of input values is available for an input parameter, determine the associated distribution of input values.
5. Calculate exposure concentrations associated with each activity.
6. Calculate full-shift TWAs based on the exposure concentration and activity duration associated with each exposure source.

7. Calculate exposure metrics (AC, SCDC, ADC, LADC) from full-shift TWAs.

For exposure models that utilize stochastic calculations, EPA performed a Monte Carlo simulation using @RISK with 100,000 iterations and the Latin Hypercube sampling method. Detailed descriptions of the model approaches used for each OES, model equations, input parameter values, and associated distributions are provided in Section 3 and Appendix E.

2.4.3.1 Occupational Exposure Limits

If monitoring data or models were not available to estimate inhalation exposures from an OES, EPA relied on relevant OELs, where available. Relevant limits may include company-specific limits, OSHA PELs, or voluntary limits, such as NIOSH RELs. When utilizing exposure limits, EPA assumed facilities operate such that the workers are exposed at the limit every day of the work year. If EPA used OELs, an explanation of the use of this limit is included in Section 3 for the relevant COU.

2.4.4 Estimating Dermal Exposures

Dermal exposure data was not reasonably available for the conditions of use in the assessment. Because TCEP is a volatile liquid that readily evaporates from the skin, EPA estimated dermal exposures using the Dermal Exposure to Volatile Liquids Model and the EPA/OPPT 2-Hand Contact with Container Surfaces Model. These models determine an APDR based on an assumed amount of liquid or solid on skin during one contact event per day and the fractional absorption for TCEP. The fractional absorption of TCEP was determined to be 23.3 percent (Abdallah et al., 2016). The amount of liquid or solid on the skin is adjusted by the weight fraction of TCEP to which the worker is exposed. Specific details of the dermal exposure assessment for each OES can be found in Section 3 and equations for estimating dermal exposures can be found in Appendix B and Appendix D.

2.4.5 Estimating Acute, Subchronic, and Chronic (Non-cancer and Cancer) Exposure

For each COU, the estimated exposures were used to calculate acute, subchronic, and chronic (non-cancer and cancer) inhalation exposures and dermal doses. These calculations require additional parameter inputs, such as years of exposure, exposure duration and frequency, and lifetime years.

For the final exposure result metrics, each of the input parameters (*e.g.*, air concentrations, dermal doses, working years, exposure frequency, lifetime years) may be a point estimate (*i.e.*, a single descriptor or statistic, such as central tendency or high-end) or a full distribution. EPA considered three general approaches for estimating the final exposure result metrics:

1. **Deterministic calculations:** EPA used combinations of point estimates of each parameter to estimate a central tendency and high-end for each final exposure metric result. EPA documented the method and rationale for selecting parametric combinations to be representative of central tendency and high-end.
2. **Probabilistic (stochastic) calculations:** EPA used a Monte Carlo simulation using the full distribution of each parameter to calculate a full distribution of the final exposure metric results and selecting the 50th and 95th percentiles of this resulting distribution as the central tendency and high-end, respectively.
3. **Combination of deterministic and probabilistic calculations:** EPA had full distributions for some parameters but point estimates of the remaining parameters. For example, EPA used a Monte Carlo simulation to estimate exposure concentrations, but only had point estimates of exposure duration and frequency, and lifetime years. In this case, EPA documented the approach and rationale for combining point estimates with distribution results for estimating central tendency and high-end results.

Equations and sample calculations for these exposures can be found in Appendix B and Appendix C, respectively.

2.5 Consideration of Engineering Controls and Personal Protective Equipment

OSHA and NIOSH recommend employers utilize the hierarchy of controls to address hazardous exposures in the workplace. The hierarchy of controls strategy outlines, in descending order of priority, the use of elimination, substitution, engineering controls, administrative controls, and lastly personal protective equipment (PPE). The hierarchy of controls prioritizes the most effective measures first which is to eliminate or substitute the harmful chemical (*e.g.*, use a different process, substitute with a less hazardous material), thereby preventing or reducing exposure potential. Following elimination and substitution, the hierarchy recommends engineering controls to isolate employees from the hazard (*e.g.*, source enclosure, local exhaust ventilation systems), followed by administrative controls (*e.g.*, do not open machine doors when running), or changes in work practices (*e.g.*, maintenance plan to check equipment to ensure no leaks) to reduce exposure potential. Administrative controls are policies and procedures instituted and overseen by the employer to limit worker exposures. Under Section 1910.1000, OSHA requires the use of engineering or administrative controls to bring exposures to the levels permitted under the air contaminants standard (29 Code of Federal Regulations [CFR] 1910.1000). The respirators do not replace engineering controls and they are implemented in addition to feasible engineering controls (29 CFR 1910.134(a)(1)). The PPE (*e.g.*, respirators, gloves) could be used as the last means of control when the other control measures cannot reduce workplace exposure to an acceptable level.

2.5.1 Respiratory Protection

OSHA's Respiratory Protection Standard (29 CFR 1910.134) requires employers in certain industries to address workplace hazards by implementing engineering control measures and, if these are not feasible, provide respirators that are applicable and suitable for the purpose intended. Engineering and administrative controls must be implemented whenever employees are exposed above the PEL. If engineering and administrative controls do not reduce exposures to below the PEL, respirators must be worn. Respirator selection provisions are provided in Section 1910.134(d) and require that appropriate respirators are selected based on the respiratory hazard(s) to which the worker will be exposed and workplace and user factors that affect respirator performance and reliability. Assigned protection factors (APFs) are provided in Table 1 under Section 1910.134(d)(3)(i)(A) (see below in Table 2-1) and refer to the level of respiratory protection that a respirator or class of respirators could provide to employees when the employer implements a continuing, effective respiratory protection program. Implementation of a full respiratory protection program requires employers to provide training, appropriate selection, fit testing, cleaning, and changeout schedules in order to have confidence in the efficacy of the respiratory protection.

If respirators are necessary in atmospheres that are not immediately dangerous to life or health, workers must use NIOSH-certified air-purifying respirators or NIOSH-approved supplied-air respirators (SARs) with the appropriate APF. Respirators that meet these criteria may include air-purifying respirators with organic vapor cartridges. Respirators must meet or exceed the required level of protection listed in Table 2-1. Based on the APF, inhalation exposures may be reduced by a factor of 5 to 10,000 if respirators are properly worn and fitted.

For atmospheres that are immediately dangerous to life and health, workers must use a full facepiece pressure demand self-contained breathing apparatus (SCBA) certified by NIOSH for a minimum service life of 30 minutes or a combination full facepiece pressure demand SAR with auxiliary self-contained air supply. Respirators that are provided only for escape from an atmosphere that is immediately dangerous to life and health must be NIOSH-certified for escape from the atmosphere in which they will be used.

Table 2-1. Assigned Protection Factors for Respirators in OSHA Standard (29 CFR 1910.134)

Type of Respirator	Quarter Mask	Half Mask	Full Facepiece	Helmet/ Hood	Loose-fitting Facepiece
1. Air-Purifying Respirator	5	10	50		
2. Power Air-Purifying Respirator (PAPR)		50	1,000	25/1,000	25
3. Supplied-Air Respirator (SAR) or Airline Respirator					
• Demand mode		10	50		
• Continuous flow mode		50	1,000	25/1,000	25
• Pressure-demand or other positive-pressure mode		50	1,000		
4. Self-Contained Breathing Apparatus (SCBA)					
• Demand mode		10	50	50	
• Pressure-demand or other positive-pressure mode (*e.g.*, open/closed circuit)			10,000	10,000	
Source: 29 CFR 1910.134(d)(3)(i)(A)					

The NIOSH and the U.S. Department of Labor's Bureau of Labor Statistics (BLS) conducted a voluntary survey of U.S. employers regarding the use of respiratory protective devices between August 2001 and January 2002. The survey was sent to a sample of 40,002 establishments designed to represent all private sector establishments. The survey had a 75.5 percent response rate (NIOSH, 2003). A voluntary survey may not be representative of all private industry respirator use patterns as some establishments with low or no respirator use may choose to not respond to the survey. Therefore, results of the survey may potentially be biased towards higher respirator use.

NIOSH and BLS estimated about 619,400 establishments used respirators for voluntary or required purposes (including emergency and non-emergency uses). About 281,800 establishments (45 percent) were estimated to have had respirator use for required purposes in the 12 months prior to the survey. The 281,800 establishments estimated to have had respirator use for required purposes were estimated to be approximately 4.5 percent of all private industry establishments in the United States at the time (NIOSH, 2003).

The survey found that the establishments that required respirator use had the following respirator program characteristics (NIOSH, 2003):

- 59 percent provided training to workers on respirator use,
- 34 percent had a written respiratory protection program,
- 47 percent performed an assessment of the employees' medical fitness to wear respirators, and
- 24 percent included air sampling to determine respirator selection.

The survey report does not provide a result for respirator fit testing or identify if fit testing was included in one of the other program characteristics.

Of the establishments that had respirator use for a required purpose within the 12 months prior to the survey, NIOSH and BLS found (NIOSH, 2003):

- Non-powered air purifying respirators are most common, 94 percent overall and varying from 89 to 100 percent across industry sectors;
- Powered air-purifying respirators represent a minority of respirator use, 15 percent overall and varying from 7 to 22 percent across industry sectors; and
- Supplied air respirators represent a minority of respirator use, 17 percent overall and varying from 4 to 37 percent across industry sectors.

Of the establishments that used non-powered air-purifying respirators for a required purpose within the 12 months prior to the survey, NIOSH and BLS found (NIOSH, 2003):

- A high majority use dust masks, 76 percent overall and varying from 56 to 88 percent across industry sectors.
- A varying fraction use half-mask respirators, 52 percent overall and varying from 26 to 66 percent across industry sectors.
- A varying fraction use full-facepiece respirators, 23 percent overall and varying from 4 to 33 percent across industry sectors.

Table 2-2 summarizes the number and percent of all private industry establishments and employees that used respirators for a required purpose within the 12 months prior to the survey and includes a breakdown by industry sector (NIOSH, 2003).

Table 2-2. Number and Percent of Establishments and Employees Using Respirators Within 12 Months Prior to Survey

Industry	Establishments		Employees	
	Number	Percent of All Establishments	Number	Percent of All Employees
Total Private Industry	281,776	4.5%	3,303,414	3.1%
Agriculture, Forestry, and Fishing	13,186	9.4%	101,778	5.8%
Mining	3,493	11.7%	53,984	9.9%
Construction	64,172	9.6%	590,987	8.9%
Manufacturing	48,556	12.8%	882,475	4.8%
Transportation and Public Utilities	10,351	3.7%	189,867	2.8%
Wholesale Trade	31,238	5.2%	182,922	2.6%
Retail Trade	16,948	1.3%	118,200	0.5%
Finance, Insurance, and Real Estate	4,202	0.7%	22,911	0.3%
Services	89,629	4.0%	1,160,289	3.2%

2.5.2 Glove Protection

OSHA's hand protection standard (29 CFR 1910.138) requires employers select and require employees to use appropriate hand protection when expected to be exposed to hazards such as those from skin absorption of harmful substances; severe cuts or lacerations; severe abrasions; punctures; chemical burns; thermal burns; and harmful temperature extremes. Dermal protection selection provisions are provided in Section 1910.138(b) and require that appropriate hand protection is selected based on the performance characteristics of the hand protection relative to the task(s) to be performed, conditions present, duration of use, and the hazards to which employees will be exposed.

Unlike respiratory protection, OSHA standards do not provide PFs associated with various hand protection PPE, such as gloves, and data about the frequency of effective glove use – that is, the proper use of effective gloves – is very limited in industrial settings. Initial literature review suggests that there is unlikely to be sufficient data to justify a specific probability distribution for effective glove use for a chemical or industry. Instead, the impact of effective glove use is explored by considering different percentages of effectiveness.

EPA made assumptions about glove use and associated PF. Where workers wear gloves, workers are exposed to TCEP-based products that may penetrate the gloves, such as seepage through the cuff from improper donning of the gloves, and if the gloves occlude the evaporation of TCEP from the skin. Where workers do not wear gloves, workers are exposed through direct contact with TCEP.

Gloves only offer barrier protection until the chemical breaks through the glove material. Using a conceptual model, Cherrie et al. (2004) proposed a glove workplace protection factor – the ratio of estimated uptake through the hands without gloves to the estimated uptake though the hands while wearing gloves: this protection factor is driven by flux, and thus varies with time. The European Centre For Ecotoxicology and Toxicology of Chemicals' Targeted Risk Assessment model, Version 3.0 (ECETOC TRA v3) represents the protection factor of gloves as a fixed, APF equal to 5, 10, or 20 (Marquart et al., 2017) where, similar to the APF for respiratory protection, the inverse of the protection factor is the fraction of the chemical that penetrates the glove. It should be noted that the described PFs are not based on experimental values or field investigations of PPE effectiveness, but rather professional judgements used in the development of the ECETOC TRA v3 model. EPA did not identify reasonably available information on PPE usage to corroborate the PFs used in this model.

As indicated in Table 2-3, use of protection factors above one is recommended only for glove materials that have been tested for permeation against the TCEP-containing liquids associated with the COU. EPA has not found information that would indicate specific activity training (*e.g.*, procedure for glove removal and disposal) for tasks where dermal exposure can be expected to occur in a majority of sites in industrial only OESs, so the PF of 20 would usually not be expected to be achieved.

Table 2-3. Glove Protection Factors for Different Dermal Protection Strategies from ECETOC TRA v3

Dermal Protection Characteristics	Affected User Group	Indicated Efficiency (%)	Protection Factor (PF)
a. Any glove/gauntlet without permeation data and without employee training	Both industrial and professional users	0	1

Dermal Protection Characteristics	Affected User Group	Indicated Efficiency (%)	Protection Factor (PF)
b. Gloves with available permeation data indicating that the material of construction offers good protection for the substance		80	5
c. Chemically resistant gloves (*i.e.*, as b above) with "basic" employee training		90	10
d. Chemically resistant gloves in combination with specific activity training (*e.g.*, procedure for glove removal and disposal) for tasks where dermal exposure can be expected to occur	Industrial users only	95	20

2.6 Evidence Integration for Environmental Releases and Occupational Exposures

Evidence integration for the environmental release and occupational exposure assessment includes analysis, synthesis and integration of information and data to produce estimates of environmental releases and occupational inhalation and dermal exposures. During evidence integration, EPA considered the likely location, duration, intensity, frequency, and quantity of releases and exposures while also considering factors that increase or decrease the strength of evidence when analyzing and integrating the data. Key factors EPA considered when integrating evidence includes the following:

1. **Data Quality:** EPA only integrated data or information rated as *high, medium, or low* obtained during the data evaluation phase. Data and information rated as *uninformative* are not used in exposure evidence integration. In general, higher rankings are given preference over lower ratings; however, lower ranked data may be used over higher ranked data when specific aspects of the data are carefully examined and compared. For example, a lower ranked data set that precisely matches the OES of interest may be used over a higher ranked study that does not as closely match the OES of interest.
2. **Data Hierarchy:** EPA used both measured and modeled data to obtain accurate and representative estimates (*e.g.*, central-tendency, high-end) of the environmental releases and occupational exposures resulting directly from a specific source, medium, or product. If available, measured release and exposure data are given preference over modeled data, with the highest preference given to data that are both chemical-specific and directly representative of the OES/exposure source.

EPA considered data quality and data hierarchy equally when determining evidence integration strategies. For example, EPA may have given preference to high quality modeled data directly applicable to the OES being assessed over low quality measured data that is not specific to the OES. The final integration of the environmental release and occupational exposure evidence combined decisions regarding the strength of the available information, including information on plausibility and coherence across each evidence stream.

2.7 Summary of Weight of Scientific Evidence for Environmental Release Estimates

For each OES, EPA considered the assessment approach, quality of the data and models, strengths, limitations, assumptions, and key sources of uncertainties to determine a weight of scientific evidence

(WoSE) rating. EPA considered factors that increase or decrease the strength of the evidence supporting the release estimate—including quality of the data/information, applicability of the release data to the OES (including considerations of temporal and locational relevance) and the representativeness of the estimate for the whole industry. The best professional judgment is summarized using the descriptors of robust, moderate, slight, or indeterminant, according to the 2021 Draft Systematic Review Protocol (U.S. EPA, 2021). For example, a conclusion of moderate is appropriate where there is measured release data from a limited number of sources such that there is a limited number of data points that may not cover most or all the sites within the OES. A conclusion of slight is appropriate where there is limited information that does not sufficiently cover all sites within the OES, and the assumptions and uncertainties are not fully known or documented. See the 2021 Draft Systematic Review Protocol (U.S. EPA, 2021) for additional information on WoSE conclusions. Table 2-4 summarizes the WoSE ratings for each media of release for each OES. Details on the basis EPA used to determine the rating are provided in Section 3 for each OES.

Table 2-4. Summary of the Weight of Scientific Evidence Ratings for Environmental Releases

OES	Release Media	Reported Data[a]	Data Quality Rating for Reported Data	Modeling	Data Quality Rating for Modeling[b]	Weight of Scientific Evidence Conclusion
Manufacture (Import) – Repackaging	Fugitive air emissions	✗	N/A	✓	Medium	Moderate
	Stack air emissions	✗	N/A	✓	Medium	
	Direct discharges to surface water	✗	N/A	✗	N/A	
	Indirect discharges to POTW or non-POTW WWT	✗	N/A	✓	Medium	
	Land disposal	✗	N/A	✗	N/A	
Processing – Incorporation into paints and coatings – 1-part coatings	Fugitive air emissions	✗	N/A	✓	Medium	Moderate
	Stack air emissions	✗	N/A	✓	Medium	
	Direct discharges to surface water	✗	N/A	✗	N/A	
	Indirect discharges to POTW or non-POTW WWT	✗	N/A	✓	Medium	
	Land disposal	✗	N/A	✓	N/A	
Processing – Incorporation into paints and coatings – 2-part Reactive coatings	Fugitive air emissions	✗	N/A	✓	Medium	Moderate
	Stack air emissions	✗	N/A	✓	Medium	
	Direct discharges to surface water	✗	N/A	✗	N/A	
	Indirect discharges to POTW or non-POTW WWT	✗	N/A	✓	Medium	
	Land disposal	✗	N/A	✓	N/A	
Processing – Formulation of TCEP-containing reactive resins (for	Fugitive air emissions	✗	N/A	✓	Medium	Moderate
	Stack air emissions	✗	N/A	✓	Medium	
	Direct discharges to surface water	✗	N/A	✗	N/A	

OES	Release Media	Reported Data[a]	Data Quality Rating for Reported Data	Modeling	Data Quality Rating for Modeling[b]	Weight of Scientific Evidence Conclusion
use in 2-part systems)	Indirect discharges to POTW or non-POTW WWT	×	N/A	✓	Medium	
	Land disposal	×	N/A	✓	N/A	
Processing – Processing into 2-part resin article	Fugitive air emissions	×	N/A	✓	Medium	Moderate
	Stack air emissions	×	N/A	✓	Medium	
	Direct discharges to surface water	×	N/A	×	N/A	
	Indirect discharges to POTW or non-POTW WWT	×	N/A	×	N/A	
	Land disposal	×	N/A	✓	N/A	
Processing – Recycling e-waste	Fugitive air emissions	×	N/A	×	N/A	N/A
	Stack air emissions	×	N/A	×	N/A	
	Direct discharges to surface water	×	N/A	×	N/A	
	Indirect discharges to POTW or non-POTW WWT	×	N/A	×	N/A	
	Land disposal	×	N/A	×	N/A	
Distribution – Distribution in Commerce	Fugitive air emissions	×	N/A	×	N/A	N/A
	Stack air emissions	×	N/A	×	N/A	
	Direct discharges to surface water	×	N/A	×	N/A	
	Indirect discharges to POTW or non-POTW WWT	×	N/A	×	N/A	
	Land disposal	×	N/A	×	N/A	
	Fugitive air emissions	×	N/A	×	N/A	N/A

OES	Release Media	Reported Data[a]	Data Quality Rating for Reported Data	Modeling	Data Quality Rating for Modeling[b]	Weight of Scientific Evidence Conclusion
Industrial Use – Installing article (containing 2-part resin) for aerospace applications	Stack air emissions	×	N/A	×	N/A	
	Direct discharges to surface water	×	N/A	×	N/A	
	Indirect discharges to POTW or non-POTW WWT	×	N/A	×	N/A	
	Land disposal	×	N/A	×	N/A	
Commercial Use – Use of Paints and Coatings – Spray Application OES	Fugitive air emissions	×	N/A	✓	Medium	Moderate
	Stack air emissions	×	N/A	✓	Medium	
	Direct discharges to surface water	×	N/A	×	N/A	
	Indirect discharges to POTW or non-POTW WWT	×	N/A	✓	Medium	
	Land disposal	×	N/A	×	N/A	
Commercial Use – Lab Chemical – Use of Laboratory Chemicals	Fugitive air emissions	×	N/A	✓	High	Moderate
	Stack air emissions	×	N/A	✓	High	
	Direct discharges to surface water	×	N/A	×	N/A	
	Indirect discharges to POTW or non-POTW WWT	×	N/A	✓	High	
	Land disposal	×	N/A	×	N/A	
Commercial Use – *Placeholder for Legacy/Historic uses	Fugitive air emissions	×	N/A	×	N/A	N/A
	Stack air emissions	×	N/A	×	N/A	
	Direct discharges to surface water	×	N/A	×	N/A	
	Indirect discharges to POTW or non-POTW WWT	×	N/A	×	N/A	

OES	Release Media	Reported Data[a]	Data Quality Rating for Reported Data	Modeling	Data Quality Rating for Modeling[b]	Weight of Scientific Evidence Conclusion
	Land disposal	×	N/A	×	N/A	
Disposal	Fugitive air emissions	×	N/A	×	N/A	N/A
	Stack air emissions	×	N/A	×	N/A	
	Direct discharges to surface water	×	N/A	×	N/A	
	Indirect discharges to POTW or non-POTW WWT	×	N/A	×	N/A	
	Land disposal	×	N/A	×	N/A	

[a] Reported data includes data obtained from EPA databases (*i.e.*, TRI, DMR, NEI) and facility release data from literature sources.

[b] Data quality ratings for models include ratings of underlying literature sources used to select model approaches and input values/distributions such as a GS/ESD used in tandem with Monte Carlo simulations.

2.8 Summary of Weight of Scientific Evidence for Occupational Exposures

For the WoSE for occupational exposures, EPA considered the same factors as discussed for environmental releases in Section 2.7. Table 2-5 summarizes the WoSE ratings for the occupational exposures for each OES. Details on the basis EPA used to determine the rating are provided in Section 3 for each OES.

Table 2-5. Summary of the Weight of Scientific Evidence Ratings for Occupational Exposures

OES	Inhalation Exposure										Dermal Exposure				
	Monitoring					Modeling			Weight of the Scientific Evidence Conclusion		Monitoring		Modeling	Weight of the Scientific Evidence Conclusion	
	Worker	# Data Points	ONU	# Data Points	Data Quality Rating	Worker	ONU	Data Quality Rating[a]	Worker	ONU	Worker	Data Quality Rating	Worker	Worker	ONU
Manufacture (Import) – Repackaging	×	N/A	×	N/A	N/A	✓	×	Medium	Moderate	Slight	×	N/A	✓	Moderate	N/A
Processing – Incorporation into paints and coatings – 1-part coatings	×	N/A	×	N/A	N/A	✓	×	Medium	Moderate to Robust	Slight	×	N/A	✓	Moderate	N/A
Processing – Incorporation into paints and coatings – 2-part Reactive coatings	×	N/A	×	N/A	N/A	✓	×	Medium	Moderate to Robust	Slight	×	N/A	✓	Moderate	N/A
Processing – Formulation of TCEP-containing reactive resins (for use in 2-part systems)	×	N/A	×	N/A	N/A	✓	×	Medium	Moderate to Robust	Slight	×	N/A	✓	Moderate	N/A
Processing – Processing into 2-part resin article	×	N/A	×	N/A	N/A	✓	×	Medium	Moderate	Slight	×	N/A	✓	Moderate	N/A
Processing – Recycling e-waste	✓	55	✓	21	High	×	×	N/A	Moderate to Robust	Moderate to Robust	×	N/A	✓	Moderate	N/A

OES	Inhalation Exposure										Dermal Exposure				
	Monitoring					Modeling			Weight of the Scientific Evidence Conclusion		Monitoring		Modeling	Weight of the Scientific Evidence Conclusion	
	Worker	# Data Points	ONU	# Data Points	Data Quality Rating	Worker	ONU	Data Quality Rating[a]	Worker	ONU	Worker	Data Quality Rating	Worker	Worker	ONU
Distribution – Distribution in Commerce															
Industrial Use – Installing article (containing 2-part resin) for aerospace applications	✓	1 (surrogate)	×	N/A	High	×	×	N/A	Slight	Slight	×	N/A	×	N/A	N/A
Commercial Use – Use of Paints and Coatings – Spray Application OES	✓	Surrogate Spray GS	×	N/A	High	×	×	N/A	Moderate	Slight	×	N/A	✓	Moderate	N/A
Commercial Use – Lab Chemical – Use of Laboratory Chemicals	×	N/A	×	N/A	N/A	✓	×	High	Moderate	Slight	×	N/A	✓	Moderate	N/A
Commercial Use – *Placeholder for Legacy/Historic uses															
Disposal															

Note: Where EPA was not able to estimate an ONU inhalation exposure from monitoring data or models, this was assumed equivalent to the central tendency experienced by workers for the corresponding OES; dermal exposure for ONUs was not evaluated because they are not expected to be in direct contact with TCEP.

[a] Data quality ratings for models include ratings of underlying literature sources used to select model approaches and input values/distributions such as a GS/ESD used in tandem with Monte Carlo simulations.

3 ENVIRONMENTAL RELEASE AND OCCUPATIONAL EXPOSURE ASSESSMENTS BY OCCUPATIONAL EMISSION SCENARIOS

3.1 Import – Repackaging

3.1.1 Process Description

In the 2016 CDR, a single site, Aceto Corporation in Port Washington, NY, reported importing TCEP (U.S. EPA, 2019). The 2020 CDR had no reporters for TCEP (U.S. EPA, 2020a). EPA did not identify other data on current import volumes or import sites from systematic review. Therefore, EPA assumed TCEP may still be imported at volumes below the CDR reporting threshold (see Section 2.2 for details) and assessed the following two potential scenarios: 1) one site importing 25,000 lb; and 2) one site importing 2,500 lb. These scenarios are meant to estimate a generic import site and do not necessarily represent the total number of import sites or total import volume of TCEP.

EPA did not identify data to determine the types of TCEP products that may be imported/repackaged, nor the types of containers used to import TCEP. EPA expects that TCEP may be imported as either a neat liquid or as part of a formulation (*e.g.*, coatings). Based on the low production volume, EPA expects that TCEP and TCEP-containing products will be imported in drums or smaller containers rather than larger bulk containers. TCEP and TCEP-containing products imported in drums may be stored in warehouses where they may be repackaged into smaller containers for use in smaller quantities prior to distribution to processors and end-users (NICNAS, 2001; J6 Polymers, 2021). EPA does not expect TCEP and TCEP-containing products imported in containers smaller than drums to be repackaged prior to distribution.

A typical repackaging site first stores imported drums in warehouses until orders for the chemical are received, then the chemical product is pumped out of the drums into several smaller containers (OECD, 2009c). Quality control sampling of the TCEP product may also occur at the repackaging site. After repackaging, empty drums will be cleaned, disposed of, or reconditioned for reuse and the smaller containers containing the chemical product will be shipped offsite for downstream processing or use. No changes to chemical composition will occur during repackaging.

EPA did not identify information from systematic review for repackaging site operating data (*i.e.*, daily throughputs or operating days per year). The number of drums repackaged per day can vary depending on customer demand. The upper end of operating days is expected to be but not exceed 250 days per year based on 5 days of work per week and 50 weeks of work per year. Figure 3-1 provides an illustration of the repackaging process.

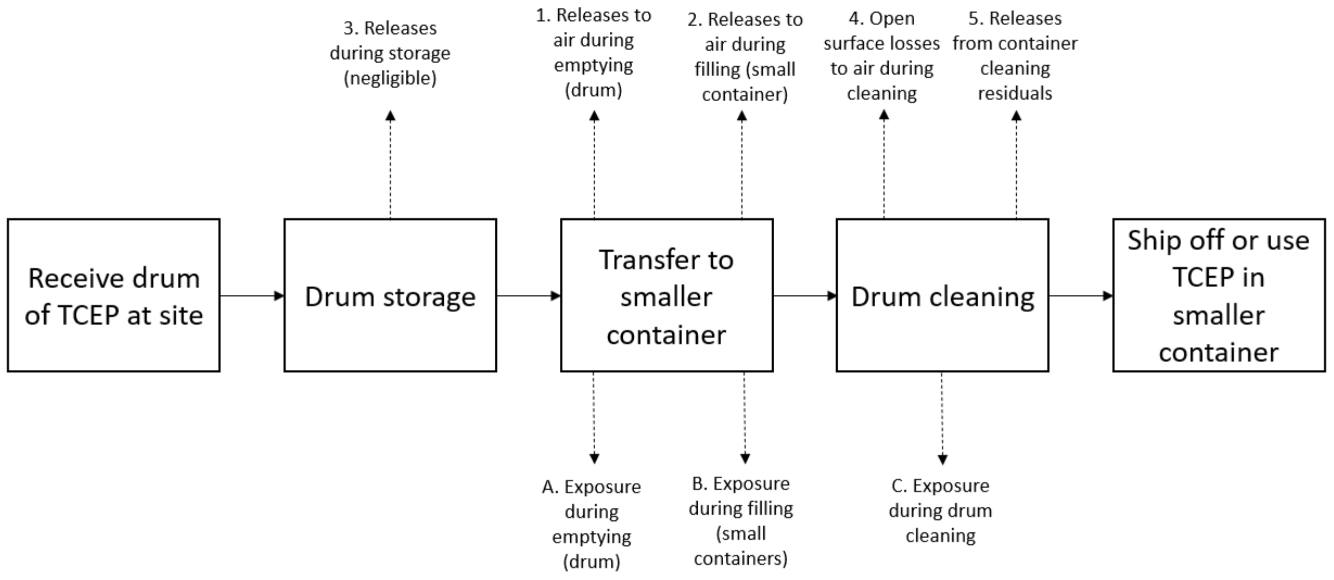

Figure 3-1. Repackaging Flow Diagram

3.1.2 Facility Estimate

The 2016 CDR data included a single reporting site, Aceto Corporation in Port Washington, NY, importing TCEP, with no downstream industry sectors identified (U.S. EPA, 2019). TCEP was not reported in 2020 CDR (U.S. EPA, 2020a). EPA did not identify other data on current import volumes or import sites from systematic review. Therefore, EPA assumed TCEP may still be imported at volumes below the CDR reporting threshold (see Section 2.2 for details) and assessed the following two potential scenarios: 1) one site importing 25,000 lb; and 2) one site importing 2,500 lb. EPA modeled environmental releases and occupational exposures for these hypothetical scenarios as a conservative estimate. Based on TCEP’s physical properties, EPA assumes TCEP is imported in its pure form which is a neat liquid at 25 °C (see Table 2-1 in the TCEP Risk Evaluation (U.S. EPA, 2024)). EPA additionally assumed that the number of operating days is equivalent to the number of drums imported per year (*i.e.*, one drum repackaged per day) but not to exceed 250 operating days per year. If the number of drums exceeds 250, EPA expects that more than one drum will be repackaged each day.

3.1.3 Release Assessment

3.1.3.1 Environmental Release Points

EPA expects releases to occur during the emptying of drums, cleaning of emptied drums, and filling of smaller containers. EPA estimated releases from Import – Repackaging using a Monte Carlo simulation with 100,000 iterations and the Latin Hypercube sampling method using the models and approaches described in Appendix E.2. Input parameters for the models were determined using data from literature and the *Emission Scenario Document on Transport and Storage of Chemicals* (OECD, 2009c). EPA used this method to estimate releases for individual release points and summed the individual releases to each environmental media to estimate total annual and daily facility releases. Specific release points considered for estimating releases are shown numbered as 1 through 5 in Figure 3-1. EPA expects fugitive or stack air releases from unloading, filling, and cleaning containers during repackaging. EPA expects releases in wastewater treated onsite or discharged to a POTW from cleaning containers. EPA expects releases during storage to be negligible compared to other sources of release.

3.1.3.2 Environmental Release Assessment Results

Appendix E.2 includes the model equations and input parameters used in the Monte Carlo simulation for this COU. EPA estimated TCEP releases by simulating two potential throughput scenarios: 1) one site importing and processing 2,500 lb; and 2) one site importing and processing 25,000 lb. Table 3-1 summarizes the estimated release results for Import – Repackaging based on the two scenarios applied. The high-ends are the 95th percentile of the respective simulation output and the central tendencies are the 50th percentile.

Table 3-1. Summary of Modeled Environmental Releases for the Import – Repackaging of TCEP

Modeled Scenario	Environmental Media	Annual Release (kg/site-yr)		Number of Release Days[a]		Daily Release (kg/site-day)	
		Central Tendency	High-End	Central Tendency	High-End	Central Tendency	High-End
Scenario 1: One site; 2,500 lb throughput	Fugitive or stack air[b]	1.4E–03	2.2E–03	4	4	3.2E–04	6.0E–04
	Wastewater to onsite treatment or discharge to POTW	27	32	4	4	6.3	9.9
Scenario 2: One site; 25,000 lb throughput	Fugitive or stack air[b]	1.2E–02	1.9E–02	38	32	3.2E–04	6.0E–04
	Wastewater to onsite treatment or discharge to POTW	275	320	39	29	7.1	11

[a] EPA assumes that the number of operating days is equivalent to the number of drums imported per year (*i.e.*, one drum repackaged per day) but not to exceed 250 operating days per year. The number of release days presented in this table is based on simulation outputs for the annual release divided by the daily release (grouped by high-end or central tendency estimate), rounded to the closest integer. Annual totals may not add exactly due to rounding.

[b] Hours of release per day is based on typical container sizes for import and small containers. Per Table 4-11 in U.S. EPA (1991), drum and small container sizes range from 20–100 and 5–20 gallons, respectively. Drum and small containers have typical unloading rates of 20 and 60 containers/hour, respectively. Due to variability in the container sizes used in the model, the hours of release may vary (model results for hours of release ranged from 0.12–0.43 hours/container-day).

3.1.3.3 Weight of Scientific Evidence for Environmental Releases

Releases to the environment are assessed using the assumptions and values from the *Emission Scenario Document on Transport and Storage of Chemicals* (OECD, 2009c), which the systematic review process rated medium for data quality. EPA used EPA/OPPT models combined with Monte Carlo simulations to estimate releases to the environment, with media of release assessed using assumptions from the ESD and EPA/OPPT models. EPA believes a strength of the Monte Carlo simulation approach is that variation in model input values and a range of potential releases values is more likely than a discrete value to capture actual releases at sites. The primary limitation to EPA's approach is the uncertainty in the representativeness of values toward the true distribution of potential releases. In addition, EPA lacks TCEP facility production volume data and number of importing/repackaging sites; therefore, throughput estimates are based on CDR reporting thresholds with an overall release using a hypothetical scenario of a single facility. Additional limitations to this assessment are that EPA could not estimate the number of release days per year associated with repackaging operations, so the release days per year estimates are based on engineering assumptions such as a site throughput of imported containers. Based on this information, EPA has concluded that the WoSE for this assessment is moderate and provides a plausible estimate of releases in consideration of the strengths and limitations of reasonably available data.

3.1.4 Occupational Exposure Assessment

3.1.4.1 Workers Activities

During repackaging, workers are potentially exposed to TCEP when transferring TCEP from the import drums into smaller containers. Workers may also be exposed via inhalation of vapor or dermal contact with liquids when cleaning import drums following emptying. EPA did not find information that indicates the extent that engineering controls and worker PPE are used at facilities that repackage TCEP from import drums into smaller containers.

ONUs include employees (*e.g.*, supervisors, managers) at the import site, where repackaging occurs, that do not directly handle TCEP. Therefore, the ONUs are expected to have lower inhalation exposures, lower vapor-through-skin uptake, and no expected dermal exposure.

3.1.4.2 Numbers of Workers and Occupational Non-Users

EPA used data from the BLS and the U.S. Census' SUSB specific to the OES to estimate the number of workers and ONUs per site potentially exposed to TCEP during repackaging (U.S. Census Bureau, 2015; U.S. BLS, 2016). This approach involved the identification of relevant Standard Occupational Classification (SOC) codes within the BLS data for the identified NAICS codes. Section 2.4.2 includes further details regarding methodology for estimating the number of workers and ONUs per site. EPA assigned the NAICS code 424690 – Other Chemical and Allied Products Merchant Wholesalers for this OES based on the process description. Table 3-2 summarizes the per site estimates for this OES based on the methodology described. As addressed in Section 3.1.2, EPA did not identify site-specific data for the number of facilities in the Unites States repackaging TCEP; therefore, EPA did not estimate the total number of workers and ONUs exposed from this OES.

Table 3-2. Estimated Number of Workers Potentially Exposed to TCEP During Import – Repackaging

NAICS Code	Exposed Workers per Site[a]	Exposed ONUs per Site[a]
424690 – Other Chemical and Allied Products Merchant Wholesalers	1	0.4

[a] Number of workers and ONUs per site are calculated by dividing the exposed number of workers or ONUs by the number of establishments. The number of workers per site is rounded to the nearest integer. The number of ONUs per site is shown as 0.4, as it rounds down to zero.

3.1.4.3 Occupational Inhalation Exposure Results

EPA did not identify inhalation monitoring data to assess exposures during repackaging of TCEP. Therefore, EPA estimated inhalation exposures during Import – Repackaging using a Monte Carlo simulation with 100,000 iterations and the Latin Hypercube sampling method using the models and approaches described in Appendix E.2. Input parameters for the models were determined using data from literature and the *Emission Scenario Document on Transport and Storage of Chemicals* (OECD, 2009c). EPA estimated inhalation exposures of TCEP by simulating two potential scenarios: 1) one site importing and processing 2,500 lb; and 2) one site importing and processing 25,000 lb.

For this scenario, EPA applied the EPA Mass Balance Inhalation Model to exposure points described in the *Emission Scenario Document on Transport and Storage of Chemicals* (OECD, 2009c), particularly for the emptying of drums, filling of containers, and cleaning of drums process described in the process description (see Section 3.1). The EPA Mass Balance Inhalation Model estimates the concentration of the chemical in the breathing zone of the worker based on a vapor generation rate (G). An 8-hour TWA is then estimated and averaged over eight hours assuming no exposure occurs outside of those activities. Appendix E.2 also describes the model equations and other input parameters used in the Monte Carlo simulation for this OES.

EPA used the vapor generation rate and exposure duration parameters from the *Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Volume 1* (U.S. EPA, 1991) (hereinafter referred to as the "1991 CEB Manual") in addition to those used in the EPA Mass Balance Inhalation Model to determine a time-weighted exposure for each exposure point. EPA estimated the TWA inhalation exposure for a full work-shift (EPA assumed an 8-hour work-shift) as an output of the Monte Carlo simulation by summing the time-weighted inhalation exposures for each of the exposure points and assuming TCEP exposures were zero outside these activities. Table 3-3 summarizes the estimated 8-hour TWA exposures, AC, ADC, LADC, and $ADC_{subchronic}$ for repackaging TCEP based on the two production volume scenarios. The high-end exposures presented in Table 3-3 are the 95th percentiles of the respective simulation output, and the central tendency exposures are the 50th percentiles. Equations for calculating AC, ADC, LADC, and $ADC_{subchronic}$ are presented in Appendix B.1.

The estimated exposures assume that TCEP is imported to the site in its pure form and repackaged into smaller containers, with no engineering controls present. Actual exposures may differ based on worker activities, TCEP throughputs, and facility processes.

Table 3-3. Summary of Modeled Worker Inhalation Exposures for the Import – Repackaging of TCEP

Modeled Scenario	Exposure Concentration Type	Central Tendency (mg/m^3)	High-End (mg/m^3)	Data Quality Rating of Air Concentration Data
Scenario 1: One site; 2,500 lb throughput	8-hr TWA exposure concentration	1.1E–02	4.1E–02	N/A – Modeled data
	AC based on 8-hr TWA	7.5E–03	2.8E–02	
	ADC based on 8-hr TWA	8.9E–05	3.1E–04	
	LADC based on 8-hr TWA	3.4E–05	1.2E–04	
	$ADC_{subchronic}$ based on 8-hr TWA	1.1E–03	3.7E–03	
Scenario 2: One site; 25,000 lb throughput	8-hr TWA exposure concentration	1.1E–02	4.1E–02	
	AC based on 8-hr TWA	7.6E–03	2.8E–02	
	ADC based on 8-hr TWA	8.0E–04	2.7E–03	
	LADC based on 8-hr TWA	3.0E–04	1.1E–03	
	$ADC_{subchronic}$ based on 8-hr TWA	5.6E–03	2.0E–02	

Modeled Scenario	Exposure Concentration Type	Central Tendency (mg/m^3)	High-End (mg/m^3)	Data Quality Rating of Air Concentration Data
AC = Acute concentration; ADC = Average daily concentration; LADC = Lifetime average daily concentration; ADC$_{subchronic}$ = Subchronic average daily concentration				

3.1.4.4 Occupational Dermal Exposure Results

EPA estimated dermal exposures for this OES using the Dermal Exposure to Volatile Liquid Model and a fraction absorbed value of 23.3 percent described in Section 2.4.4 based on the dermal absorption data from Abdallah et al. (2016) (see Section 2.4.4 and Appendix D). The maximum concentration evaluated for this dermal exposure is 100 percent since TCEP is expected to be received at site in its pure form. Table 3-4 summarizes the APDR, ARD, CRD and SCRD for TCEP repackaged during import activities. The high-ends are based on a higher loading rate of TCEP (2.1 mg/cm^2-event) and two-hand contact, and the central tendencies are based on a lower loading rate of TCEP (1.4 mg/cm^2-event) and one-hand contact. OES-specific parameters for dermal exposures are described in Appendix D.

Table 3-4. Summary of Calculated Worker Dermal Exposures for the Import – Repackaging of TCEP

Modeled Scenario	Exposure Concentration Type	Central Tendency	High-End
Average adult worker (2,500 lb/yr)	APDR (mg/day)	175	524
	Dermal DD (mg/kg-day)	2.2	6.5
	ADD, non-cancer (mg/kg-day)	2.4E–02	0.13
	Chronic ADD, cancer (mg/kg-day)	9.5E–03	6.4E–02
	Subchronic ADD (mg/kg-day)	0.3	1.5
Average adult worker (25,00 lb/yr)	APDR (mg/day)	175	524
	Dermal DD (mg/kg-day)	2.2	6.5
	ADD, non-cancer (mg/kg-day)	0.2	1.2
	Chronic ADD, cancer (mg/kg-day)	9.0E–02	0.6
	Subchronic ADD (mg/kg-day)	1.6	4.8
Female of reproductive age (2,500 lb/yr)	APDR (mg/day)	145	435
	Dermal DD (mg/kg-day)	2.0	6.0
	ADD, non-cancer (mg/kg-day)	0.2	1.1
	Chronic ADD, cancer (mg/kg-day)	8.3E–02	0.6
	Subchronic ADD (mg/kg-day)	1.5	4.4
Female of reproductive age (25,000 lb/yr)	APDR (mg/day)	145	435
	Dermal DD (mg/kg-day)	2.0	6.0
	ADD, non-cancer (mg/kg-day)	2.2E–2	0.1

Modeled Scenario	Exposure Concentration Type	Central Tendency	High-End
	Chronic ADD, cancer (mg/kg-day)	8.7E–03	5.9E–02
	Subchronic ADD (mg/kg-day)	0.3	1.4
APDR = Acute potential dose rate; DD = Daily dose; ADD = Average daily dose			

3.1.4.5 Weight of Scientific Evidence for Occupational Exposures

EPA considered the assessment approach, the quality of the data, and uncertainties in assessment results to determine a WoSE conclusion for the inhalation exposure estimates. EPA used assumptions and values from the *Emission Scenario Document on Transport and Storage of Chemicals* (OECD, 2009c), which the systematic review process rated medium for data quality, to assess inhalation exposures. EPA used EPA/OPPT models combined with Monte Carlo simulations to estimate inhalation exposures. A strength of the Monte Carlo simulation approach is that variation in model input values and a range of potential exposure values is more likely than a discrete value to capture actual exposure at sites. The primary limitation is the uncertainty in the representativeness of values toward the true distribution of potential inhalation exposures. In addition, EPA lacks TCEP facility production volume data; and therefore, throughput estimates are based on CDR reporting thresholds. Also, EPA could not estimate the number of exposure days per year associated with repackaging operations, so the exposure days per year estimates are based on an assumed site throughput of imported containers. Based on these strengths and limitations, EPA has concluded that the WoSE for this assessment is moderate and provides a plausible estimate of exposures.

3.2 Incorporation Into Paints and Coatings

3.2.1 Process Description

TCEP is a component in coating products for commercial (non-consumer) use, including 1-part coatings and 2-part reactive coatings (PPG, 2010; FCC, 2016a; Vimasco, 2016; CharCoat, 2017; Duratec, 2018; J6 Polymers, 2018c). The 2020 CDR had no reporters for TCEP (U.S. EPA, 2020a), and the 2016 CDR had one reporter, Aceto Corporation in Port Washington, NY, which reported an industry sector of “not known or reasonably ascertainable” (U.S. EPA, 2019). EPA did not identify other data on current import volumes or import sites from systematic review. Therefore, EPA assumed TCEP may still be imported and used for paint and coating formulation at volumes below the CDR reporting threshold (see Section 2.2 for details) and assessed the following two potential scenarios: 1) one site using 25,000 lb of TCEP for paint and coating formulation; and 2) one site using 2,500 lb of TCEP for paint and coating formulation. These scenarios are meant to estimate a generic paint and coating manufacturer site that would not be subject to CDR reporting, and the scenarios do not necessarily represent the total number of paint and coating manufacturing sites using TCEP or total throughput of TCEP.

EPA did not identify data to determine the concentration of TCEP products that may be imported to formulation sites, nor the types of containers used to import TCEP. Based on the low production volume, EPA expects that TCEP and TCEP-containing products will be imported in drums or smaller containers rather than larger bulk containers, with material in drums then transferred to mixing vessels during formulation (NICNAS, 2001; OECD, 2009a; U.S. EPA, 2014b).

Based on the identified products, EPA expects that TCEP may be used in both 1-part and 2-part reactive coatings. EPA expects that the general processes for the formulation of 1-part coatings and 2-part reactive coatings to be similar. Incorporation into paint and coating formulations typically takes place in closed industrial mixing vessels as a batch blending or mixing process, with no reactions or chemical changes occurring to the additive (*i.e.*, TCEP) during the mixing process (NICNAS, 2001; OECD, 2009a; U.S. EPA, 2014b). Blending or mixing operations typically take place in the closed vessel over the course of 7–72 hours for 1-part coatings and 8–24 hours for 2-part reactive products (OECD, 2009a; U.S. EPA, 2014b). As part of process operations, operators may collect quality control samples once per batch (OECD, 2009a; U.S. EPA, 2014b). In the case of 1-part coatings, the manufacturer will transfer the blended formulation through an in-line filter, which EPA expects to be changed out once per batch (U.S. EPA, 2014b). The manufacturer will then transfer the blended formulation to product containers for sale or distribution as a coating product (OECD, 2009a; U.S. EPA, 2014b). Manufacturers will dispose of off-specification product when the coating does not meet quality or desired standards (OECD, 2009a; U.S. EPA, 2014b).

EPA assesses an overall concentration range of 0.1–5 percent of TCEP by mass in 1-part products and 10–25 percent of TCEP by mass in 2-part reactive coating products based on a review of available safety and technical data sheets from TCEP-containing coating products identified by EPA (specific concentrations and products provided in Appendix E.3.17). EPA also expects product container sizes to range from 1 quart up to 100-gallon drums based on of the information in the safety and technical data sheets from TCEP-containing coating products (container sizes and products provided in Appendix E.3.10).

EPA did not identify TCEP-specific operating data for paint and coatings manufacturing sites from systematic review (*i.e.*, daily throughputs or operating days/year). Sites are expected to operate 24 hours a day, 7 days a week (*i.e.* multiple shifts) with operating days as necessary up to 250 days per year. Figure 3-2 provides an illustration of the paint and coating manufacturing process.

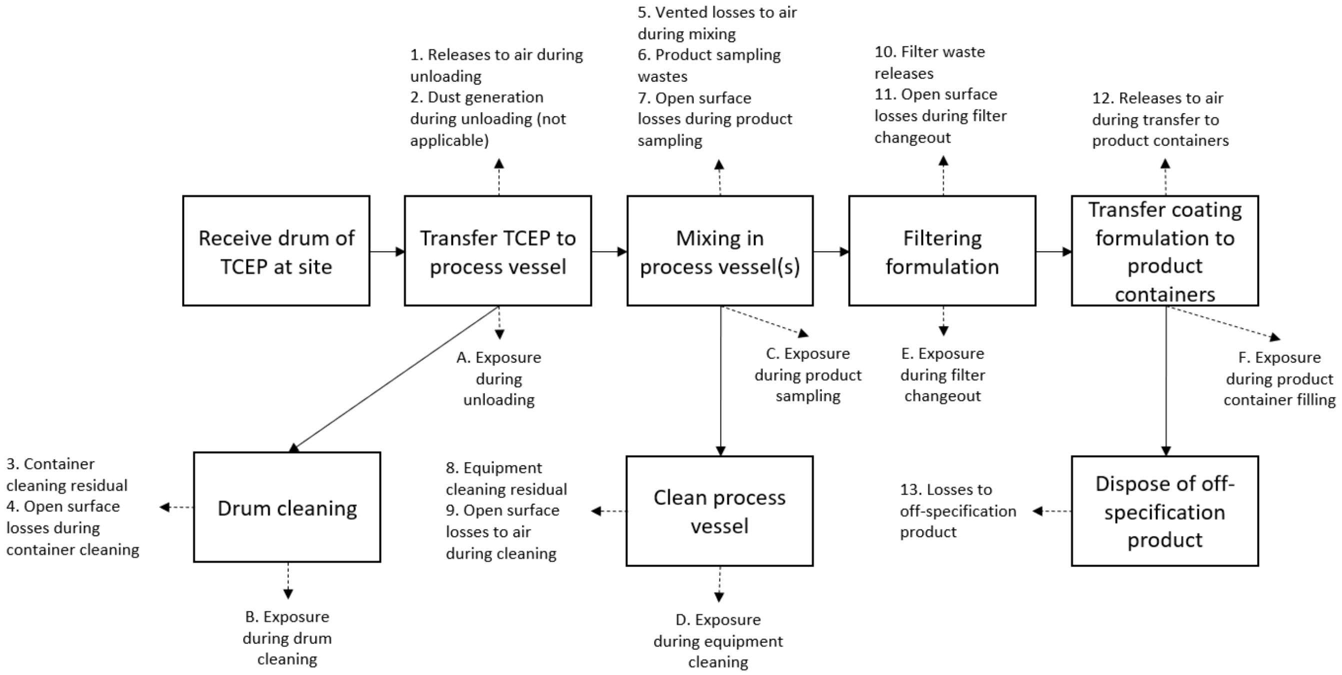

Figure 3-2. Paint and Coating Manufacturing Flow Diagram

3.2.2 Facility Estimates

The 2016 CDR data included a single reporting site, Aceto Corporation in Port Washington, NY, importing TCEP, with no downstream industry sectors identified (U.S. EPA, 2019). The 2020 CDR had no reporters for TCEP (U.S. EPA, 2020a). EPA assessed TCEP-containing paint and coating products from a review of available safety and technical data sheets (PPG, 2010; FCC, 2016a; PPG, 2016; Vimasco, 2016; CharCoat, 2017; Duratec, 2018). From the available data, EPA could not identify the number of receiving facilities or individual facility throughput for TCEP used in the manufacture of paints and coatings. Based on the absence of site-specific data, EPA modeled environmental releases and occupational exposures for a hypothetical scenario in which a single site receives and processes TCEP, with the overall throughput of TCEP at CDR reporting thresholds of 2,500 lb per year or 25,000 lb per year. EPA expects that paint and coating manufacturing sites receive TCEP as a raw material in its pure form, which is a neat liquid at 25 °C (see Table 2-1 in the TCEP Risk Evaluation (U.S. EPA, 2024)). EPA assumed that site operate 24 hours a day, 7 days a week (*i.e.*, multiple shifts) with operating days as necessary up to 250 days per year.

3.2.3 Release Assessment

3.2.3.1 Environmental Release Points

EPA expects releases to occur during the formulation of TCEP-containing paints and coatings. EPA estimated releases from incorporating TCEP into paints and coatings using a Monte Carlo simulation with 100,000 iterations and the Latin Hypercube sampling method using the models and approaches described in Appendix E.2. Input parameters for models were determined using data from literature, the *Draft Formulation of Waterborne Coatings – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2014a) (hereinafter referred to as the "GS for Formulation of Waterborne Coatings") and the *Emission Scenario Document on the Formulation of Adhesives* (OECD, 2009a). Specific release points considered for estimating releases are shown numbered as 1 through 13 in Figure 3-2. EPA expects releases may occur to different media for 1-part and 2-part reactive coatings based on the release point. EPA assessed process equipment cleaning residuals and off-specification wastes as waste disposal for 2-part reactive coatings and as released to water for 1-part coatings. Additionally, EPA did not assess releases to air or to disposal during filter changeout for 2-part reactive coatings since EPA does not expect filters to be used during formulation of this type of coatings. EPA did not assess releases from dust generation during unloading due to the expected liquid physical state of TCEP, and EPA expects releases from product sampling wastes to be negligible compared to other release points. Appendix E.3 describes the specific media assessed for each release point.

3.2.3.1 Environmental Release Assessment

Appendix E.3 includes the model equations and input parameters used in the Monte Carlo simulation for this COU. EPA estimated releases of TCEP by simulating two potential throughput scenarios: 1) one site processing TCEP at a total throughput of 2,500 lb of TCEP; and 2) one site processing TCEP at a total throughput of 25,000 lb of TCEP.

Table 3-5 summarizes the estimated release results for formulation of 1-part and 2-part reactive coatings based on the two scenarios applied. The high-end release estimates are the 95th percentile of the respective simulation output and the central tendency release estimates are the 50th percentile.

Table 3-5. Summary of Modeled Environmental Releases for the Formulation of TCEP-containing 1-part or 2-part Reactive Coatings

Modeled Scenario	Environmental Media	Annual Release (kg/site-yr)		Number of Release Days[a]		Daily Release (kg/site-day)	
		Central Tendency	High-End	Central Tendency	High-End	Central Tendency	High-End
1-part Coatings							
Scenario 1: One site; 2,500 lb throughput	Fugitive or stack air[b]	9.3E–03	3.9E–02	6	4	1.6E–03	9.6E–03
	Wastewater to onsite treatment or discharge to POTW	63	71	6	2	10	35
	Waste Disposal	11	22	7	2	1.5	9.3
Scenario 2: One site; 25,000 lb throughput	Fugitive or stack air[b]	8.5E–02	0.4	52	36	1.6E–03	1.0E–02
	Wastewater to onsite treatment or discharge to POTW	626	712	57	13	11	56
	Waste disposal	113	215	68	18	1.7	12
2-part Reactive Coatings							
Scenario 1: One site; 2,500 lb throughput	Fugitive air[c]	3.8E–03	8.3E–03	1	1	3.7E–03	7.9E–03
	Stack air[c]	4.0E–03	2.1E–02	1	1	3.8E–03	2.0E–02
	Wastewater to onsite treatment or discharge to POTW	27	32	1	1	27	32
	Waste disposal	34	34	1	1	34	34
Scenario 2: One site; 25,000 lb throughput	Fugitive air[c]	2.8E–02	5.8E–02	4	4	6.8E–03	1.6E–02
	Stack air[c]	2.4E–02	0.1	4	4	5.6E–03	2.9E–02
	Wastewater to onsite treatment or discharge to POTW	275	320	4	2	66	148
	Waste disposal	340	340	4	2	85	170

[a] The output for number of release days from the simulation was provided as a distribution. The number of release days presented in this table is based on simulation outputs for the annual release divided by the daily release (grouped by high-end or central tendency estimate), rounded to the closest integer. Annual totals may not add exactly due to rounding.

[b] EPA expects releases to air to occur for 7–24 hours per day. This time of release per day is based on the typical batch time of 7–72 hours per batch for 1-part coatings. Air releases also occur during container cleaning, equipment cleaning, curing/drying time, and transfer operations.

[c] EPA expects releases to air to occur for 8–24 hours per day. This time of release per day is based on the typical batch time of 8–24 hours per batch for 2-part reactive coatings. Air releases also occur during container cleaning, equipment cleaning, curing/drying time, filter media changeout, and transfer operations.

3.2.3.2 Weight of Scientific Evidence for Environmental Releases

Releases to the environment are assessed separately for 1-part coating products and 2-part reactive coating products. EPA used the GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a), which has a high data quality rating from the systematic review process, to assess releases for 1-part coating formulations. EPA used the *Emission Scenario Document on the Formulation of Adhesives* (OECD, 2009a; U.S. EPA, 2014a), which also has a high data quality rating from the systematic review process, to assess releases for 2-part reactive coating formulations. EPA used EPA/OPPT models combined with Monte Carlo modeling to estimate releases to the environment, with media of release assessed using assumptions from the GS, ESD, and EPA/OPPT models. A strength of the Monte Carlo stimulation approach is that variation in model input values and a range of potential releases values is more likely than a discrete value to capture actual releases at sites. Additionally, EPA used TCEP-specific data on concentrations in paint and coating products and product densities in the analysis to provide more accurate estimates than the generic values provided by the ESDs. The safety and product data sheets these values were obtained from have high data quality ratings from the systematic review process. The primary limitation of EPA's approach is the uncertainty in the representativeness of values toward the true distribution of potential releases. In addition, EPA lacks TCEP facility production volume data and number of processing sites; therefore, throughput estimates are based on CDR reporting thresholds with an overall release using a hypothetical scenario of a single facility. Additional limitations to this assessment are that EPA could not estimate an overall number of release days per year associated with all release points, so the release days per year estimates are based on engineering assumptions and batch formulation times. Based on this information, EPA has concluded that the WoSE for this assessment is moderate and provides a plausible estimate of releases in consideration of the strengths and limitations of reasonably available data.

3.2.4 Occupational Exposure Assessment

3.2.4.1 Worker Activities

During the formulation of TCEP-containing coatings, workers are potentially exposed to TCEP during the following activities: transferring TCEP from transport containers into formulation equipment, sampling coating product, and filling product containers. For the 2-part reactive coatings, the filter changeout activity potentially exposes workers to TCEP. During cleaning activities, workers may also be exposed via inhalation of vapor or dermal contact with TCEP-containing residuals in transport containers or formulation equipment. EPA does not expect significant worker inhalation exposure to TCEP after the coating has been packaged because TCEP vapor generation from the coating will be sealed in product containers. For this OES, ONUs would include supervisors, managers, and other employees that may be in the formulation area but do not perform tasks with direct contact with TCEP.

3.2.4.2 Number of Workers and Occupational Non-Users

EPA used data from the BLS and the U.S. Census' SUSB specific to the OES (U.S. Census Bureau, 2015; U.S. BLS, 2016) to estimate the number of workers and ONUs per site potentially exposed to TCEP during formulation of TCEP-containing coatings. This approach involved the identification of relevant Standard Occupational Classification (SOC) codes within the BLS data for the identified NAICS codes. Section 2.4.2 includes further details regarding methodology for estimating the number of workers and ONUs per site. EPA assigned the NAICS code 325510 – Paint and Coating Manufacturing for this OES based on the process description. Table 3-6 summarizes the per site estimates for this OES based on the methodology described. As addressed in Section 3.2.2, EPA did not identify site-specific data for the number of facilities in the United States incorporating TCEP into paint and coating formulations.

Table 3-6. Estimated Number of Workers Potentially Exposed to TCEP During Formulation of 1-part and 2-part Reactive Coatings

NAICS Code	Exposed Workers per Site[a]	Exposed ONUs per Site[a]
325510 – Paint and Coating Manufacturing	14	5

[a] Number of workers and ONUs per site are calculated by dividing the exposed number of workers or ONUs by the number of establishments. The number of workers per site is rounded to the nearest integer. The number of ONUs per site is shown as 5.4, as it rounds down to 5.

3.2.4.3 Occupational Inhalation Exposure Results

EPA did not identify inhalation monitoring data for processing TCEP as a component in formulations of paints and coatings based on systematic review of literature sources. Therefore, EPA estimated inhalation exposures using a Monte Carlo simulation with 100,000 iterations and the Latin Hypercube sampling method using the models and approaches described in Appendix E.3. Input parameters for the models were determined using data from literature and the GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a), and the *Emission Scenario Document on the Formulation of Adhesives* (OECD, 2009a). EPA estimated inhalation exposures of TCEP by simulating two potential scenarios: 1) one site importing and processing 2,500 lb; and 2) one site importing and processing 25,000 lb. EPA also assumed that pure TCEP is imported to the site and incorporated into the final formulation by a batch mixing process, with no engineering controls present. EPA used product data from TCEP-containing paints and coatings to estimate the concentration of TCEP in the final product and the final product density as inputs to the Monte Carlo simulation. Actual exposures may differ based on worker activities, TCEP throughputs, and facility processes.

For this scenario, EPA applied the EPA Mass Balance Inhalation Model to exposure points described in the GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) and the *Emission Scenario Document on the Formulation of Adhesives* (OECD, 2009a). The EPA Mass Balance Inhalation Model estimates the concentration of the chemical in the breathing zone of the worker based on a vapor generation rate (G). An 8-hour TWA is then estimated and averaged over eight hours assuming no exposure occurs outside of those activities. Inhalation exposures from formulation of TCEP-containing 1-part and 2-part Reactive coatings were assessed separately as the literature data for model inputs were different for the two coating types. EPA generally does not expect the formulation of the two coating types to occur at the same site, such that different workers would be exposed from each formulation process. See Appendix E.3 for the specific differences between the parameters and product values, the model equations, and other input parameters used in the Monte Carlo simulation for this OES.

EPA used the EPA Mass Balance Inhalation Model to determine a time-weighted exposure for each exposure point. EPA estimated the time-weighted average inhalation exposure for a full work-shift (EPA assumed an 8-hour work-shift) as an output of the Monte Carlo simulation by summing the time-weighted inhalation exposures for each of the exposure points and assuming no exposures outside these activities. Table 3-7 summarizes the estimated 8-hour TWA exposures, AC, ADC, LADC, and $ADC_{subchronic}$ for formulating TCEP-containing coatings based on the two scenarios applied. The high-end exposures presented in Table 3-7 are the 95th percentile of the respective simulation output, and the central tendency exposures are the 50th percentile. Equations for calculating AC, ADC, LADC, and $ADC_{subchronic}$ are presented in Appendix B.1.

Table 3-7. Summary of Modeled Worker Inhalation Exposures for the Formulation of 1-part and 2-part Reactive Coatings

Modeled Scenario	Exposure Concentration Type	Central Tendency (mg/m^3)	High-End (mg/m^3)	Data Quality Rating of Air Concentration Data
1-part Coatings				
Scenario 1: One site; 2,500 lb throughput	8-hr TWA exposure concentration	1.7E–02	0.1	N/A – Modeled data
	AC based on 8-hr TWA	1.1E–02	7.1E–02	
	ADC based on 8-hr TWA	1.9E–04	8.0E–04	
	LADC based on 8-hr TWA	7.3E–05	3.2E–04	
	ADC$_{subchronic}$ based on 8-hr TWA	2.2E–03	9.2E–03	
Scenario 2: One site; 25,000 lb throughput	8-hr TWA exposure concentration	1.7E–02	0.1	
	AC based on 8-hr TWA	1.1E–02	7.4E–02	
	ADC based on 8-hr TWA	1.7E–03	7.1E–03	
	LADC based on 8-hr TWA	6.4E–04	2.8E–03	
	ADC$_{subchronic}$ based on 8-hr TWA	7.7E–03	4.3E–02	
2-part Reactive Coatings				
Scenario 1: One site; 2,500 lb throughput	8-hr TWA exposure concentration	9.6E–02	0.4	N/A – Modeled data
	AC based on 8-hr TWA	6.5E–02	0.3	
	ADC based on 8-hr TWA	1.9E–04	7.9E–04	
	LADC based on 8-hr TWA	7.1E–05	3.1E–04	
	ADC$_{subchronic}$ based on 8-hr TWA	2.3E–03	9.6E–03	
Scenario 2: One site; 25,000 lb throughput	8-hr TWA exposure concentration	0.1	0.5	
	AC based on 8-hr TWA	8.6E–02	0.4	
	ADC based on 8-hr TWA	1.0E–03	4.2E–03	
	LADC based on 8-hr TWA	3.8E–04	1.7E–03	
	ADC$_{subchronic}$ based on 8-hr TWA	1.2E–02	5.1E–02	
AC = Acute concentration; ADC = Average daily concentration; LADC = Lifetime average daily concentration; ADC$_{subchronic}$ = Subchronic average daily concentration				

3.2.4.4 Occupational Dermal Exposure Results

EPA estimated dermal exposures for this OES using the Dermal Exposure to Volatile Liquid Model and a fraction absorbed value of 23.3 percent described in Section 2.4.4 based on the dermal absorption data from (Abdallah et al., 2016) (see Section 2.4.4 and Appendix D). The maximum concentration evaluated for this dermal exposure is 100 percent for both 1-part and 2-part reactive coatings since pure TCEP is expected to be received at site. Table 3-8 summarizes the APDR, ARD, CRD and SCRD for TCEP incorporated into paint and coating formulations, with separate values for 1-part or 2-part reactive coatings. The high-ends are based on a higher loading rate of TCEP (2.1 mg/cm^2-event) and two-hand contact, and the central tendencies are based on a lower loading rate of TCEP (1.4 mg/cm^2-event) and one-hand contact. OES-specific parameters for dermal exposures are described in Appendix D.

Table 3-8. Summary of Calculated Worker Dermal Exposures for the Formulation of 1-part and 2-part Reactive Coatings

Modeled Scenario	Exposure Concentration Type	Central Tendency	High-End
1-part Coatings			
Average adult worker (2,500 lb/yr)	APDR (mg/day)	175	524
	Dermal DD (mg/kg-day)	2.2	6.5
	ADD, non-cancer (mg/kg-day)	3.6E–02	0.7
	Chronic ADD, cancer (mg/kg-day)	1.4E–02	0.3
	Subchronic ADD (mg/kg-day)	0.4	4.8
Average adult worker (25,000 lb/yr)	APDR (mg/day)	175	524
	Dermal DD (mg/kg-day)	2.2	6.5
	ADD, non-cancer (mg/kg-day)	0.3	4.5
	Chronic ADD, cancer (mg/kg-day)	0.1	2.3
	Subchronic ADD (mg/kg-day)	1.6	4.8
Female of reproductive age (2,500 lb/yr)	APDR (mg/day)	145	435
	Dermal DD (mg/kg-day)	2.0	6.0
	ADD, non-cancer (mg/kg-day)	3.3E–02	0.6
	Chronic ADD, cancer (mg/kg-day)	1.3E–02	0.3
	Subchronic ADD (mg/kg-day)	0.4	4.4
Female of reproductive age (25,000 lb/yr)	APDR (mg/day)	145	435
	Dermal DD (mg/kg-day)	2.0	6.0
	ADD, non-cancer (mg/kg-day)	0.3	4.1
	Chronic ADD, cancer (mg/kg-day)	0.1	2.1
	Subchronic ADD (mg/kg-day)	1.5	4.4
2-part Reactive Coatings			
Average adult worker (2,500 lb/yr)	APDR (mg/day)	175	524
	Dermal DD (mg/kg-day)	2.2	6.5
	ADD, non-cancer (mg/kg-day)	6.0E–03	3.6E–02
	Chronic ADD, cancer (mg/kg-day)	2.4E–03	1.8E–02
	Subchronic ADD (mg/kg-day)	7.3E–02	0.4
Average adult worker (25,000 lb/yr)	APDR (mg/day)	175	524
	Dermal DD (mg/kg-day)	2.2	6.5
	ADD, non-cancer (mg/kg-day)	2.4E–02	0.2

Modeled Scenario	Exposure Concentration Type	Central Tendency	High-End
	Chronic ADD, cancer (mg/kg-day)	9.5E–03	0.1
	Subchronic ADD (mg/kg-day)	0.3	2.6
Female of reproductive age (2,500 lb/yr)	APDR (mg/day)	145	435
	Dermal DD (mg/kg-day)	2.0	6.0
	ADD, non-cancer (mg/kg-day)	5.5E–03	3.3E–02
	Chronic ADD, cancer (mg/kg-day)	2.2E–03	1.7E–02
	Subchronic ADD (mg/kg-day)	6.7E–02	0.4
Female of reproductive age (25,000 lb/yr)	APDR (mg/day)	145	435
	Dermal DD (mg/kg-day)	2.0	6.0
	ADD, non-cancer (mg/kg-day)	2.2E–02	0.2
	Chronic ADD, cancer (mg/kg-day)	8.7E–03	1.0E–01
	Subchronic ADD (mg/kg-day)	0.3	2.4
APDR = Acute potential dose rate; DD = Daily dose; ADD = Average daily dose			

3.2.4.5 Weight of Scientific Evidence for Occupational Exposures

EPA considered the assessment approach, the quality of the data, and uncertainties in assessment results to determine a WoSE conclusion for the 8-hr TWA inhalation exposure estimates. EPA used the GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) to assess inhalation exposures for 1-part coating formulations, which has a high data quality rating from the systematic review process. EPA used the *Emission Scenario Document on the Formulation of Adhesives* (OECD, 2009a) to assess inhalation exposures for 2-part reactive coating formulations, which also has a high data quality rating from the systematic review process. EPA used EPA/OPPT models combined with a Monte Carlo simulation to estimate inhalation exposure parameters. A strength of the Monte Carlo stimulation approach is that variation in model input values and a range of potential exposure values is more likely than a discrete value to capture actual exposure at sites. Another strength was the ability to separately estimate exposures for 1-part and 2-part reactive coatings. EPA used TCEP-specific data on concentrations in paint and coating products and product densities in the analysis to provide more accurate estimates than the generic values provided by the ESDs. The safety data sheets (SDSs) these values were obtained from have high data quality ratings from the systematic review process. The primary limitation is the uncertainty in the representativeness of values toward the true distribution of potential inhalation exposures. In addition, EPA lacks TCEP facility production volume data; and therefore, throughput estimates are based on CDR reporting thresholds. Also, EPA could not estimate the number of exposure days per year associated with processing operations, so the exposure days per year estimates are based on engineering assumptions and batch formulation times. Based on these strengths and limitations, EPA has concluded that the WoSE for this assessment is moderate to robust and provides a plausible estimate of exposures.

3.3 Use In Paints and Coatings

3.3.1 Process Description

TCEP is an additive component in coating products for commercial and industrial use, including 1-part coatings and 2-part reactive coatings (PPG, 2010; FCC, 2016a; PPG, 2016; Vimasco, 2016; CharCoat, 2017; Duratec, 2018). Industrial and commercial sites apply TCEP-containing products as a flame retardant coating to achieve flame spread or fire protection standards for structural and electrical components, such as masonry surfaces or cables (PPG, 2010; FCC, 2016a; PPG, 2016; Vimasco, 2016; CharCoat, 2017; Duratec, 2018).

The 2020 CDR had no reporters for TCEP (U.S. EPA, 2020a), and the 2016 CDR had one reporter, Aceto Corporation in Port Washington, NY, which reported an industry sector of "not known or reasonably ascertainable" (U.S. EPA, 2019). EPA did not identify other data on current import volumes or import sites from systematic review. Therefore, EPA assumed TCEP or TCEP-containing paint and coating products may still be imported and used at volumes below the CDR reporting threshold (see Section 2.2 for details) and assessed overall throughputs of TCEP at 25,000 lb and 2,500 lb for use in paints and coatings. EPA did not find information on TCEP-specific use rates and EPA expects TCEP-containing paint and coating application rates at commercial and industrial sites to vary depending on the specific needs of the site. The Specific Emission Release Category (SpERC) documents developed by the European Council of the Paint, Printing Ink, and Artist's Colours Industry (CEPE) for industrial application of coatings by spraying and professional application of inks and coatings by spraying estimate coating use rates of 1,000 kg and 100 kg per site, per day, respectively (CEPE, 2020a, 2020b). These scenarios are meant to estimate generic site(s) that apply TCEP-containing paints and coatings and the scenarios do not necessarily represent the total number of paint and coating sites using TCEP or total throughput of TCEP.

EPA expects that coatings containing TCEP as an additive component arrive at the end user site in containers ranging from approximately 1 quart up through 100 gallon drums based on the relevant ESD and review of available TDSs from TCEP-containing coating products identified by EPA (specific container sizes discussed in Appendix E.4.11). EPA assesses an overall concentration range of 0.1 to 25 percent of TCEP by mass in paint and coating products based on a review of available safety and technical data sheets from TCEP-containing coating products identified by EPA (specific concentrations and products provided in Appendix E.4.13). Upon receiving of the TCEP-containing coating product, an operator will transfer the coating product from the container to the application equipment. Coating application methods for TCEP-containing paints and coatings include spray gun, brush, and trowel coating for use on structures or equipment (PPG, 2008; FCC, 2011; CharCoat, 2019). Spray gun applications may include an air (*e.g.*, low volume/high pressure), air-assisted, or airless spray system (U.S. EPA, 2004; OECD, 2009a; U.S. EPA, 2014a). EPA did not identify the prevalence of these various application methods. The operator will then apply the coating to the substrate and TCEP will remain in the coating as an additive in the dried/cured coating on the substrate. EPA expects that coating applications occur over the course of an 8-hour workday for one or two days at a given site, accounting for multiple coats and typical drying or curing times listed for TCEP-containing coatings (PPG, 2008; FCC, 2011; CharCoat, 2019). Figure 3-3 provides an illustration of the process for commercial use of paints and coatings.

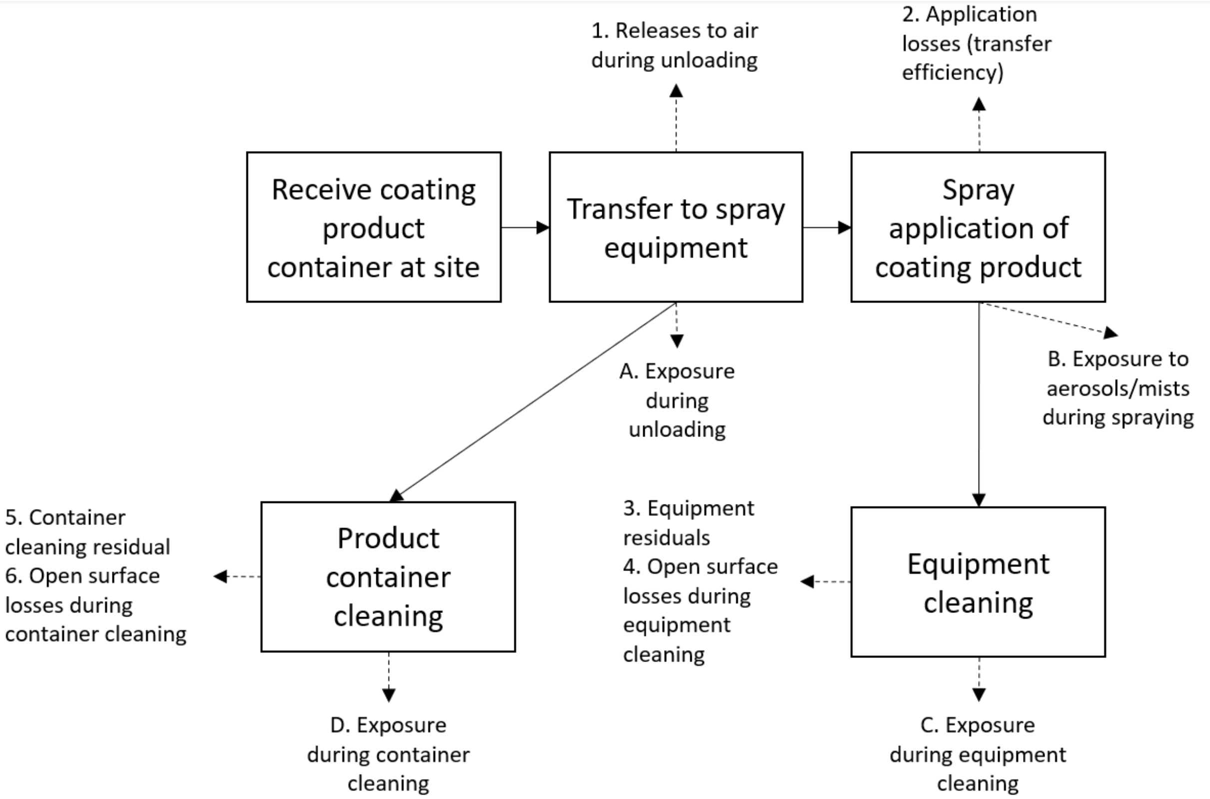

Figure 3-3. Flow Diagram for Commercial Use of Paints and Coatings

3.3.2 Facility Estimates

The 2016 CDR data included a single reporting site, Aceto Corporation in Port Washington, NY, importing TCEP, with no downstream industry sectors or commercial uses identified (U.S. EPA, 2019). The 2020 CDR had no reporters for TCEP (U.S. EPA, 2020a). Therefore, EPA assumed TCEP or TCEP-containing paint and coating products may still be imported and used at volumes below the CDR reporting threshold (see Section 2.2 for details).

EPA assessed coating application rates using either 100 kg or 1,000 kg per site per day. based on the SpERC documents developed by the CEPE for industrial application of coatings by spraying and professional application of inks and coatings by spraying (CEPE, 2020a, 2020b). EPA assessed six separate scenarios:

- Number of sites calculated based on a coating use rate of 100 kg per site, per day with a TCEP throughput of 2,500 lb and 25,000 lb (two scenarios);
- Number of sites calculated based on a coating use rate of 1,000 kg per site, per day with TCEP throughput of 2,500 lb and 25,000 lb (two scenarios); and
- One site using the entire TCEP throughput at 2,500 lb and 25,000 lb (two scenarios).

These scenarios are meant to estimate a generic stie that applies TCEP-containing paints and coatings that would not be subject to CDR reporting, and the scenarios do not necessarily represent the total number of paint and coating sites using TCEP or total throughput of TCEP.

3.3.3 Release Assessment

3.3.3.1 Environmental Release Points

EPA expects releases to occur during the spray, brush, and trowel application of TCEP-containing paints and coatings. EPA did not identify use rates for the application of paints and coatings via brush and trowel therefore, EPA estimated release of TCEP-containing paints and coatings from spray application. EPA estimated releases using a Monte Carlo simulation with 100,000 iterations and the Latin Hypercube sampling method using the models and approaches described in Appendix E. Input parameters for the models were determined using data from literature, the *Emission Scenario Documents on Coatings Industry* (OECD, 2009d), *Emission Scenario Documents on Spray-Painting in Automotive Refinishing* (OECD, 2011a), and *Generic Scenario on Spray Coatings in Furniture Industry* (U.S. EPA, 2004; OECD, 2009d, 2011a). EPA used this method to estimate releases for individual release points and summed the individual releases to each environmental media to estimate total annual and daily facility releases. Specific release points considered for estimating releases are shown numbered as 1 through 6 in Figure 3-3. Based on the models and data used, EPA expects fugitive air TCEP releases during product container unloading and cleaning, application of the paint or coating, and during equipment cleaning. EPA expects TCEP releases from wastewater managed in onsite treatment or discharged to a POTW during product container cleaning and equipment cleaning.

3.3.3.2 Environmental Release Assessment Results

Appendix E.4 includes the model equations and input parameters used in the Monte Carlo simulation for this COU. EPA estimated releases of TCEP by simulating six potential throughput scenarios:

- Number of sites calculated based on a coating use rate of 100 kg per site, per day with a TCEP throughput of 2,500 lb and 25,000 lb (two scenarios);
- Number of sites calculated based on a coating use rate of 1,000 kg per site, per day with TCEP throughput of 2,500 lb and 25,000 lb (two scenarios); and
- One site using the entire TCEP throughput at 2,500 lb and 25,000 lb (two scenarios).

Table 3-9 summarizes the estimated release results for Spray Application of TCEP-containing Paints and Coatings based on the six scenarios applied. The high-end release estimates are the 95th percentile of the respective simulation output and the central tendency release estimates are the 50th percentile.

Table 3-9. Summary of Modeled Environmental Releases for the Spray Application of TCEP-containing Paints and Coatings

Modeled Scenario	# of Sites	Environmental Media	Annual Release (kg/site-yr)		Number of Release Days[a]		Daily Release (kg/site-day)	
			Central Tendency	High-End	Central Tendency	High-End	Central Tendency	High-End
Scenario 1: 100 kg/site-day; 2,500 lb throughput	22–11,333	Fugitive air[b]	1.6	16	1	2	1.2	10
		Wastewater to onsite treatment or discharge to POTW	0.3	3.3	1	2	0.2	2.0
Scenario 2: 100 kg/site-day; 25,000 lb throughput	226–112,846	Fugitive air[b]	1.7	16	1	2	1.2	9.9
		Wastewater to onsite treatment or discharge to POTW	0.3	3.3	1	2	0.2	2.0

Modeled Scenario	# of Sites	Environmental Media	Annual Release (kg/site-yr)		Number of Release Days[a]		Daily Release (kg/site-day)	
			Central Tendency	High-End	Central Tendency	High-End	Central Tendency	High-End
Scenario 3: 1,000 kg/site-day; 2,500 lb throughput	2–1,133	Fugitive air[b]	17	189	1	2	12	114
		Wastewater to onsite treatment or discharge to POTW	3.4	38	1	2	2.4	23
Scenario 4: 1,000 kg/site-day; 25,000 lb throughput	22–11,335	Fugitive air[b]	17	162	1	2	12	99
		Wastewater to onsite treatment or discharge to POTW	3.3	33	1	2	2.3	21
Scenario 5: 2,500 lb throughput	1	Fugitive air[b]	491	775	1	1	349	720
		Wastewater to onsite treatment or discharge to POTW	98	162	1	1	69	150
Scenario 6: 25,000 lb throughput	1	Fugitive air[b]	4,905	7,754	1	1	3480	7,213
		Wastewater to onsite treatment or discharge to POTW	986	1,622	1	1	689	1,497

[a] The output for number of release days was determined to be either one or two days based on review of TDSs for TCEP-containing coatings with typical applications taking one or two days. This is due to drying times required in between initial coating and a recoat of the same product. It is assumed a single job site will only use the coating product once in a given year to completely coat all given equipment/structures/items that require the coating.

[b] EPA expects releases to air to occur for a full-shift of 8 hours per day.

3.3.3.3 Weight of Scientific Evidence for Environmental Releases

Releases to the environment are assessed using EPA/OPPT generic models and spray application transfer efficiencies from GSs and ESDs. EPA combined the EPA/OPPT models with Monte Carlo modeling to estimate releases to the environment, with media of release assessed using assumptions from the EPA/OPPT models and scenario-specific assumptions that no engineering controls are used during spray application. A strength of the Monte Carlo stimulation approach is that variation in model input values and a range of potential release values is more likely than a discrete value to capture actual releases at sites. Additionally, EPA used TCEP-specific data on concentrations in paint and coating products, product densities and number of application days per site (based on drying times of coatings) in the analysis to provide more accurate estimates than the generic values provided by the ESDs. The safety and product data sheets these values were obtained from have high data quality ratings from the systematic review process. The primary limitation in EPA’s approach is the uncertainty in the representativeness of values toward the true distribution of potential releases. EPA assumes spray applications of the coatings, so the estimates may not be representative of other coating application methods. In addition, EPA lacks TCEP facility production volume data and number of application sites; therefore, national and site-specific throughput estimates are based on CDR reporting thresholds and values from industry SpERC documents. EPA applied six separate hypothetical throughput scenarios to determine a range of possible releases, but there is uncertainty which scenarios most accurately capture actual releases. Based on this information, EPA has concluded that the WoSE for this assessment is slight to moderate and provides a plausible estimate of releases in consideration of the strengths and limitations of reasonably available data.

3.3.4 Occupational Exposure Assessment

3.3.4.1 Workers Activities

During the use of TCEP-containing paints and coatings, inhalation exposures to workers may occur from mists generated during spray applications and inhalation exposures to workers and ONUs may occur from vapors generated from TCEP that volatilizes during unloading of the product, and container/equipment cleaning. Dermal exposures to liquid TCEP may occur during unloading of the product into application equipment, brush and trowel applications, and container/equipment cleaning. Workers may also have dermal exposures to mists during spray applications. EPA did not find information on the extent that engineering controls and worker PPE are used at facilities that use TCEP-containing paints and coatings. For this OES, ONUs would include supervisors, managers, and other employees that do not directly handle equipment utilizing TCEP but may be in the spray application area.

3.3.4.2 Number of Workers and Occupational Non-Users

To estimate the number of workers and ONUs per site potentially exposed to TCEP during use of TCEP-containing paints and coatings, EPA used data from the BLS and the U.S. Census' SUSB specific to the OES (U.S. Census Bureau, 2015; U.S. BLS, 2016). This approach involved the identification of relevant Standard Occupational Classification (SOC) codes within the BLS data for the identified NAICS codes. Section 2.4.2 includes further details regarding methodology for estimating the number of workers and ONUs per site. The end-use industries for TCEP coatings can vary significantly and EPA does not have information on which specific NAICS codes will use TCEP. Therefore, EPA assumed the NAICS Code 811121 – Automotive Body, Paint, and Interior Repair and Maintenance based on the *Emission Scenario Document on Spray-Painting in Automotive Refinishing* (OECD, 2011a) and the NAICS code 238320 – Painting and Wall Covering Contractors to estimate the number of workers and ONUs exposed per site for this OES. Table 3-10 summarizes the per site estimates for the NAICS Codes 811121 and 238320 based on the methodology described. The *Emission Scenario Document on Radiation Curable Coating, Inks, and Adhesives* (OECD, 2011b) estimates the number of workers exposed for industries utilizing coatings between 7–83 workers based on a separate list of applicable NAICS codes within the broader coatings industry.

Table 3-10. Estimated Number of Workers Potentially Exposed to TCEP During Spray Application

NAICS Code	Exposed Workers per Site[a]	Exposed ONUs per Site[a]
811121 – Automotive Body, Paint, and Interior Repair and Maintenance	3	0
238320 – Painting and Wall Covering Contractors	4	0

[a] Number of workers and ONUs per site are calculated by dividing the exposed number of workers or ONUs by the number of establishments. The number of workers per site is rounded to the nearest integer. The number of ONUs per site is below 0.5 per site, so it is shown as 0 due to rounding.

3.3.4.3 Occupational Inhalation Exposure Results

EPA did not identify TCEP-specific inhalation monitoring data to assess exposures during spray application of TCEP-containing paints and coatings. Therefore, EPA estimated mist inhalation exposures for the spray application activity using the mist monitoring data from the *Emission Scenario*

Document on Spray-Painting in Automotive Refinishing (OECD, 2011a) (measured as total particulate dust). Using the monitoring data from the *Emission Scenario Document on Spray-Painting in Automotive Refinishing* (OECD, 2011a), EPA estimated mist inhalation exposures for six potential scenarios: exposures calculated for 1-day application, 2-day application, and 250-day application using either 1-part or 2-part reactive paints and coatings.

EPA expects total inhalation exposures to be a contribution of both mists and vapors. However, EPA does not have information on the typical application times associated with the types of coatings TCEP is used in. Therefore, EPA assumed that the mist exposures would be the dominant exposure route and assumed spray applications would occur for the entire 8-hour shift and did not provide estimates of the contributions to exposure from vapors. The 8-hour spray duration likely overestimates application times therefore, EPA expects it to be protective of the vapor exposure activities which would only occur when the worker is not performing spray coating activities and would be a lower concentration than the estimated mist concentration.

EPA estimated the TWA inhalation exposure using a deterministic calculation for a full work-shift (EPA assumed an 8-hour work-shift) by taking the central tendency (50th percentile) and high-end (95th percentile) data points from the *Emission Scenario Document on Spray-Painting in Automotive Refinishing* (OECD, 2011a) and adjusting the concentrations based on whether the paint/coating sprayed was a 1-part or 2-part reactive paint/coating.

Table 3-11 summarizes the estimated 8-hour TWA exposures, AC, ADC, LADC, and $\text{ADC}_{\text{subchronic}}$ for the Use in Paints and Coatings TCEP-containing coatings based on the six scenarios applied. The high-ends presented in Table 3-11 are the 95th percentile of the calculated output, and the central tendencies are the 50th percentile. Equations for calculating AC, ADC, LADC, and $\text{ADC}_{\text{subchronic}}$ are presented in Appendix B.1.

The underlying data from the *Emission Scenario Document on Spray-Painting in Automotive Refinishing* (OECD, 2011a) were captured with spray booths in place, however spray booths are not expected to be used outside of the auto industry. Therefore, EPA will not assume spray booths as an engineering control for this OES. EPA used product data from TCEP-containing paints and coatings to estimate the TCEP concentration and coating product density. EPA uses both parameters as inputs for its deterministic calculation. Actual exposures may differ based on worker activities, TCEP throughputs, coating properties, and facility processes.

Table 3-11. Summary of Estimated Worker Inhalation Exposures from Use in Paints and Coatings

Modeled Scenario	Exposure Concentration Type	Central Tendency (mg/m^3)	High-End (mg/m^3)	Data Quality Rating of Air Concentration Data
Scenario 1: 1-day application; 1-part paints and coatings	8-hr TWA exposure concentration	0.2	1.1	High
	AC based on 8-hr TWA	0.1	0.8	
	ADC based on 8-hr TWA	3.1E–04	2.1E–03	
	LADC based on 8-hr TWA	1.3E–04	1.1E–03	
	$\text{ADC}_{\text{subchronic}}$ based on 8-hr TWA	3.8E–03	2.5E–02	

Modeled Scenario	**Exposure Concentration Type**	**Central Tendency (mg/m^3)**	**High-End (mg/m^3)**	**Data Quality Rating of Air Concentration Data**
Scenario 2: 2-day application; 1-part paints and coatings	8-hr TWA exposure concentration	0.2	1.1	
	AC based on 8-hr TWA	0.1	0.8	
	ADC based on 8-hr TWA	6.3E–04	4.1E–03	
	LADC based on 8-hr TWA	2.5E–04	2.1E–03	
	ADC$_{subchronic}$ based on 8-hr TWA	7.7E–03	5.0E–02	
Scenario 3: 250-day application; 1-part paints and coatings	8-hr TWA exposure concentration	0.2	1.1	
	AC based on 8-hr TWA	0.1	0.8	
	ADC based on 8-hr TWA	7.9E–02	0.5	
	LADC based on 8-hr TWA	3.1E–02	0.3	
	ADC$_{subchronic}$ based on 8-hr TWA	8.4E–02	0.6	
Scenario 4: 1-day application; 2-part reactive paints and coatings	8-hr TWA exposure concentration	0.9	5.5	
	AC based on 8-hr TWA	0.6	3.8	
	ADC based on 8-hr TWA	1.6E–03	1.0E–02	
	LADC based on 8-hr TWA	6.3E–04	5.3E–03	
	ADC$_{subchronic}$ based on 8-hr TWA	1.9E–02	0.1	
Scenario 5: 2-day application; 2-part reactive paints and coatings	8-hr TWA exposure concentration	0.9	5.5	
	AC based on 8-hr TWA	0.6	3.8	
	ADC based on 8-hr TWA	3.1E–03	2.1E–02	
	LADC based on 8-hr TWA	1.3E–03	1.1E–02	
	ADC$_{subchronic}$ based on 8-hr TWA	3.8E–02	0.3	
Scenario 6: 250-day application; 2-part reactive paints and coatings	8-hr TWA exposure concentration	0.9	5.5	
	AC based on 8-hr TWA	0.6	3.8	
	ADC based on 8-hr TWA	0.4	2.6	
	LADC based on 8-hr TWA	0.2	1.3	
	ADC$_{subchronic}$ based on 8-hr TWA	0.4	2.8	
AC = Acute concentration; ADC = Average daily concentration; LADC = Lifetime average daily concentration; ADC$_{subchronic}$ = Subchronic average daily concentration				

3.3.4.1 Occupational Dermal Results

EPA estimated dermal exposures for this OES using the Dermal Exposure to Volatile Liquid Model and a fraction absorbed value of 23.3 percent described in Section 2.4.4 based on the dermal absorption data from (Abdallah et al., 2016) (see Section 2.4.4 and Appendix D). The maximum concentration evaluated for this dermal exposure is 25 percent since that is the highest weight fraction of a TCEP-containing paint/coating product (PPG, 2010). Table 3-12 summarizes the APDR, ARD, CRD and SCRD for TCEP from industrial application of TCEP-containing paints and coatings. The high-ends are based on a higher loading rate of TCEP (2.1 mg/cm^2-event) and two-hand contact, and the central tendencies are based on a lower loading rate of TCEP (1.4 mg/cm^2-event) and one-hand contact. OES-specific parameters for dermal exposures are described in Appendix D.2.

Table 3-12. Summary of Calculated Worker Dermal Exposures from Use in Paints and Coatings

Modeled Scenario	Exposure Concentration Type	Central Tendency	High-End
1-day application			
Average adult worker	APDR (mg/day)	118	642
	Dermal DD (mg/kg-day)	1.5	8.0
	ADD, non-cancer (mg/kg-day)	4.1E–03	2.2E–02
	Chronic ADD, cancer (mg/kg-day)	1.6E–03	1.1E–02
	Subchronic ADD (mg/kg-day)	4.9E–02	0.3
Female of reproductive age	APDR (mg/day)	99	534
	Dermal DD (mg/kg-day)	1.4	7.4
	ADD, non-cancer (mg/kg-day)	3.7E–03	2.0E–02
	Chronic ADD, cancer (mg/kg-day)	1.5E–03	1.0E–02
	Subchronic ADD (mg/kg-day)	4.5E–02	0.3
2-day application			
Average adult worker	APDR (mg/day)	118	642
	Dermal DD (mg/kg-day)	1.5	8.0
	ADD, non-cancer (mg/kg-day)	8.1E–03	4.4E–02
	Chronic ADD, cancer (mg/kg-day)	3.2E–03	2.3E–02
	Subchronic ADD (mg/kg-day)	9.9E–02	0.5
Female of reproductive age	APDR (mg/day)	99	534
	Dermal DD (mg/kg-day)	1.4	7.4
	ADD, non-cancer (mg/kg-day)	7.5E–03	4.0E–02
	Chronic ADD, cancer (mg/kg-day)	3.0E–03	2.1E–02
	Subchronic ADD (mg/kg-day)	9.1E–02	0.5
250-day application			
Average adult worker	APDR (mg/day)	118	642
	Dermal DD (mg/kg-day)	1.5	8.0
	ADD, non-cancer (mg/kg-day)	1.0	5.5
	Chronic ADD, cancer (mg/kg-day)	0.4	2.8
	Subchronic ADD (mg/kg-day)	1.1	5.9
	APDR (mg/day)	99	534
	Dermal DD (mg/kg-day)	1.4	7.4

Modeled Scenario	Exposure Concentration Type	Central Tendency	High-End
Female of reproductive age	ADD, non-cancer (mg/kg-day)	0.9	5.0
	Chronic ADD, cancer (mg/kg-day)	0.4	2.6
	Subchronic ADD (mg/kg-day)	1.0	5.4
APDR = Acute potential dose rate; DD = Daily dose; ADD = Average daily dose			

3.3.4.1 Weight of Scientific Evidence for Occupational Exposures

EPA considered the assessment approach, the quality of the data, and uncertainties in assessment results to determine a WoSE conclusion for the 8-hr TWA inhalation exposure estimates. EPA used surrogate monitoring data from the *Emission Scenario Document on Coating Application via Spray-Painting in the Automotive Refinishing Industry* (OECD, 2011a), which the systematic review process rated high for data quality, to estimate inhalation exposures. EPA used SDSs and product data sheets from identified TCEP-containing products to identify product concentrations, densities, and number of application days per site (based on drying times of coatings). The safety and product data sheets have high data quality ratings from the systematic review process. The primary limitation is the lack of TCEP-specific monitoring data, with the ESD serving as a surrogate source of monitoring data representing the level of exposure that could be expected at a typical work site for the given spray application method. EPA assumes spray applications of the coatings, so the estimates may not be representative of exposure during other coating application methods. Additionally, it is uncertain whether the substrates coated, and products used to generate the surrogate data is representative of those associated with TCEP-containing coatings. EPA only assessed mist exposures to TCEP over a full 8-hour work shift to estimate the level of exposure, though other activities may result in vapor exposures other than mist and application duration may be variable depending on the job site. EPA used several hypothetical scenarios of 1-day, 2-day, or 250-day of exposure per year based on estimated days of application for coatings or anticipated working days per year in order to capture potentially variable exposure frequencies for workers at actual coating application sites. Based on these strengths and limitations, EPA has concluded that the WoSE for this assessment is moderate and provides a plausible estimate of exposures.

3.4 Incorporation into Resins

3.4.1 Process Description

TCEP is present as a flame-retardant additive component of 2-part polymer and prepolymer resin systems used in potting and casting applications as well as for production of polyurethane foam (PPG, 2010; Normet, 2015; PPG, 2016; BJB Enterprises, 2017; Rampf, 2017; J6 Polymers, 2018c). This OES represents the formulation of TCEP into these 2-part polymer resin systems, which EPA is using to assess the "Flame retardant in: Polymers (*e.g.* polyester resin)" subcategory COU. As described in Section 2.2, EPA assumed TCEP may still be imported and used for polymer resin formulation at volumes below the CDR reporting threshold and assessed the following two potential scenarios: 1) one site using 25,000 lb of TCEP for polymer resin formulation; and 2) one site using 2,500 lb of TCEP for polymer resin formulation. These scenarios are meant to estimate a generic polymer resin manufacturer site that would not be subject to CDR reporting, and the scenarios do not necessarily represent the total number of polymer resin manufacturing sites using TCEP or total throughput of TCEP.

EPA did not identify data to determine the concentration of TCEP products that may be imported to formulation sites, nor the types of containers used to import TCEP. EPA expects that polymer resin manufacturing sites receive TCEP as a raw material in its pure form, which is a neat liquid at 25 °C (see Table 2-1 in the TCEP Risk Evaluation (U.S. EPA, 2024)). Based on the low production volume, EPA expects that TCEP and TCEP-containing products will be imported in drums or smaller containers rather than larger bulk containers, with material in containers transferred to mixing vessels during formulation (NICNAS, 2001; OECD, 2011a).

Incorporation into polymer resin formulations typically takes place in closed industrial mixing vessels as a batch blending or mixing process, with no reactions or chemical changes occurring to the additive (*i.e.*, TCEP) during the mixing process (NICNAS, 2001; OECD, 2011a). Blending or mixing operations typically occur over the course of 8–24 hours (OECD, 2011a). As part of process operations, operators may collect quality control samples once per batch (OECD, 2011a). The manufacturer will then transfer the blended formulation to product containers for sale or distribution as a resin product to be used at end user sites for potting, casting, or foam product applications (PPG, 2010; OECD, 2011a; Normet, 2015; PPG, 2016; BJB Enterprises, 2017; Rampf, 2017; J6 Polymers, 2018c). Manufacturers will dispose of off-specification product when the resin does not meet quality or desired standards (OECD, 2011a).

EPA assesses an overall concentration range of 1–40 percent of TCEP by mass in formulated polymer resin products based on a review of available safety and technical data sheets from TCEP-containing resin products identified by EPA (Normet, 2015; Rampf, 2017). EPA also expects product container sizes to range from small containers less than one gallon up through various drum sizes (up to 100 gallons) based on a similar review of safety and technical data sheets from TCEP-containing resin products identified by EPA and the applicable ESD (PPG, 2008; OECD, 2011a; J6 Polymers, 2021).

EPA did not identify TCEP-specific operating data for polymer resin manufacturing sites from systematic review (*i.e.*, daily throughputs or operating days per year); therefore, EPA assumes that sites operate 24 hours a day, 7 days a week (*i.e.*, multiple shifts) with operating days as necessary up to 365 days per year for the given site throughput scenario. EPA separately estimated TCEP release and exposure days for this OES in Sections 3.4.3 and 3.4.4, respectively. Figure 3-4 provides an illustration of the polymer resin manufacturing process.

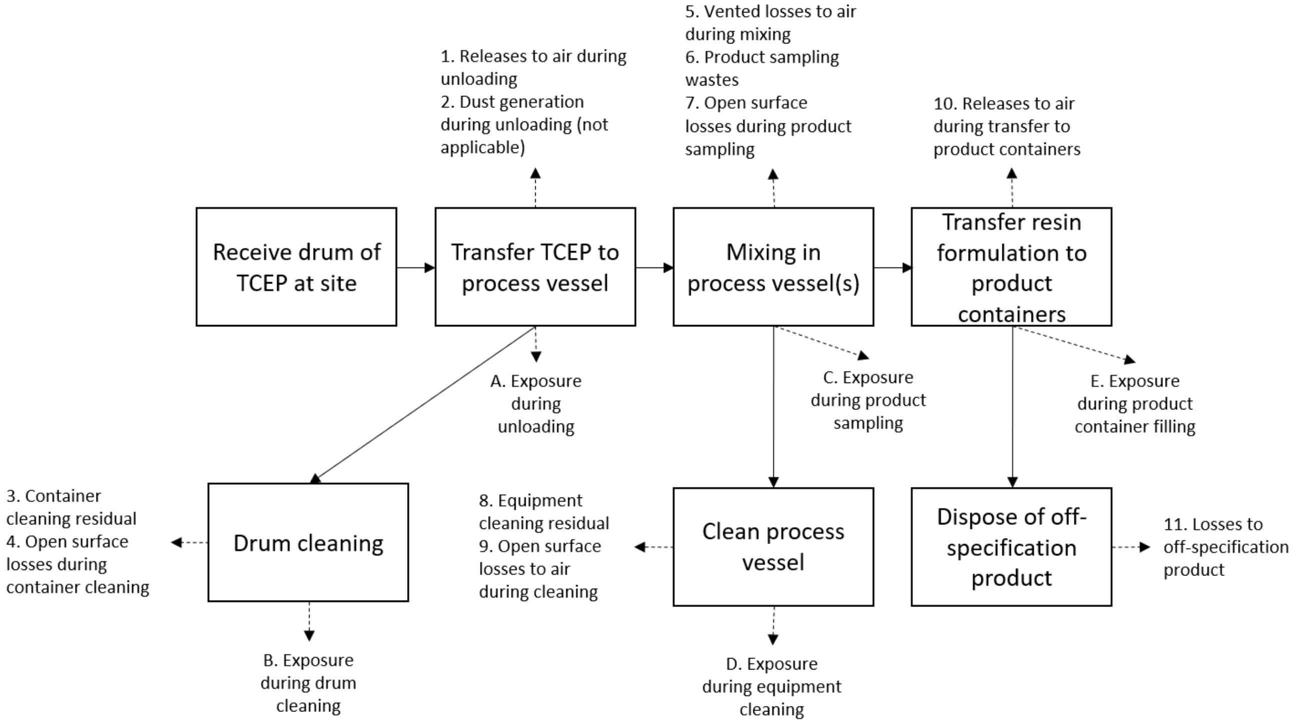

Figure 3-4. Polymer Resin Manufacturing Flow Diagram

3.4.2 Facility Estimates

The 2016 CDR data included a single reporting site, Aceto Corporation in Port Washington, NY, importing TCEP, with no downstream use industrial sectors provided (U.S. EPA, 2019). No 2020 CDR sites reported manufacturing and/or importing TCEP (U.S. EPA, 2020a). J6 Polymers, LLC (hereinafter referred to as “J6 Polymers”) in Genoa, IL, which manufactures and sells resin formulations that contain TCEP, submitted a public comment with end uses for rigid polyurethane foams and general processing information for TCEP-containing formulations (J6 Polymers, 2021). EPA was not able to determine whether J6 Polymers’ TCEP throughput and resin formulation process occurring at an unidentified toll manufacturing facility is representative of other resin formulation facilities (J6 Polymers, 2021). Based on the lack of site-specific data, EPA modeled environmental releases and occupational exposures for a hypothetical scenario in which a single site directly imports and processes TCEP at the CDR reporting thresholds of 2,500 lb per year or 25,000 lb per year.

3.4.3 Release Assessment

3.4.3.1 Environmental Release Points

EPA expects releases during the incorporation of TCEP into resin formulations; however, as discussed in Section 2.3.5, applicable release data or ELGs are not available for TCEP. Due to lack of OES-specific release data, EPA estimated releases using a Monte Carlo simulation with input parameters and equations developed using data from literature, the *Emission Scenario Document for Adhesive Formulations* (OECD, 2009a) (hereinafter referred to as the “ESD for Adhesive Formulations”), and existing EPA models. EPA used the ESD for Adhesive Formulations (OECD, 2009a) to develop the release models due to the similarity of reactive adhesives to the end uses for TCEP-containing resins, including for polyurethanes, and the formulation characteristics of reactive adhesives as “unreacted prepolymers, oligomers, or monomers that react to form a crosslinked polymer at the point of application” (OECD, 2009a). In particular, EPA used the information and data for a “Sealed Process

(Organic Solvent-Based, Reactive Adhesives)" from the ESD for Adhesive Formulations (OECD, 2009a) to inform the release assessment.

EPA used a Monte Carlo simulation to estimate releases for individual release points and summed the individual releases for total annual and daily facility releases. Specific release points are shown numbered as 1 through 11 in Figure 3-4. Based on the models and data used, EPA expects fugitive and stack air TCEP releases, TCEP releases from wastewater managed in onsite treatment or discharged to a POTW, and TCEP releases from waste disposal (*i.e.*, disposal to landfills or incineration) (OECD, 2009a).

3.4.3.2 Environmental Release Assessment Results

Appendix E.5 includes the model equations and input parameters used in the Monte Carlo simulation for this OES. Generally, EPA estimated releases of TCEP by simulating two potential throughput scenarios: 1) one site importing and processing 2,500 lb; and 2) one site importing and processing 25,000 lb. Table 3-13 summarizes the total estimated release by environmental media for incorporation into resin formulations based on the two scenarios applied. The high-end release amounts represent the 95th percentile and the central tendency release amounts represent the 50th percentile of the simulation outputs. For container cleaning residual and equipment cleaning residual release points (Release Points 3 and 8 in Figure 3-4), the ESD for Adhesive Formulations (OECD, 2009a) identified that the releases could potentially be to environmental media of either wastewater or waste disposal depending on facility practices. For the results presented in Table 3-13, EPA grouped releases from container cleaning residuals (Release Point 3) into the total for wastewater only, and EPA grouped releases from equipment cleaning residuals (Release Point 8) into the total for waste disposal only.

Table 3-13. Summary of Modeled Environmental Releases for the Incorporation of TCEP into Resin Formulations

Modeled Scenario	Environmental Media	Annual Release (kg/site-yr)		Number of Release Days[a]		Daily Release (kg/site-day)	
		Central Tendency	High-End	Central Tendency	High-End	Central Tendency	High-End
Scenario 1: One site; 2,500 lb throughput	Fugitive air[b]	4.0E–03	9.4E–03	1	1	3.3E–03	8.8E–03
	Stack air[b]	4.1E–03	2.3E–02	1	1	2.7E–03	2.1E–02
	Wastewater to onsite treatment or discharge to POTW	27	32	1	1	25	32
	Waste disposal	34	34	1	1	34	34
Scenario 2: One site; 25,000 lb throughput	Fugitive air[b]	3.1E–02	6.8E–02	6	4	5.4E–03	1.8E–02
	Stack air[b]	2.8E–02	0.2	8	5	3.7E–03	3.1E–02
	Wastewater to onsite treatment or discharge to POTW	275	320	6	2	46	145
	Waste disposal	340	340	6	2	57	170

[a] The output for number of release days from the simulation was provided as a distribution. The number of release days presented in this table is based on simulation outputs for the annual release divided by the daily release (grouped by high-end or central tendency estimate), rounded to the closest integer. Annual totals may not add exactly due to rounding.
[b] EPA expects releases to air to occur for 8 hours per day. This time of release per day is based on the typical batch time for blending/mixing operations. Air releases also occur during container cleaning, equipment cleaning, product sampling, and

Modeled Scenario	Environmental Media	Annual Release (kg/site-yr)		Number of Release Days[a]		Daily Release (kg/site-day)	
		Central Tendency	High-End	Central Tendency	High-End	Central Tendency	High-End
transfer operations. The hours per batch ranges from 8–24 hours, so the hours of release per day may be as high as 24 hours per day for each release day.							

3.4.3.3 Weight of Scientific Evidence for Environmental Releases

Releases to the environment are assessed using the *Emission Scenario Document on the Formulation of Adhesives* (OECD, 2009a), which has a high data quality rating from the systematic review process. EPA used EPA/OPPT models combined with Monte Carlo modeling to estimate releases to the environment, with media of release assessed using assumptions from the ESD and EPA/OPPT models. A strength of the Monte Carlo stimulation approach is that variation in model input values and a range of potential releases values is more likely than a discrete value to capture actual releases at sites. Additionally, EPA used SDSs and product data sheets from identified TCEP-containing resin products to identify product concentrations and densities used in the simulation. The safety and product data sheets these values were obtained from have high data quality ratings from the systematic review process. EPA believes the primary limitation to be the uncertainty in the representativeness of values toward the true distribution of potential releases. In addition, EPA lacks TCEP facility production volume data and number of processing sites; therefore, throughput estimates are based on CDR reporting thresholds with an overall release using a hypothetical scenario of a single facility. Additional limitations to this assessment are that EPA could not estimate an overall number of release days per year associated with all release points, so the release days per year estimates are based on engineering assumptions and batch formulation times. Based on this information, EPA has concluded that the WoSE for this assessment is moderate and provides a plausible estimate of releases in consideration of the strengths and limitations of reasonably available data.

3.4.4 Occupational Exposure Assessment

3.4.4.1 Worker Activities

During the formulation of TCEP-containing resins, workers are potentially exposed to TCEP when transferring TCEP from transport containers into process vessels, taking QC samples, and packaging formulated resin products into containers (OECD, 2009a). Workers may also be exposed via inhalation of vapor or dermal contact with liquids when cleaning residuals from transport containers or process vessels (OECD, 2009a). EPA did not identify engineering controls and worker PPE used at TCEP-containing resin formulation facilities.

For this OES, ONUs would include supervisors, managers, and other employees that may be in the formulation area but do not perform tasks with direct contact with receiving TCEP, processing into formulation, or handling of the formulated product.

3.4.4.2 Number of Workers and Occupational Non-Users

EPA used data from the BLS and the U.S. Census' SUSB to estimate the number of workers and ONUs per site potentially exposed to TCEP during incorporation into resins (U.S. BLS, 2016). This approach involved identifying relevant Standard Occupational Classification (SOC) codes in BLS data for the COU identified NAICS codes. Section 2.4.2 includes the detailed methodology for estimating the number of workers and ONUs per site. Generally, EPA assigned the NAICS code 325211, Plastics Material and Resin Manufacturing, to this OES based on the process description. Table 3-14 summarizes the workers and ONUs per-facility estimates for this OES. As addressed in Section 3.4.2, EPA did not identify data for the number of facilities in the Unites States incorporating TCEP into resin formulations.

Table 3-14. Estimated Number of Workers Potentially Exposed to TCEP During Incorporation into Resins

NAICS Code	Exposed Workers per Site	Exposed ONUs
325211 – Plastics Material and Resin Manufacturing	27	12

3.4.4.3 Occupational Inhalation Exposure Results

EPA did not identify inhalation monitoring data for processing TCEP as a component in formulations based on systematic review of literature sources. Therefore, EPA estimated inhalation exposures using Monte Carlo simulations based on the OES. EPA estimated inhalation exposures of TCEP by simulating two potential scenarios: 1) one site importing and processing 2,500 lb; and 2) one site importing and processing 25,000 lb. EPA also assumed that pure TCEP is imported to the site and incorporated into the final formulation by a batch mixing process, with no engineering controls present. EPA used product data from TCEP-containing resins to estimate the concentration of TCEP in the final product and the final product density as inputs to the Monte Carlo simulation. Actual exposures may differ based on worker activities, TCEP throughputs, and facility processes.

For this scenario, EPA applied the EPA Mass Balance Inhalation Model to exposure points described in the *Emission Scenario Document for Adhesive Formulation* (OECD, 2009a), particularly for sealed/closed processes. The EPA Mass Balance Inhalation Model estimates the amount of chemical inhaled by a worker during a vapor-generating activity. EPA estimated the inhalation exposure for each exposure point using a vapor generation rate (G) and exposure duration based on the *Emission Scenario Document for Adhesive Formulation* (OECD, 2009a). EPA calculated vapor generation rates for exposures using the same equations applied for estimating air releases associated with the same activity, with possible vapor generation rate models and default values presented in the *Emission Scenario Document for Adhesive Formulation* (OECD, 2009a). The Monte Carlo simulation varies the following parameters: ventilation rate, mixing factor, air speed, saturation factor, container sizes, opening diameters (*e.g.*, mixing tanks, containers), batch size, time per batch, TCEP product concentration, product density, working years, and operating hours. Appendix E.5 provides specifics on how the model parameters were varied and how the model equations, along with other input parameters, were implemented in the Monte Carlo simulation for this OES.

EPA used the vapor generation rate and exposure duration parameters from the *Emission Scenario Document for Adhesive Formulation* (OECD, 2009a) and the EPA Mass Balance Inhalation Model to determine a time-weighted average (TWA) exposure for each exposure point. EPA assumed the same worker performed each activity throughout their work shift and estimated the 8-hr TWA by combining the exposures from each exposure point and averaging over 8-hrs within the Monte Carlo simulation. EPA assumed workers had no exposure outside each exposure activity. Table 3-15 summarizes the estimated 8-hr TWA exposures, AC, ADC, LADC, and $ADC_{subchronic}$ for incorporating TCEP into resin formulations based on the two throughput scenarios. The high-end values represent the 95th percentile and the central tendency values represent the 50th percentile of the simulation outputs. Methods for calculating 8-hour TWA, AC, ADC, LADC, and $ADC_{subchronic}$ are presented in Section 2.4.5.

Table 3-15. Summary of Modeled Worker Inhalation Exposures for the Incorporation of TCEP into Resin Formulations

Modeled Scenario	Exposure Concentration Type	Central Tendency (mg/m^3)	High-End (mg/m^3)	Data Quality Rating of Air Concentration Data
Scenario 1: One site; 2,500 lb throughput	8-hr TWA exposure concentration	7.4E–02	0.4	N/A – Modeled data
	AC based on 8-hr TWA	5.1E–02	0.3	
	ADC based on 8-hr TWA	1.8E–04	8.4E–04	
	LADC based on 8-hr TWA	6.9E–05	3.3E–04	
	ADC$_{subchronic}$ based on 8-hr TWA	2.2E–03	1.0E–02	
Scenario 2: One site; 25,000 lb throughput	8-hr TWA exposure concentration	9.4E–02	0.5	
	AC based on 8-hr TWA	6.4E–02	0.4	
	ADC based on 8-hr TWA	4.8E–03	1.1E–03	
	LADC based on 8-hr TWA	4.2E–04	1.9E–03	
	ADC$_{subchronic}$ based on 8-hr TWA	1.2E–02	5.3E–02	

AC = Acute concentration; ADC = Average daily concentration; LADC = Lifetime average daily concentration; ADC$_{subchronic}$ = Subchronic average daily concentration

3.4.4.1 Occupational Dermal Exposure Results

EPA estimated dermal exposures for this OES using the Dermal Exposure to Volatile Liquid Model and a fraction absorbed value of 23.3 percent described in Section 2.4.4 based on the dermal absorption data from (Abdallah et al., 2016) (see Section 2.4.4 and Appendix D). The maximum concentration evaluated for this dermal exposure is 100 percent since TCEP is expected to be received at site in its pure form. Table 3-16 summarizes the APDR, ARD, CRD and SCRD for TCEP incorporated into resin formulations. The high-ends are based on a higher loading rate of TCEP (2.1 mg/cm^2-event) and two-hand contact, and the central tendencies are based on a lower loading rate of TCEP (1.4 mg/cm^2-event) and one-hand contact. OES-specific parameters for dermal exposures are described in Appendix D.2.

Table 3-16. Summary of Calculated Worker Dermal Exposures for the Incorporation of TCEP into Resin Formulations

Modeled Scenario	Exposure Concentration Type	Central Tendency	High-End
Average adult worker (2,500 lb/yr)	APDR (mg/day)	175	524
	Dermal DD (mg/kg-day)	2.2	6.5
	ADD, non-cancer (mg/kg-day)	6.0E–03	0.1
	Chronic ADD, cancer (mg/kg-day)	2.4E–03	5.5E–02
	Subchronic ADD (mg/kg-day)	7.3E–02	1.3
Average adult worker (25,000 lb/yr)	APDR (mg/day)	175	524
	Dermal DD (mg/kg-day)	2.2	6.5
	ADD, non-cancer (mg/kg-day)	3.6E–02	1.0
	Chronic ADD, cancer (mg/kg-day)	1.4E–02	0.5
	Subchronic ADD (mg/kg-day)	0.4	4.8
Female of reproductive age (2,500 lb/yr)	APDR (mg/day)	145	435
	Dermal DD (mg/kg-day)	2.0	6.0
	ADD, non-cancer (mg/kg-day)	5.5E–03	9.9E–02
	Chronic ADD, cancer (mg/kg-day)	2.2E–03	5.1E–02
	Subchronic ADD (mg/kg-day)	6.7E–02	1.2
Female of reproductive age (25,000 lb/yr)	APDR (mg/day)	145	435
	Dermal DD (mg/kg-day)	2.0	6.0
	ADD, non-cancer (mg/kg-day)	3.3E–02	0.9
	Chronic ADD, cancer (mg/kg-day)	1.3E–02	0.5
	Subchronic ADD (mg/kg-day)	0.4	4.4
APDR = Acute potential dose rate; DD = Daily dose; ADD = Average daily dose			

3.4.4.1 Weight of Scientific Evidence for Occupational Exposures

EPA considered the assessment approach, the quality of the data, and uncertainties in assessment results to determine a WoSE conclusion for the 8-hr TWA inhalation exposure estimates. EPA used the *Emission Scenario Document on the Formulation of Adhesives* (OECD, 2009a) to assess inhalation exposures, which EPA expects to be representative of resin formulation and also has a high data quality rating from the systematic review process. EPA used EPA/OPPT models combined with Monte Carlo stimulation to estimate inhalation exposures. A strength of the Monte Carlo stimulation approach is that variation in model input values and a range of potential exposure values is more likely than a discrete value to capture actual exposure at sites. EPA used SDSs from identified TCEP-containing resin products to identify product concentrations and densities. The SDSs have high data quality ratings from the systematic review process. The primary limitation is the uncertainty in the representativeness of values toward the true distribution of potential inhalation exposures. EPA lacks TCEP facility production volume data; and therefore, throughput estimates are based on CDR reporting thresholds. Also, EPA could not estimate the number of exposure days per year associated with processing operations, so the exposure days per year estimates are based on engineering assumptions and batch formulation times. Based on these strengths and limitations, EPA has concluded that the WoSE for this assessment is moderate to robust and provides a plausible estimate of exposures.

3.5 Incorporation into Articles

3.5.1 Process Description

TCEP is present as a flame-retardant and plasticizer additive in polymer resins used in potting and casting applications as well as for production of polyurethane foam (Normet, 2015; BJB Enterprises, 2017; Rampf, 2017; J6 Polymers, 2021). This OES represents the incorporation of TCEP-containing resins into articles, which EPA is using to assess the "Processing – Incorporation into Article" category COU. EPA identified that these TCEP-containing plastic and foam products are currently used as articles for aircraft and aerospace applications or automobile replacement parts (AIA, 2019; U.S. EPA, 2020c). As described in Section 2.2, EPA assumed TCEP may still be imported and used for polymer resin formulation in aircraft and aerospace applications at volumes below the CDR reporting threshold and assessed the following two potential scenarios: 1) one site using 25,000 lb of TCEP for potting and casting polymer resins; and 2) one site using 2,500 lb of TCEP for potting and casting polymer resins. These scenarios are meant to estimate a generic site where TCEP-containing resin is used to form a plastic or foam article for use in aircraft or aerospace vehicles, and the scenarios do not necessarily represent the total number of resin article manufacturing sites using TCEP-containing resins or total throughput of TCEP for this use.

Resin article manufacturing sites may receive TCEP as an additive in formulated liquid resin with an overall concentration of 1–40 percent by mass (TCEP is only present in one of the components for a 2-component resin system) based on a review of available safety and technical data sheets from TCEP-containing resin products identified by EPA (specific concentrations and products provided in Appendix E.6.12). EPA expects the final concentration of TCEP in the article to be lower than in the component due to mixing the 2-component resin systems, resulting in dilution of TCEP. EPA expects container sizes for the liquid resin to arrive in volumes ranging from one quart up through various drum sizes (up to 100 gallons), based on a review of available safety and technical data sheets from TCEP-containing resin products identified by EPA (specific container sizes provided in Appendix E.6.7).

Operators will apply liquid resins using a syringe or pour method, with resin components initially unloaded from containers and into the syringe or a mixing cup (OECD, 2015). The operator then manually dispenses the resin from the syringe or mixing cup into the mold or the article component (substrate) and allows the resin to cure as a batch operation (OECD, 2015). Curing times varying depending on the product; TCEP-containing products identified by EPA show set times or post-cure times up to 24 hours near room temperature (FCC, 2016a). After the resin cures, TCEP resides within the solid article matrix as a discrete molecule (NICNAS, 2001). The operator may immediately use the component or article or store it for later use or distribution.

EPA did not identify TCEP-specific operating data for resin article manufacturing sites (*i.e.*, daily throughputs or operating days per year); therefore, EPA assumes that one container (one quart up to 100 gallons) of TCEP-containing resin received at the site is used per batch, with one batch occurring per day up to a maximum of 250 operating days per year. Figure 3-5 provides an illustration of the resin article manufacturing process.

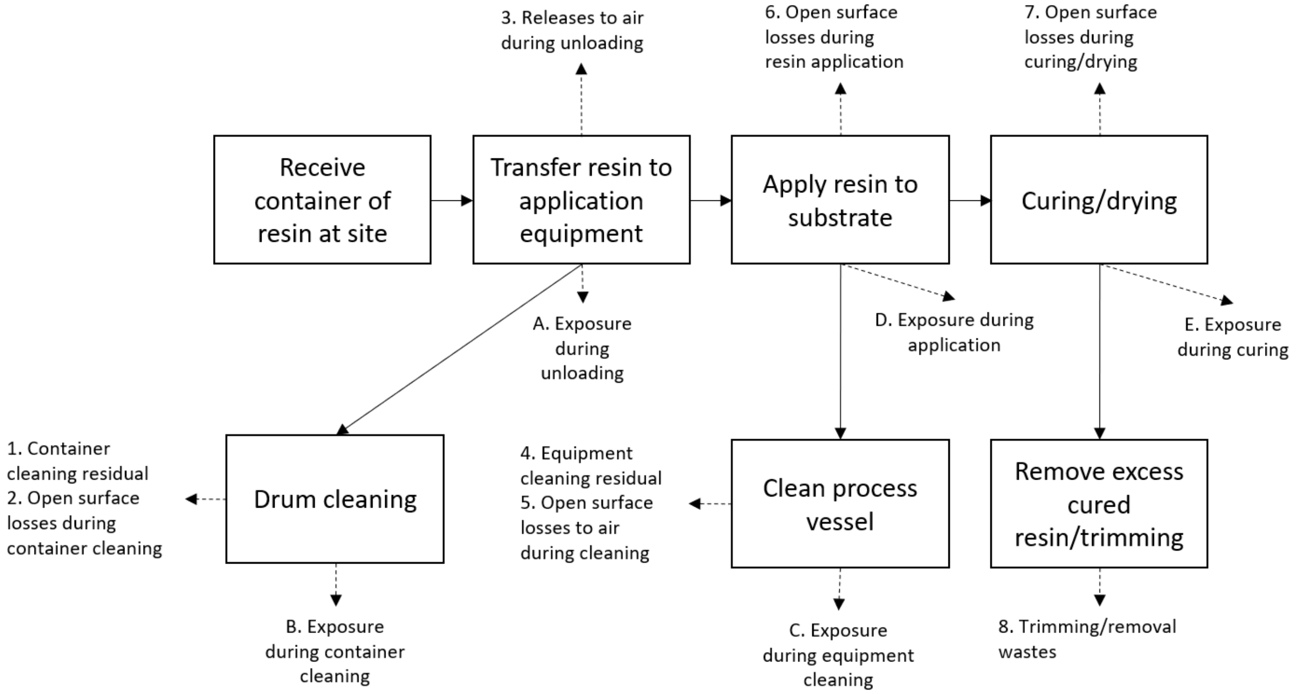

Figure 3-5. Resin Article Manufacturing Flow Diagram

3.5.2 Facility Estimates

The 2016 CDR data included a single reporting site, Aceto Corporation in Port Washington, NY, importing TCEP, with no downstream use industrial sectors identified (U.S. EPA, 2019). No 2020 CDR sites reported manufacturing and/or importing TCEP (U.S. EPA, 2020a). J6 Polymers in Genoa, IL, which manufactures and sells resin formulations that contain TCEP, submitted a public comment denoting end uses for rigid polyurethane foams in the aerospace and defense industries and containing general processing information for TCEP-containing formulations (J6 Polymers, 2021). The public comment submitted by J6 Polymers did not specify the number of receiving facilities or individual facility throughput for TCEP used in the manufacture of resin articles. Based on the lack of site-specific data, EPA modeled environmental releases and occupational exposures for a hypothetical scenario in which a single site receives and processes resin formulation containing TCEP at CDR reporting thresholds of 2,500 lb per year or 25,000 lb per year.

3.5.3 Release Assessment

3.5.3.1 Environmental Release Points

EPA expects releases during the incorporation of TCEP-containing resins into aircraft and aerospace articles; however, as discussed in Section 2.3 applicable release data or ELGs are not available for TCEP. Due to lack of OES-specific release data, EPA estimated releases using a Monte Carlo simulation with input parameters and equations developed using data from literature, the *Emission Scenario Document on the Use of Adhesives* (OECD, 2015), and existing EPA models. EPA used the *Emission Scenario Document on the Use of Adhesives* (OECD, 2015) to develop the release models due to the similarity of reactive adhesives to the end uses for TCEP-containing resins, including for polyurethanes, and the characteristics of reactive adhesives as “unreacted prepolymers, oligomers, or monomers that react to form a crosslinked polymer at the point of application.” In particular, EPA used the information and data for “Syringe or Bead Application” from the *Emission Scenario Document on the Use of*

Adhesives (OECD, 2015) to inform the release assessment based on the assumption of potting and casting applications as opposed to spray or roll coating.

EPA used the Monte Carlo simulation method to estimate releases for individual release points and summed the individual releases to estimate total annual and daily facility releases. Specific release points considered for estimating releases are shown numbered as 1 through 8 in Figure 3-5. Based on the models and data used, EPA expects fugitive or stack air TCEP releases and TCEP releases from waste disposal (*i.e.*, disposals to landfill and incineration) (OECD, 2015).

3.5.3.2 Environmental Release Assessment Results

Appendix E.6 includes the model equations and input parameters used in the Monte Carlo simulation for this OES. EPA estimated releases of TCEP by simulating two potential throughput scenarios: 1) one site processing resins containing TCEP at a total throughput of 2,500 lb of TCEP; and 2) one site processing resins containing TCEP at a total throughput of 25,000 lb of TCEP. Table 3-17 summarizes the total estimated release by environmental media for incorporation into articles based on the two scenarios applied. The high-end release amounts represent the 95th percentile and the central tendency release amounts represent the 50th percentile of the simulation outputs.

Table 3-17. Summary of Modeled Environmental Releases for the Incorporation of TCEP into Articles

Modeled Scenario	Environmental Media	Annual Release (kg/site-yr)		Number of Release Days[a]		Daily Release (kg/site-day)	
		Central Tendency	High-End	Central Tendency	High-End	Central Tendency	High-End
Scenario 1: One site; 2,500 lb throughput	Fugitive or stack air[b]	1.8E–02	0.1	55	113	3.3E–04	9.9E–04
	Waste disposal	37	43	92	17	0.4	2.5
Scenario 2: One site; 25,000 lb throughput	Fugitive or stack air[b]	0.2	1.1	232	250	7.8E–04	4.5E–03
	Waste disposal	365	429	245	167	1.5	2.6

[a] The output for number of release days from the simulation was provided as a distribution. The number of release days presented in this table is based on simulation outputs for the annual release divided by the daily release (grouped by high-end or central tendency estimate), rounded to the closest integer. Annual totals may not add exactly due to rounding.

[b] EPA expects releases to air to occur for 8 hours per day. This time of release per day is based on the typical batch time of 1 batch/day. Air releases also occur during container cleaning, equipment cleaning, curing/drying time and transfer operations.

3.5.3.3 Weight of Scientific Evidence for Environmental Releases

Releases to the environment are assessed using the *Emission Scenario Document on the Use of Adhesives* (OECD, 2015), which EPA expects to be representative of resin application and curing and has a high data quality rating from the systematic review process. EPA used EPA/OPPT models combined with Monte Carlo modeling to estimate releases to the environment, with media of release assessed using assumptions from the ESD and EPA/OPPT models. EPA believes a strength of the Monte Carlo stimulation approach is that variation in model input values and a range of potential releases values is more likely than a discrete value to capture actual releases at sites. Additionally, EPA used safety and product data sheets from identified TCEP-containing resin products to identify product concentrations and densities. Curing time for resins was estimated using product information from one of the identified TCEP-containing resin products. The safety and product data sheets have high data quality ratings from the systematic review process. EPA believes the primary limitation to be the uncertainty in the representativeness of values toward the true distribution of potential releases. There is also uncertainty in the use of the curing time from a single product to represent all potential products. EPA assumed syringe and bead application methods for this OES which may not accurately capture releases using other application methods. In addition, EPA lacks TCEP facility production volume data and number of processing sites; therefore, throughput estimates are based on CDR reporting thresholds with an overall release using a hypothetical scenario of a single facility. Additional limitations to this assessment are that EPA could not estimate the number of release days per year associated with the processing operations, so the release days per year estimates are based on engineering assumptions and the site throughput of 2-part resin containers. Based on this information, EPA has concluded that the WoSE for this assessment is moderate and provides a plausible estimate of releases in consideration of the strengths and limitations of reasonably available data.

3.5.4 Occupational Exposure Assessment

3.5.4.1 Worker Activities

During the incorporation of TCEP-containing resins into aircraft and aerospace articles, workers are potentially exposed to TCEP when transferring resins from transport containers into application equipment, during application of the resin, and during curing of the resin (OECD, 2015). Workers may also be exposed via inhalation of vapor or dermal contact with liquids when cleaning transport containers or application equipment following use (OECD, 2015). EPA does not expect significant worker inhalation exposure to TCEP after the resin has cured because TCEP vapor generation from the resin will be limited by the hardened polymer matrix. EPA did not identify engineering controls and worker PPE used at facilities that incorporate TCEP-containing resins into articles.

ONUs include supervisors, managers, and other employees that may be in the formulation area but do not perform tasks that result in the same level of exposures as workers that engage in tasks related to the handling of the TCEP-containing resin.

3.5.4.2 Number of Workers and Occupational Non-Users

EPA used data from the BLS and the U.S. Census’ SUSB to estimate the number of workers and ONUs per site potentially exposed to TCEP during incorporation of TCEP-containing resins into aerospace and aircraft articles (U.S. BLS, 2016). This approach involved identifying relevant SOC codes within the BLS data for the identified NAICS codes. Section 2.4.2 includes the detailed methodology for estimating the number of workers and ONUs per facility. EPA assigned the NAICS code 326400, Aerospace Product and Parts Manufacturing, for this OES as a relevant industry based on the process description.

Table 3-18 summarizes the worker and ONU per-facility estimates for this OES. As addressed in Section 3.5.2, EPA did not identify data for the number of facilities in the United States incorporating TCEP into resin formulations.

Table 3-18. Estimated Number of Workers Potentially Exposed to TCEP During Incorporation of Resins into Articles

NAICS Code	Exposed Workers per Site	Exposed ONUs per Site
326400 – Aerospace Product and Parts Manufacturing	75	64

3.5.4.3 Occupational Inhalation Exposure Results

EPA did not identify inhalation monitoring data for incorporation of TCEP-containing resins into aircraft and aerospace articles based on systematic review of literature sources. Therefore, EPA estimated inhalation exposures using Monte Carlo simulations based on the OES. EPA estimated inhalation exposures of TCEP by simulating two potential scenarios: 1) one site processing resins containing TCEP at a total throughput of 2,500 lb of TCEP; and 2) one site processing resins containing TCEP at a total throughput of 25,000 lb of TCEP. EPA also assumed that the TCEP-containing resin is incorporated into the article by a syringe or bead application, with no engineering controls present. EPA used product data from TCEP-containing resins to estimate TCEP concentration in resins, resin product density, and demold or set times for resin curing as inputs to the Monte Carlo simulation. EPA assumed a constant TCEP vapor generation rate during resin curing, with exposure ending once the resin cures as determined by demold or set time. Actual exposures may differ based on worker activities, TCEP throughputs, resin cure properties, and facility processes.

For this scenario, EPA applied the EPA Mass Balance Inhalation Model to exposure points described in the *Emission Scenario Document on the Use of Adhesives* (OECD, 2015), particularly for syringe and bead applications described in the ESD. The EPA Mass Balance Inhalation Model estimates the amount of chemical inhaled by a worker during a vapor-generating activity. EPA estimated the inhalation exposure for each exposure point using a vapor generation rate (G) and exposure duration based on the *Emission Scenario Document on the Use of Adhesives* (OECD, 2015) or product-specific data. EPA calculated vapor generation rates for exposures using the same equations applied for estimating air releases associated with the same activity, with possible vapor generation rate models and default values presented in the *Emission Scenario Document on the Use of Adhesives* (OECD, 2015). Inhalation exposures during application of the resin were assessed together with exposures during curing of the resin since the *Emission Scenario Document on the Use of Adhesives* (OECD, 2015) did not present an applicable methodology for assessing inhalation exposures to vapors during syringe or bead application. The *Emission Scenario Document on the Use of Adhesives* (OECD, 2015) suggests that inhalation exposures to vapors during non-spray applications and subsequent curing is a data gap in cases where monitoring data is not available. To assess exposures during syringe or bead application and curing of the resin, EPA used existing vapor generation rate models and product-specific data. The Monte Carlo simulation varies the following parameters: ventilation rate, mixing factor, air speed, saturation factor, container sizes, time for resin curing, concentration of TCEP in the resin, resin density, and working years. Appendix E.6 provides specifics on how the model parameters were varied and how the model equations, along with other input parameters, were implemented in the Monte Carlo simulation for this OES.

EPA used the vapor generation rate and exposure duration parameters from the *Emission Scenario Document on the Use of Adhesives* (OECD, 2015) and EPA Mass Balance Inhalation Model to determine a TWA exposure for each exposure point. EPA assumed the same worker performed each activity throughout their work shift and estimated the 8-hr TWA by combining the exposures from each exposure point and averaging over 8-hrs within the Monte Carlo simulation. EPA assumed workers had no exposure outside each exposure activity. Exposure durations for equipment cleaning and resin curing were adjusted to fit a total exposure duration of a full 8-hour work-shift in cases where the total summed exposure duration exceeded eight hours. Table 3-19 summarizes the estimated 8-hour TWA exposures, AC, ADC, LADC, and $\text{ADC}_{\text{subchronic}}$ for incorporating TCEP-containing resins into articles based on the two throughput scenarios. The high-end values represent the 95th percentile and the central tendency values represent the 50th percentile of the simulation outputs. Methods for calculating 8-hour TWA, AC, ADC, LADC, and $\text{ADC}_{\text{subchronic}}$ are presented in Section 2.4.5.

Table 3-19. Summary of Modeled Worker Inhalation Exposures for the Incorporation of TCEP into Articles

Modeled Scenario	Exposure Concentration Type	Central Tendency (mg/m^3)	High-End (mg/m^3)	Data Quality Rating of Air Concentration Data
Scenario 1: One site; 2,500 lb throughput	8-hr TWA exposure concentration	3.4E–03	1.8E–02	N/A – Modeled data
	AC based on 8-hr TWA	2.3E–03	1.2E–02	
	ADC based on 8-hr TWA	3.9E–04	2.3E–03	
	LADC based on 8-hr TWA	1.5E–04	9.2E–04	
	$\text{ADC}_{\text{subchronic}}$ based on 8-hr TWA	1.6E–03	8.1E–03	
Scenario 2: One site; 25,000 lb throughput	8-hr TWA exposure concentration	4.0E–03	1.9E–02	
	AC based on 8-hr TWA	2.7E–03	1.3E–02	
	ADC based on 8-hr TWA	1.7E–03	7.8E–03	
	LADC based on 8-hr TWA	6.5E–04	3.1E–03	
	$\text{ADC}_{\text{subchronic}}$ based on 8-hr TWA	2.0E–03	9.4E–03	

AC = Acute concentration; ADC = Average daily concentration; LADC = Lifetime average daily concentration; $\text{ADC}_{\text{subchronic}}$ = Subchronic average daily concentration

3.5.4.4 Occupational Dermal Exposure Results

EPA estimated dermal exposures for this OES using the Dermal Exposure to Volatile Liquid Model and a fraction absorbed value of 23.3 percent described in Section 2.4.4 based on the dermal absorption data from (Abdallah et al., 2016) (see Section 2.4.4 and Appendix D). The maximum concentration evaluated for this dermal exposure is 40 percent since that is the highest weight fraction of a TCEP-containing resin incorporated into an article for this COU (Rampf, 2017). Table 3-20 summarizes the APDR, ARD, CRD and SCRD for TCEP during incorporation of TCEP-containing resins into articles. The high-ends are based on a higher loading rate of TCEP (2.1 mg/cm^2-event) and two-hand contact, and the central tendencies are based on a lower loading rate of TCEP (1.4 mg/cm^2-event) and one-hand contact. OES-specific parameters for dermal exposures are described in Appendix D.2.

Table 3-20. Summary of Calculated Worker Dermal Exposures for the Incorporation of TCEP into Articles

Modeled Scenario	Exposure Concentration Type	Central Tendency	High-End
Average adult worker (2,500 lb/yr)	APDR (mg/day)	70	209
	Dermal DD (mg/kg-day)	0.9	2.6
	ADD, non-cancer (mg/kg-day)	0.2	1.8
	Chronic ADD, cancer (mg/kg-day)	6.8E–02	0.9
	Subchronic ADD (mg/kg-day)	0.6	1.9
Average adult worker (25,000 lb/yr)	APDR (mg/day)	70	209
	Dermal DD (mg/kg-day)	0.9	2.6
	ADD, non-cancer (mg/kg-day)	0.6	1.8
	Chronic ADD, cancer (mg/kg-day)	0.2	0.9
	Subchronic ADD (mg/kg-day)	0.6	1.9
Female of reproductive age (2,500 lb/yr)	APDR (mg/day)	58	174
	Dermal DD (mg/kg-day)	0.8	2.4
	ADD, non-cancer (mg/kg-day)	0.2	1.6
	Chronic ADD, cancer (mg/kg-day)	6.3E–02	0.8
	Subchronic ADD (mg/kg-day)	0.6	1.8
Female of reproductive age (25,000 lb/yr)	APDR (mg/day)	58	174
	Dermal DD (mg/kg-day)	0.8	2.4
	ADD, non-cancer (mg/kg-day)	0.5	1.6
	Chronic ADD, cancer (mg/kg-day)	0.2	0.8
	Subchronic ADD (mg/kg-day)	0.6	1.8
APDR = Acute potential dose rate; DD = Daily dose; ADD = Average daily dose			

3.5.4.5 Weight of Scientific Evidence for Occupational

EPA considered the assessment approach, the quality of the data, and uncertainties in assessment results to determine a WoSE conclusion for the 8-hr TWA inhalation exposure estimates. EPA used the *Emission Scenario Document on the Use of Adhesives* (OECD, 2015) to assess inhalation exposures, which EPA expects to be representative of resin application and curing and also has a high data quality rating from the systematic review process. EPA used safety and product data sheets from identified TCEP-containing resin products to identify product concentrations, densities, and curing times. EPA used EPA/OPPT models combined with Monte Carlo modeling to estimate inhalation exposures. A strength of the Monte Carlo stimulation approach is that variation in model input values and a range of potential exposure values is more likely than a discrete value to capture actual exposure at sites. EPA used SDSs from identified TCEP-containing resin products to identify product concentrations and densities, and curing time was estimated using product information from one of the identified TCEP-containing resin products. The safety and product data sheets have high data quality ratings from the systematic review process. The primary limitation is the uncertainty in the representativeness of values toward the true distribution of potential inhalation exposures. The curing time exposure duration and worker activities associated with product application and curing are also uncertain; EPA assumes syringe and bead application methods for this OES. Additionally, EPA lacks TCEP facility production volume data; and therefore, throughput estimates are based on CDR reporting thresholds. Also, EPA could not estimate the number of exposure days per year associated with resin application and curing operations, so the exposure days per year estimates are based on an assumed site throughput of 2-part resin containers. Based on these strengths and limitations, EPA has concluded that the WoSE for this assessment is moderate and provides a plausible estimate of exposures.

3.6 Use and Installation of Articles

3.6.1 Process Description

TCEP is present in the cured resin or foam components of articles that are installed in aircrafts or aerospace vehicles (AIA, 2019; U.S. EPA, 2020b). This OES represents the installation of TCEP-containing articles into aircrafts or aerospace vehicles and the automotive sector for industrial uses, which EPA is using to assess the “Aircraft interiors and aerospace products” subcategory COU within the “Industrial Use” life cycle stage. Examples of possible TCEP uses in aircraft and aerospace products includes its presence as a flame retardant in articles (AIA, 2019; U.S. EPA, 2020b). The 2020 CDR had no reporters for TCEP, though J6 Polymers, LLC, which incorporates TCEP into resin products for creating rigid polyurethane foams for aerospace and defense industries, stated that its customers use ten pounds of TCEP per year on average (U.S. EPA, 2020a; J6 Polymers, 2021). EPA did not identify information on the number of customers. The total number of sites within the aircraft and aerospace assembly industry can be determined from the applicable NAICS code 3364, Aerospace Product and Parts Manufacturing; however, the proportion of these sites using TCEP-containing articles is unknown.

EPA expects that the TCEP-containing articles are used as received at the site, with minimal or no reshaping or processing of the article prior to manual installation into the aircraft or aerospace vehicle. The concentration of TCEP in the article is dependent upon upstream manufacturing processes such as component mixing ratios during incorporation of resins into the article, with typical concentrations of flame retardants in plastic articles, including foams, reported to be 5–20 percent in a NICNAS risk assessment report and 0–15 percent in a Commission for Environmental Cooperation (CEC) report (NICNAS, 2001; CEC, 2015). Concentrations reported in samples of several consumer products from the United States showed concentrations of TCEP typically under one percent, though EPA expects products for industrial applications would have higher loadings of TCEP (TERA, 2013). The concentration of TCEP in the final articles is expected to be lower than in the initial liquid resin formulation due to the mixing of resin parts and/or addition of other compounds in the final article.

EPA did not identify TCEP-specific data for end-use sites (*i.e.*, daily throughputs or operating days per year). Therefore, EPA assumes end-use sites operate 5 days per week and 250 days per year. EPA did not estimate TCEP throughputs at end-use sites because this parameter was not needed for the occupational exposure estimates included in this risk evaluation. Releases are not expected as discussed in Section 3.6.3. Figure 3-6 provides an illustration of the installation of articles process.

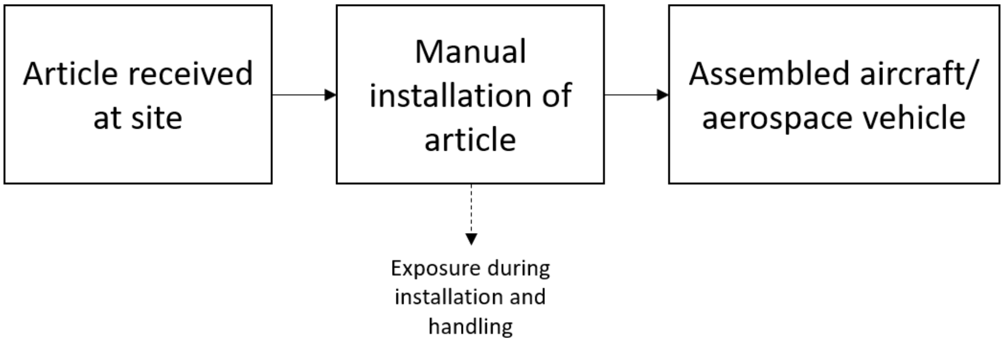

Figure 3-6. Installation of Articles Flow Diagram

3.6.2 Facility Estimates

The 2016 CDR data included a single reporting site, Aceto Corporation in Port Washington, NY, importing TCEP, with no downstream use industrial sectors or commercial uses identified (U.S. EPA, 2019). No 2020 CDR sites reported manufacturing and/or importing TCEP (U.S. EPA, 2020a). EPA assumes that facilities installing articles containing TCEP are classified under the applicable NAICS code 3364, Aerospace Product and Parts Manufacturing. Based on the 2020 County Business Patterns data published by the U.S. Census Bureau, there are 1,844 establishments classified under the NAICS code 3364, which provides a high-end estimate for the number of facilities that may install articles containing TCEP.

3.6.3 Release Assessment

EPA does not expect significant releases to occur during the installation of TCEP-containing aircraft and aerospace articles into or onto the relevant transportation equipment. As discussed in Section 2.3, applicable release data or ELGs are not available for TCEP. After TCEP-containing resins have cured, EPA expects TCEP release will be limited by the hardened polymer matrix. EPA anticipates that release may occur via the mechanism of “blooming”, or volatilization from the cured resin surface, during the service life of the aircraft or aerospace article, but EPA expects that releases via this mechanism during installation activities will be negligible (NICNAS, 2001; OECD, 2009b). EPA does not account for TCEP releases from blooming within an OES since releases are expected to be disperse and dependent upon end use and service life of the product.

3.6.4 Occupational Exposure Assessment

3.6.4.1 Worker Activities

During the installation of aircraft and aerospace articles, workers are potentially exposed to TCEP when manually handling articles manufactured with TCEP-containing resins. EPA expects that inhalation exposures may occur from TCEP that volatilizes from the surface of the article or particulate generated from the article during handling. EPA did not find information that indicates the extent that engineering controls and worker PPE are used at facilities that install aircraft and aerospace articles in the United States.

ONUs include supervisors, managers, and other employees that may be in the manufacturing area but do not perform tasks that result in the same level of exposures as workers that engage in tasks related to the handling of the TCEP-containing articles.

3.6.4.2 Number of Workers and Occupational Non-Users

EPA used data from the BLS and the U.S. Census' SUSB to estimate the number of workers and ONUs per site potentially exposed to TCEP during installation of aerospace and aircraft articles (U.S. BLS, 2016). This approach involved the identification of relevant SOC codes within the BLS data for the identified NAICS codes. Section 2.4.2 includes further details regarding methodology for estimating the number of workers and ONUs per site. EPA assigned the NAICS code 326400, Aerospace Product and Parts Manufacturing, for this OES based on the applicable end users for the TCEP-containing articles as described in the process description.

Table 3-21 summarizes the per-facility estimates for this OES based on the methodology described. As addressed in Section 3.6.2, EPA did not identify data for the number of facilities in the United States installing aerospace and aircraft articles containing TCEP, though a high-end estimate may be 1,844 establishments.

Table 3-21. Estimated Number of Workers Potentially Exposed to TCEP During Installation of Aerospace and Aircraft Articles

NAICS Code	Exposed Workers per Site	Exposed ONUs per Site
326400 – Aerospace Product and Parts Manufacturing	75	64

3.6.4.3 Occupational Inhalation Exposure Results

EPA did not identify inhalation monitoring data for installation of aircraft and aerospace articles based on the systematic review of literature sources. However, EPA estimated inhalation exposures for this OES using monitoring data for TCEP exposures during furniture manufacturing. EPA expects that inhalation exposures during furniture manufacturing occur from handling or contacting TCEP-containing foams or cured resin products, which is comparable to inhalation exposures expected during installation of TCEP-containing foam or resin products for aircraft or aerospace applications.

EPA used surrogate monitoring data provided in an exposure study conducted by Mäkinen et al. (2009) in furniture workshops to estimate inhalation exposures for this OES. The study used monitoring data collected via personal and stationary samples with either Institute of Occupational Medicine (IOM) or OSHA Versatile Sampler (OVS) sampler types. To compile available data, EPA considered the personal sampling data more relevant to estimating worker exposures. Additionally, the study did not provide sufficient metadata to compile the IOM and OVS sampler results, so EPA used data from the OVS sampler, which accounted for a combination of TCEP vapor and particulate phases. The Mäkinen et al. (2009) study included one personal sampling data point collected with an OVS sampler in the furniture workshop, which was collected during upholstering activities.

The study did not provide sampling time for individual data points, so EPA conservatively assumed a full 8-hour work-shift exposure duration at the concentration measured by the single data point. EPA used this data point to estimate worker inhalation exposure to TCEP as an 8-hour TWA, AC, ADC, LADC, and $\mathrm{ADC}_{\mathrm{subchronic}}$ during installation of aircraft and aerospace articles. EPA calculated point estimates of the 8-hour TWA, AC, ADC, and $\mathrm{ADC}_{\mathrm{subchronic}}$ based on the single data point from the Mäkinen et al. (2009) study. EPA determined a high-end and a central tendency LADC based on a high-end and central tendency number of working years applied to the single data point from the Mäkinen et al. (2009) study. Table 3-22 summarizes the estimated values for each of these parameters. Equations for calculating 8-hour TWA, AC, ADC, LADC, and ADC$_{subchronic}$ are presented in Section 2.4.5.

Table 3-22. Summary of Estimated Worker Inhalation Exposures for the Installation of Articles based on Surrogate Monitoring Data

Exposure Concentration Type	Estimated Value (mg/m^3)	Data Quality Rating of Air Concentration Data
8-hr TWA exposure concentration	1.3E–05	High
AC based on 8-hr TWA	8.8E–06	
ADC based on 8-hr TWA	6.1E–06	
LADC based on 8-hr TWA – Central tendency[a]	2.4E–06	
LADC based on 8-hr TWA – High-end[a]	3.1E–06	
ADC$_{subchronic}$ based on 8-hr TWA	6.5E–06	

AC = Acute concentration; ADC = Average daily concentration; LADC = Lifetime average daily concentration; ADC$_{subchronic}$ = Subchronic average daily concentration

[a] EPA used the same 8-hour TWA to calculate the central tendency and high-end LADC. The difference between the central tendency and high-end calculation is the use of a larger number of working years for the high-end LADC.

3.6.4.4 Occupational Dermal Exposure Results

EPA expects that the TCEP-containing articles are used as received at the site, with minimal or no reshaping or processing of the article prior to manual installation into an aircraft or aerospace vehicle. No significant generation of dust or powders is expected therefore, EPA does not expect any dermal exposure for this COU.

3.6.4.5 Weight of Scientific Evidence for Occupational Exposures

EPA considered the assessment approach, the quality of the data, and uncertainties in assessment results to determine a WoSE conclusion for the 8-hour TWA inhalation exposure estimates. EPA used inhalation air concentration data to assess inhalation exposures, which has a high data quality rating from the systematic review process. The primary limitations of these data include the uncertainty of the representativeness of these data toward the true distribution of inhalation concentrations in this scenario since the data was from a surrogate occupational activity of upholstering furniture. In addition, EPA used only a single data point without exposure duration to estimate the inhalation exposure, with the 8-hour exposure duration assumed for TWA calculation. EPA also assumed 250 exposure days per year based on TCEP exposure each working day for a typical worker schedule; it is uncertain whether this captures actual worker schedules and exposures. Based on these strengths and limitations, EPA has concluded that the WoSE for this assessment is slight, yet still provides a plausible estimate of exposures.

3.7 Recycling

3.7.1 Process Description

EPA expects that TCEP may be present as an additive in components of electronics and electrical equipment that is recycled. Multiple studies show detections of TCEP at electronics and electrical equipment waste (e-waste) recycling facilities at concentrations ranging from 1.0×10^{-7} to 1.1×10^{-3} mg/m^3, though the source of the TCEP at each facility is not specified (Sjödin et al., 2001; Yang et al., 2013; NIOSH, 2018; Grimes et al., 2019; Stubbings et al., 2019; NCBI, 2020). EPA did not identify information regarding volume of TCEP-containing articles that are recycled or the total volume of TCEP contained in the recycled articles. According to the NAICS code 562920 – "Materials Recovery Facilities" there are 1,455 recycling facilities in the United States (U.S. BLS, 2016) however only a subset of electronic waste facilities is expected to handle TCEP-containing products. The exact number of TCEP-handling facilities is unknown.

E-waste recycling activities include receiving e-waste at the facility, dismantling or shredding the e-waste, and sorting the recycled articles and generated scrap materials (Sjödin et al., 2001; Yang et al., 2013; NIOSH, 2018). EPA expects that TCEP-containing material from the recycling process is typically treated or disposed following the initial processing and not reprocessed or reused (Yang et al., 2013). EPA did not identify any data for the weight fraction of TCEP in e-waste.

EPA did not identify TCEP-specific operating data for e-waste recycling facilities (*i.e.*, operating days per year); therefore, EPA assumes that operations occur eight hours per day and up to a maximum of 250 operating days per year. Figure 3-7 provides an illustration of the electronic waste recycling process.

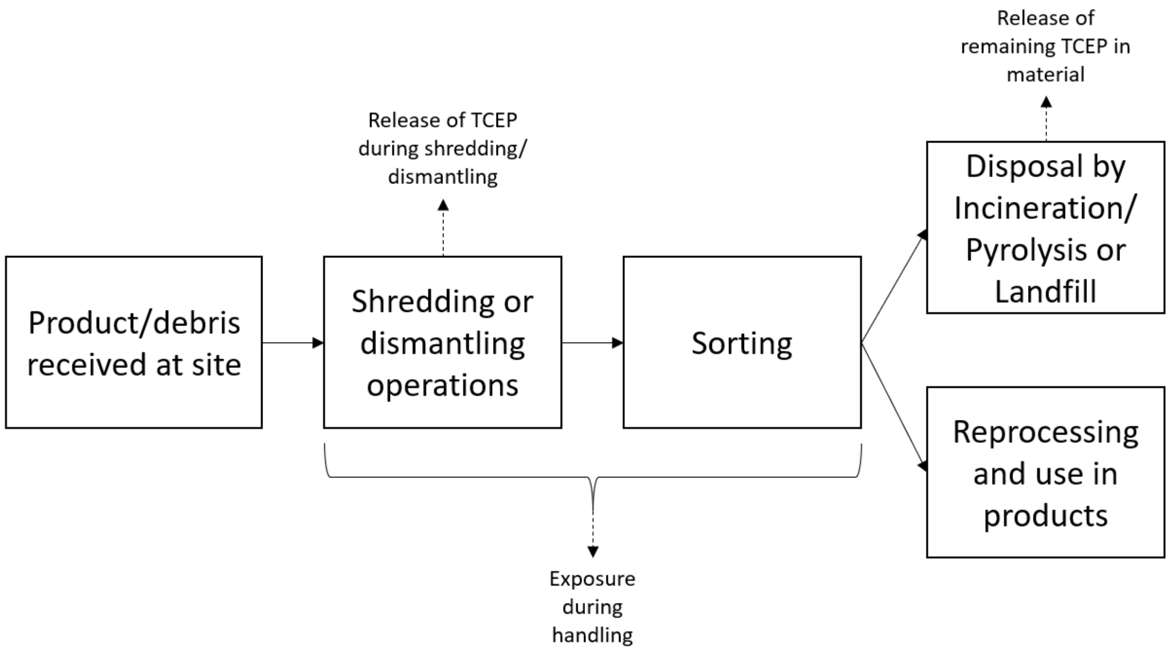

Figure 3-7. Electronic Waste Recycling Flow Diagram

3.7.2 Facility Estimates

The 2016 CDR data included a single reporting site, Aceto Corporation in Port Washington, NY, importing TCEP, with no downstream use industrial sectors identified (U.S. EPA, 2019). No 2020 CDR sites reported manufacturing and/or importing TCEP (U.S. EPA, 2020a). EPA did not identify information regarding the volume of TCEP-containing articles that are recycled or the total volume of TCEP contained in the recycled articles. However, EPA identified electronics recycling sources that indicate TCEP is detected in the e- waste and recycling industry (Sjödin et al., 2001; Yang et al., 2013; NIOSH, 2018; Grimes et al., 2019; Stubbings et al., 2019; NCBI, 2020). According to the NAICS code 562920 – "Materials Recovery Facilities" there are 1,455 recycling facilities in the United States (U.S.

BLS, 2016) however only a subset of electronic waste facilities is expected to handle TCEP-containing products. The exact number of TCEP-handling facilities is unknown.

3.7.3 Release Assessment

3.7.3.1 Environmental Release Points

EPA did not assess environmental releases for the recycling COU. EPA did not find data to quantify releases of TCEP from e-waste facilities. The total releases are expected to be low as the overall volume of TCEP in e-waste products is low, only a fraction of the products is recycled, and recycling will likely be dispersed over many e-waste sites. TCEP was found to be present at multiple electronic recycling facilities based on systematic review. These sources did not provide data on the volume of TCEP-contained electronics processed at any of the facilities identified.

3.7.4 Occupational Exposure Assessment

3.7.4.1 Worker Activities

During the recycling process, workers are potentially exposed to TCEP when manually handling TCEP-containing electronic articles. These articles are received at the recycling site where they are shredded, dismantled, and sorted based on site-specific requirements. EPA expects that inhalation exposure may occur from TCEP that volatilizes from the surfaces of the electronic articles or particulate generated from the shredding and dismantling process. EPA did not find information on the engineering controls and worker PPE used while handling TCEP at electronics recycling facilities in the United States.

ONUs include supervisors, managers, and other employees that may be in the recycling area but do not perform tasks that result in the same level of exposures as workers that engage in tasks related to the handling of TCEP-containing electronic articles.

3.7.4.2 Number of Workers and Occupational Non-Users

EPA used data from the BLS and the U.S. Census' SUSB to estimate the number of workers and ONUs per site potentially exposed to TCEP during electronic recycling (U.S. BLS, 2016). This approach involved the identification of relevant SOC codes within the BLS data for the identified NAICS code. Section 2.4.2 includes further details regarding the methodology for estimating the number of workers and ONUs per site. EPA assigned the NAICS code 562920 – Materials Recovery Facilities, for this OES. Table 3-23 summarizes the per site estimates for this OES based on the methodology described. As addressed in Section 3.7.2, EPA did not identify data for the number of facilities in the United States recycling TCEP-containing electronics.

Table 3-23. Estimated Number of Workers Potentially Exposed to TCEP During Recycling of Electronics

NAICS Code	Exposed Workers per Site	Exposed ONUs per Site
562920 – Materials Recovery Facilities	2	2

3.7.4.3 Occupational Inhalation Exposure Results

EPA identified inhalation monitoring data for electronic waste recycling based on systematic review of literature sources. EPA used monitoring data provided in an exposure study conducted by Mäkinen et al. (2009) in a circuit board factory and two electronics dismantling facilities to estimate inhalation exposures for this OES. Additionally, EPA used monitoring data provided in two health hazard evaluation reports that measured TCEP in an electronic recycling facility in 2015 and 2016 (NIOSH, 2018; Grimes et al., 2019).

Mäkinen et al. (2009) collected data via PBZ and stationary samples with either IOM or OVS sampler types. EPA used the PBZ sampling data for estimating worker exposures and stationary samples for estimating ONU exposures. EPA used the OVS sampler data as it accounted for total TCEP exposure from both vapor and particulate phases whereas the IOM samples only account TCEP exposure from both vapor and particulate phases whereas the IOM samples only account for the particulate phase. The Mäkinen et al. (2009) study included six personal sampling data points and five stationary data points, which were all collected during activities in electronics or electronic dismantling facilities.

The 2015 and 2016 HHE reports each collected PBZ samples using an IOM sampler type. Specifically, the HHE reports took PBZ samples in shipping and receiving, resale, office, shredding and sorting, and disassembly locations at the electronics recycling facility. The HHE Reports describe shipping and receiving as job activities as processing paperwork associated with incoming electronic and unloading truck. These workers would periodically work in the shredding and sorting work area. Office and resale employees would occasionally enter recycling warehouse but would not perform any activities associated with direct exposure to TCEP. Shredding and sorting employees directly handled electronic components and placed them into the shredder to be sorted once dispelled by the shredder. Disassembly workers would manually disassemble and separated computer components such as circuit boards, hard drives, copper wiring, and other parts. Based on these descriptions, EPA assessed employees in the shredding and sorting, and disassembly areas as workers and the shipping and receiving, office, and resale employees as ONUs. The HHE Reports included 65 PBZ data points, 16 of which EPA assessed as ONU data points and the remaining 49 as worker data points (NIOSH, 2018; Grimes et al., 2019). The two HHE reports only provided summary statistics (minimum, maximum, median) rather than discrete samples. Therefore, EPA could not create a full distribution of monitoring results across the sources to use in estimating central tendency and high-end exposures. However, across the three sources, 43 of the 49 worker data points were reported as below the LOD and 15 of the 16 ONU data points were reported as below the LOD. Because over 50 percent of the data for both workers and ONUs from all three sources were reported as below the LOD, EPA determined that the 50th percentile value would also be below the LOD. Therefore, EPA estimated the central tendency at the LOD of 1.0×10^{-7}. To estimate high-end exposure for workers, EPA used the 95th percentile of the discrete PBZ data available from the Mäkinen et al. (2009) study. To estimate high-end exposure for ONU, EPA used the 95th percentile of the discrete stationary data available from the Mäkinen et al. (2009) study. While neither value is not the true 95th percentile of the overall distribution, EPA expects it to fall within its definition of high-end exposures of greater than the 90th percentile of the data but less than the maximum as the Mäkinen et al. (2009) study data were generally three orders of magnitude higher than the results from the HHE reports. Table 3-24 presents the inhalation exposure results based on the available monitoring data.

Table 3-24. Summary of Estimated Worker Inhalation Exposures for the Electronic Recycling Monitoring Data

Worker Type	Exposure Concentration Type	Estimated Value (mg/m^3)		Data Quality Rating of Air Concentration Data
		Central Tendency	High-End	
Average adult worker	8-hr TWA exposure concentration	1.0E–07	9.7E–04	High
	AC based on 8-hr TWA	6.8E–08	6.6E–04	
	ADC based on 8-hr TWA	4.7E–08	4.5E–04	
	LADC based on 8-hr TWA	1.9E–08	2.3E–04	
	$ADC_{subchronic}$ based on 8-hr TWA	5.0E–08	4.8E–04	
ONU	8-hr TWA exposure concentration	1.0E–07	1.9E–04	
	AC based on 8-hr TWA	6.8E–08	1.3E–04	
	ADC based on 8-hr TWA	4.7E–08	8.9E–05	
	LADC based on 8-hr TWA	1.9E–08	4.5E–05	
	$ADC_{subchronic}$ based on 8-hr TWA	5.0E–08	9.5E–05	

3.7.4.4 Occupational Dermal Exposure Results

EPA estimated high-end worker dermal potential dose rate in accordance with the EPA/OPPT Direct 2-Hand Dermal Contact with Container Surfaces (Solids) Model (U.S. EPA, 2015) and the fraction absorbed value of 23.3 percent from dermal absorption data in (Abdallah et al., 2016) (see Section 2.4.4 and Appendix D). The high-end potential dose rate from this model is equal to 1,110 mg/day which is the quantity of solids retained on a worker's skin during an event that results in the worker's contact with the solids; the frequency of such events is assumed to be once per day (U.S. EPA, 2013). The EPA/OPPT Direct 2-Hand Dermal Contact with Container Surfaces (Solids) Model (U.S. EPA, 2015) does not include a central tendency value of the potential dose rate although this model is based on data reported in Lansink et al. (1996) and both the high-end and central tendency values of these data are given in Lansink et al. (1996). The central tendency potential dose rate that is associated with the high-end potential dose rate of 1,110 mg/day is equal to 450 mg/day. The central tendency value of 450 mg is reported in Lansink et al. (1996) as cited in Marquart et al. (2006). This central tendency value pertains to the gathering of closed bags of powder and is designated as the typical case exposure (Marquart et al., 2006).[2]

The maximum concentration evaluated for this dermal exposure is 1.4×10^{-5} percent based on the highest TCEP weight fraction detected on patch samples of various surfaces within a circuit board factory (Marquart et al., 2006). Table 3-25 summarizes the APDR, ARD, CRD and SCRD for TCEP during electronic recycling. OES-specific parameters for dermal exposures are described in Appendix D.2.

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[2] The high-end value of 1,110 mg also pertains to the gathering of closed bags of powder. This value corresponds to the value of 1,050 mg reported in Marquart et al. (2006) as the reasonable worst case exposure pertaining to the gathering of closed bags of powder and obtained from Lansink et al. (1996). EPA did not directly cite Lansink et al. (1996) because, as stated in Marquart et al. (2006), this report has not been published in a scientific journal.

Table 3-25. Summary of Calculated Worker Dermal Exposures for Electronic Recycling

Modeled Scenario	Exposure Concentration Type	Central Tendency	High-End
Average adult worker (2,500 lb/yr)	APDR (mg/day)	1.5E–03	3.5E–03
	Dermal DD (mg/kg-day)	1.8E–05	4.4E–05
	ADD, non-cancer (mg/kg-day)	1.3E–05	3.0E–05
	Chronic ADD, cancer (mg/kg-day)	5.0E–06	1.5E–05
	Subchronic ADD (mg/kg-day)	1.3E–05	3.2E–05
Average adult worker (25,000 lb/yr)	APDR (mg/day)	1.5E–03	3.5E–03
	Dermal DD (mg/kg-day)	1.8E–05	4.4E–05
	ADD, non-cancer (mg/kg-day)	1.3E–05	3.0E–05
	Chronic ADD, cancer (mg/kg-day)	5.0E–06	1.5E–05
	Subchronic ADD (mg/kg-day)	1.3E–05	3.2E–05
Female of reproductive age (2,500 lb/yr)	APDR (mg/day)	1.2E–03	2.9E–03
	Dermal DD (mg/kg-day)	1.7E–05	4.0E–05
	ADD, non-cancer (mg/kg-day)	1.2E–05	2.7E–05
	Chronic ADD, cancer (mg/kg-day)	4.6E–06	1.4E–05
	Subchronic ADD (mg/kg-day)	1.2E–05	2.9E–05
Female of reproductive age (25,000 lb/yr)	APDR (mg/day)	1.2E–03	2.9E–03
	Dermal DD (mg/kg-day)	1.7E–05	4.0E–05
	ADD, non-cancer (mg/kg-day)	1.2E–05	2.7E–05
	Chronic ADD, cancer (mg/kg-day)	4.6E–06	1.4E–05
	Subchronic ADD (mg/kg-day)	1.2E–05	2.9E–05
APDR = Acute potential dose rate; DD = Daily dose; ADD = Average daily dose			

3.7.4.5 Weight of Scientific Evidence for Occupational Exposures

EPA considered the assessment approach, the quality of the data, and uncertainties in assessment results to determine a WoSE conclusion for the full-shift TWA inhalation exposure estimates. The primary strength is the use of directly applicable monitoring data, which is preferrable to other assessment approaches such as modeling or the use of OELs. EPA used both PBZ and stationary air concentration data to assess inhalation exposures, with each of the data sources having a high data quality rating from the systematic review process. Data from these sources were TCEP-specific and for the e-waste recycling industry, though it is uncertain whether the measured concentrations accurately represent the entire industry. The primary limitations of these data include the uncertainty of the representativeness of these data toward the true distribution of inhalation concentrations in this scenario, and that over 50 percent of the data for both workers and ONUs from all three sources were reported as below the LOD. EPA also assumed 8 exposure hours per day and 250 exposure days per year based on continuous TCEP exposure each working day for a typical worker schedule; it is uncertain whether this captures actual worker schedules and exposures. Based on these strengths and limitations, EPA has concluded that the WoSE for this assessment is moderate to robust and provides a plausible estimate of exposures.

3.8 Waste Handling

3.8.1 Waste Disposal – Landfill or Incineration for Ongoing Condition of Uses

Waste handling, disposal, and or treatment, for OESs that may still considered as ongoing (*e.g.*, Incorporation into Paints and Coatings, Resins, Articles, etc.) are covered in their relevant sections. This includes water and air releases and well as "waste disposal." Waste Disposal, in the context of TCEP, refers to either landfill or incineration and results from the potential given by the ESD or GS used for that OES. The throughput proportion to either landfill or incineration is not listed in these ESDs or GSs so it may be assumed that these waste streams go to one or both endpoints.

3.8.2 End of Service Life Disposal of Products Containing TCEP

During the TCEP Risk Evaluation process it was found that several of the Commercial Use COUs included during scoping that TCEP is no longer actively incorporated into. These COUs are:

- Furnishing, Cleaning, Treatment/Care Products
    - Fabric and textile products
    - Foam Seating and Bedding Products
- Construction, Paint, Electrical, and Metal Products
    - Building/construction materials – insulation
    - Building/construction materials – wood and engineered wood products – wood resin composites

EPA has confirmed from literature sources that TCEP was used for these purposes in the past but was phased out of these uses starting in the late 1980s or early 1990s in favor of other flame retardants or flame-retardant formulations. This phase out of TCEP began prior to what the expected service life of these products would be. EPA does not have historical data to estimate the TCEP throughput used for these products nor the amounts of these products that have already reached the end of their service life and subsequently already been disposed of. EPA assumes that what is still in use of these products represents a fraction of the overall amount of TCEP that was used for these purposes and that, given the nature of these types of products (*e.g.*, insulation and furniture), they will ultimately go to a landfill for final disposal.

3.8.2.1 Construction, Paint, Electrical, and Metal Products

During scoping, rigid polyurethane foams for insulation, specifically commercial roofing insulation, was identified as a potential application for TCEP (IARC, 1990). This source further stated that foams (for furniture and roof insulation) were the major use of TCEP. Further investigation showed that by the TCEP use had peaked prior to the 1990s (EC, 2009) and that TCPP has replaced TCEP in polyurethane applications such as rigid foams used in insulation and flexible foams and upholstery used in furniture (IPCS, 1998). Industries that EPA corresponded with during the risk evaluation process also confirmed the shift away from TCEP occurring along similar timelines.

According to a joint public comment submitted by the American Chemistry Council's (ACC) Center for the Polyurethanes Industry (CPI), the North American Modern Building Alliance (NAMBA) and the Polyisocyanurate Insulation Manufacturers Association (PIMA), TCEP was used for this application, however, it the public comment stated that this use occurred predominately during the 1970s and 1980s and phase out of TCEP began prior to the 1990s. TCEP was phased out and replaced with TCPP, which has become the most commonly used chemical flame retardant in the manufacture of polyiso insulation produced in North America. TCPP is the chemical flame retardant used in the manufacture of polyiso insulation today. They stated that, to their knowledge, “the last, limited commercial sale of TCEP to the polyiso industry occurred on or about 2009 based on industry records.” They further stated that “it should be noted that any use of TCEP by the polyiso industry that occurred after the initial transition period in the early 1990s (*i.e.*, mid-1990s to the 2000s) constituted a small portion of the overall volume of product manufactured and sold during this period. Furthermore, certain producers of polyiso insulation never used TCEP in their products relying on TCPP as the chemical flame retardant in product formulations. Finally, PIMA is unaware of any imports of polyiso products produced outside of the United States or Canada that would be responsible for introducing TCEP-based formulations into the market” (ACC, 2021).

This is also further collaborated by the lack of any CDR/IUR data for this use. While this does not confirm it was no longer used for these types of products after the phase out of TCEP, it does provide credibility that it was not used in large quantities after the phase out of TCEP in roofing insulation foams occurred in the 1990s.

Given the history/timeline of TCEPs use in rigid foam insulation for commercial roofing application as well as the expected lifespan of this type of roof, which is approximately 17–20 years it is not expected that there will be replacement activities that would generate significant releases and/or exposures going forward as much of this would have already made its way into a landfill, which is the expected destination for this type of waste stream (ACC, 2021).

In summary, the shift away from TCEP in roofing applications (prior to the 1990s) predates the average life expectancy of a roof, EPA does not have enough data to determine how much TCEP was used for this purpose in the past or how much of this past use is still in service today. It is expected that what remains in service today is only a small fraction of the overall historic use and that it will ultimately be sent to a landfill.

Regarding TCEPs use in engineered wood products, specifically wood resin products, there is only limited evidence of this occurring, and all sources cited during scoping are from the 1980s. It is possible that TCEP was used in the resins that bond wood products together, however, there is not enough information to quantify how prevalent this was. Sources describes the major uses of TCEP as being “in foams, such as the flexible foams used in automobiles and furniture and rigid foams for building insulation” (IARC, 1990). This implies any use in engineered wood products to have been a minor use, it is also unclear what applications these wood products may have been used in. It is possible they were only used in niche uses such as furniture production as opposed to larger scale uses in building construction.

Based on the weight of the evidence presented above EPA believes that while some minor exposures and releases could occur sporadically from the disposal of rigid foam products (*e.g.*, roofing insulation) or from the disposal of engineered wood products that contained TCEP or TCEP-containing flame retardant mixtures, EPA believes that this use of TCEP has ceased. Furthermore, EPA believes it is reasonable to conclude that this cessation occurred long enough ago such that the majority of the TCEP-containing products are no longer in use or in any supply chains that could potentially provide them to the types of industries and/or commercial enterprises that would use them.

EPA does understand that the potential for exposures and releases during the end of service life disposal of the application does exist, however, the data needed to estimate these is not reasonably available to us. There are no historical records of the quantities of TCEP that were used in these products. The use of

TCEP in rigid foams for roofing insulation appears to have been the major historical use of TCEP prior to the early 2000s. The amount of dust that would be generated during the removal of roofing insulation is likely to be minimal, as the insulation would be removed mostly intact to save time and effort on cleanup (ACC, 2021). Since TCEP would be already incorporated into the polymer matrix of the products dermal exposure would likely be very minimal if it occurred at all.

3.8.2.2 Furnishing, Cleaning, Treatment/Care Products

During scoping, TCEP was identified in items including fabric and textile products as well as foam seating and bedding products (IPCS, 1998). It was indicated that TCEP is used as a flame-retardant additive for flexible and rigid polyurethane and polyisoanate foams, carpet backing, paints and lacquers, epoxy, phenolic and amino resins, wood-resin composites such as particle boards, and in some cases as a coating for the back of upholstery. However, the source further indicated the major uses of TCEP appears to be in foams, such as the flexible foams used in automobiles and furniture and rigid foams for building insulation (IARC, 1990). Therefore, the past use of TCEP in wood-resin composites and upholstery are considered minor uses that did not result in large production volume, and the major historical use of TCEP in flexible and rigid foams occurred predominately prior to the early 1990's and that TCEP has been phased out of these products in favor of other flame retardants (EC, 2009). More recent research on the presence of TCEP in flexible foam products has shown low concentrations of TCEP in specific products include mattresses, seats, and carpet backing (Fang et al., 2013). TCEP concentration ranged, approximately, from less than 1 to 7 percent, by weight (see Section 5.1.2 in TCEP Risk Evaluation {U.S. EPA, 2024, 11151775) though most of the measurements were on the lower end of this range. It is known that TCEP is contained, in small quantities, in other commercially available flame-retardant formulations; an example of this could be a flame retardant known commercially as 2,2-bis(chloromethyl)-propane-1,3-diyltetrakis(2-chloroethyl) biphosphate (V6), which is a dimer of TCEP.

According to the EU RE of V6, contains between 4.5 and 7.5 percent TCEP (w/w). The EU Risk Assessment of V6 provides a lifecycle of V6 consistent with the assumption that V6 was predominately used in flexible polyurethane foams used in the automotive and furniture industries, with high end automobiles being the major use due to the higher cost of V6 relative to other flame retardants {EU, 2008, 10284991}.

The most likely source of TCEP for flexible foam, fabric, textile, and other applications is the past use of recycled foam that contained TCEP as part of other flame-retardant mixtures, such as V6. The foam that is recycled is from the original manufacture of the foam; when it is trimmed down for final shaping of a product the scraps can be recycled and used in a wide variety of applications. These foams can contain many different types of flame retardants or none at all and it is not possible to determine, with reasonable certainty, the exact flame retardants that are used in the various application. According to the EU Risk Assessment for V6, scrap foam is suitable for applications including vibration sound dampening, sport mats, cushioning, packaging and carpet underlay (EU, 2008).

The EU Risk Assessment of V6 indicates that while these operations occurred in the EU, as much as 25 percent of the throughput may have been exported to the US, it is not clear how much of this throughput contained flame-retardant chemicals or the exact products they were used in. It was indicated that TCEP alone was not used in these types of products (EU, 2008). Due to the low levels of TCEP in many of the items sampled, it is assumed that the presence of TCEP in these types of products results, primarily, from the presence of TCEP as an impurity of other flame-retardant mixtures such as V6, this is further collaborated by other sources as well (Fang et al., 2013).

Furthermore, in the EU, it has been indicated that V6 is now available with no TCEP impurity since approximately 2005 (EU, 2008), it is therefore assumed that further importation of products potentially containing TCEP into the US from the EU is no longer occurring or will occur in the future. The EU Risk Assessment of V6 provides sources that indicate lifetimes for furniture of five to ten years and PUR-specific lifetimes for furnishing/mattresses of greater than ten years. It is expected that these products still in service in the US will ultimately make their way into a landfill, but the data needed, such as the amount of TCEP and specific items/articles that were created, to quantify this is not reasonably available.

A domestic source that was identified during scoping as potentially relevant was NIOSH HHE-2014-0131-3268, "Evaluation of Occupational Exposure to Flame Retardants at Four Gymnastics Studios." This source discussed the investigation and findings from four gymnastic studios regarding the potential for employee exposure to flame retardants from polyurethane foam blocks, mats, and other padded equipment in the gymnastics studios. These studios were investigated in June 2014, October 2014, and April 2015. The investigation was prompted by the owner of the studios as opposed to any type of complaints. The site was investigated before and after the replacement and cleaning occurred to determine if the measures taken could be considered as an effective way of mitigating potential exposures to flame retardant chemicals.

During the evaluation, the owner replaced the foam blocks in the pits with foam blocks reported by the manufacturer to be free of some types of flame retardants, and thoroughly cleaned the gymnastics studio. All the new foam products that were installed during this period were certified by CertiPUR-US, which is a nonprofit organization that conducts voluntary testing and analysis of flexible urethane foams and certifies that products are made without PBDEs, tris(1,3-dichloro-2-propyl) phosphate (TDCPP), or TCEP flame retardants. It was determined that the replacement foam did not contain any of the seven most common flame retardants (TDCPP, Firemaster 550 [contains TBB and TBPH], Firemaster 600, tris(1-chloro-2-propyl) phosphate [TCPP], tris-isobutylated triphenyl phosphate [TBPP], PentaBDE, and V6 [a chlorinated organophosphate containing TCEP]). Key findings from this report are as follows:

- Handwipe samples showed a decrease of TCEP from pre shift to post shift; this indicates that employees were exposed to TCEP before their shift started, TCEP has been detected in dust samples from homes and cars (Fang et al., 2013).
- Two of the facilities conducted hand wipe sampling of employees before and after removing old foam blocks and cleaning of accumulated dust from the bottom of the foam pits. TCEP was not detected during this sampling.
- Samples of both the old and new foam did not detect TCEP. This appears to indicate that TCEP was in fact phased out of these types of foams well before the time of the inspection.
- The only source of TCEP, which was only found in two of the four gymnasiums investigated, were from surface wipe samples taken from windowsills in the facilities. TCEP was detected in a windowsill of an office area and a gymnastics area at Facility #4 and in a windowsill of a gymnastics area at Facility #1. It is not possible to know, with reasonable certainty, when the last time these areas were cleaned and therefore how long ago TCEP-containing foams were present within these studios or if the source of TCEP was even from the foams themselves. Post cleaning and replacement of the foams did not detect any TCEP in these same locations.

A similar study measured 1.6–1.9 μg/g dry weight (dw) of TCEP in polyurethane foam blocks in a Seattle gym. TCEP was detected at a mean concentration of 1.18 μg/g dw was detected in gym dust concentrations across four gyms. Dust samples were collected from the homes of four gym instructors. TCEP was found at a mean concentration of 2.5 µg/g dw at the instructors' residences (La Guardia and Hale, 2015). This source seems to provide an explanation as to how the gym employees were exposed to TCEP before beginning their work shift.

Based on the weight of the evidence presented above EPA believes that while some minor exposures and releases could occur from flexible foam products (*i.e.*, foam in many common gymnasium products, carpet backing/underlayment, and furniture/automobile cushions) that the use of TCEP, or TCEP-containing flame retardant mixtures has ceased in these products. Furthermore, EPA believes that this cessation of TCEP use, which began prior to the 1990s, as well as the apparent domestic removal of TCEP from other flame-retardant formulations as well, occurred long enough ago such that the majority of the TCEP-containing products are no longer in use or in any supply chains that could potentially provide them to the types of industries and/or commercial enterprises that would use them. While some releases and exposures could occur during the disposal of the wide variety of items that TCEP has found its way in to, these are expected to be minimal and dispersed and not expected to lead to risk, this is further supported by the findings of the consumer risk section(s).

3.9 Distribution in Commerce

3.9.1 Process Description

For purposes of assessment in this risk evaluation, distribution in commerce of TCEP consists of the transportation associated with the moving of sealed containers of TCEP or sealed packages of TCEP-containing products. EPA expects TCEP to be transported from import sites to downstream processing and use sites, or for final disposal of TCEP. The steps of loading and unloading that are assessed during other COUs/OESs consists of unloading TCEP into the formulation process and loading refers to packaging the finished product prior to shipment. Regarding loading and unloading activities that occur during a distribution in commerce scenario would only refer to loading or unloading sealed containers from a transport vehicle. More broadly under TSCA, "distribution in commerce" and "distribute in commerce" are defined under TSCA section 3(5).

3.10 Use of Laboratory Chemicals

3.10.1 Process Description

TCEP is used as a laboratory chemical, such as in a chemical standard or reference material during analyses (Chem Service, 2015; Santa Cruz Biotechnology, 2018; TCI America, 2018; Sigma-Aldrich, 2019). In the 2016 and 2020 CDR, there were no reporters for TCEP that had an industrial function category (IFC) for laboratory chemicals (U.S. EPA, 2019, 2020a). EPA did not identify other data on current laboratory use volumes or laboratory sites from systematic review. Therefore, EPA assumed TCEP may still be used at volumes below the CDR reporting threshold (see Section 2.2 for details) and assessed the following two potential scenarios: 1) laboratories utilizing 25,000 lb of TCEP; and 2) laboratories utilizing 2,500 lb of TCEP. EPA estimated the number of sites, which is described further below, for each of these scenarios. These scenarios are meant to estimate a generic laboratory site and do not necessarily represent the total number of sites or total volume of TCEP as a laboratory chemical.

EPA expects that Laboratory TCEP products are pure TCEP or TCEP present as an impurity in other products. EPA expects TCEP to be a neat liquid when present in its pure form at 25 °C (see Table 2-1 in the TCEP Risk Evaluation (U.S. EPA, 2024)). Based on the low production volume and typical laboratory chemical container sizes, EPA expects that TCEP is imported to laboratories in 1-gallon containers (U.S. EPA, 2022). Workers may remove TCEP from these containers by hand-pouring or pipette and either adding to the appropriate labware in its pure form to be diluted later or added to dilute other chemicals already in the labware (U.S. EPA, 2022). Workers may store the solution at the laboratory until it is required for a laboratory analysis. Laboratories run analytical tests using laboratory instrumentation equipment and the TCEP-containing solution. After the tests are complete, all chemicals used during the experiment are disposed and all labware is cleaned for reuse. Figure 3-8 provides an illustration of a generic laboratory process (U.S. EPA, 2022).

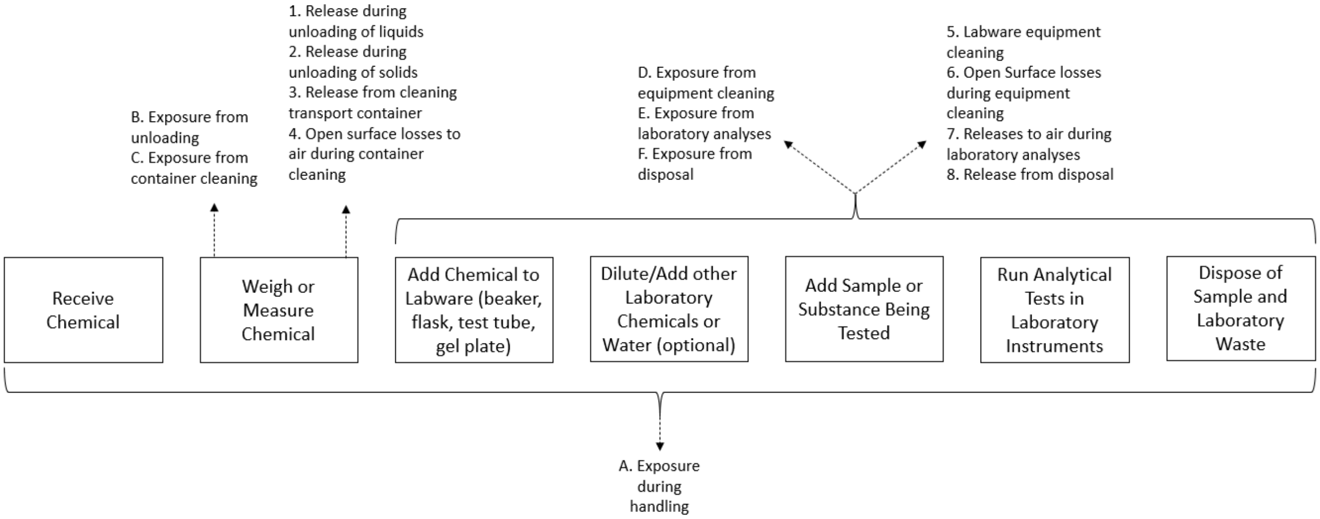

Figure 3-8. Laboratory Chemical Flow Diagram

EPA did not identify some information from systematic review for TCEP-specific laboratory chemical use data (*i.e.*, operating days per year, number of sites), however EPA did identify information regarding usage of TCEP as a laboratory standard used for calibration of equipment and testing samples that may contain TCEP. One study identified the use of small quantities, purchased from a laboratory supplier, of reagent grade TCEP for calibrating solid-phase microextraction fibers that can then be used to detect TCEP in air sampling equipment (Tollback et al., 2010). Another study also purchased reagent grade TCEP for use in creating calibration curves to test for various organophosphates that could be contained withing nail polishes (Tokumura et al., 2019). This study used TCEP in the ng/mL level to create a calibration curve. Given the usage profile identified during systematic review, EPA assumes that the daily throughput follows the lower end of the distribution of 0.5 to 4,000 mL of TCEP per site-day based on the Draft Use of Laboratory Chemicals GS (U.S. EPA, 2022). Specifically, EPA used the result of the 1st and 5th percentiles of this distribution, in lieu of the high-end and central tendency, to model the releases and exposures that could occur during this OES. The GS also estimates the number of operating days based on data from the U.S. BLS Occupational Employment Statistics and assumed shift durations of 8-, 10-, and 12-hour shifts, yielding a number of operating days of 260 days/yr, 208 days/yr, and 174 days/yr, respectively (U.S. EPA, 2022). The maximum number of laboratory sites in the United States based on the Draft Use of Laboratory Chemicals GS is 40,639 sites. While EPA does not have TCEP-specific data for laboratory use, Section 3.10.2 provides estimates for the number of laboratory sites that utilize TCEP.

3.10.2 Facility Estimates

The 2016 CDR data included a single reporting site, Aceto Corporation in Port Washington, NY, importing TCEP, with no downstream industry sectors identified (U.S. EPA, 2019). TCEP was not reported in 2020 CDR (U.S. EPA, 2020a). EPA did not identify other data on current laboratory use volumes or number of sites from systematic review. Therefore, EPA assumed TCEP may still be imported at volumes below the CDR reporting threshold (see Section 2.2 for details). In conjunction with the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023), EPA assessed the following two potential scenarios: 1) an annual production volume of TCEP of 25,000 lb across all laboratories; and 2) an annual production volume of TCEP of 2,500 lb across all laboratories. EPA estimated the number of sites from the use of laboratory chemicals using a Monte Carlo simulation with 100,000 iterations and the Latin Hypercube sampling method using the models and approaches described in Appendix E.7. Input parameters for the models were determined using data from literature and the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023).

EPA assumed liquid chemicals are expected to have daily throughput distributions presented in Table 3-26 below according to the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023).

Table 3-26. Daily Throughput of Laboratory Stock Solutions

Physical Form of Chemical of Interest	$Q_{stock\_site\_day}$[a] (g or mL of reagent/site-day)		
	Low-End[b]	**Median**[c]	**High-End**[d]
Liquid	0.5 mL	*2,000 mL (default)*	4,000 mL

[a] Based on data from the Draft Use of Laboratory Chemicals GS (U.S. EPA, 2023)

[b] This is the minimum value of the available throughput data

[c] This is the median value of the available throughput data

[d] This is the maximum value of the available throughput data

When present in its pure form, TCEP is expected to be imported to laboratory sites as a neat liquid at 25 °C (see Table 2-1 in the TCEP Risk Evaluation (U.S. EPA, 2024)). Since TCEP is in its pure form and a liquid, the distribution presented in Table 3-26 for liquid stock solutions is a one-to-one conversion to the daily throughput of TCEP at a laboratory site.

EPA assessed the number of operating days associated with laboratories using employment data obtained through the U.S. BLS Occupational Employment Statistics (U.S. BLS, 2016). Per the U.S. BLS website, operating duration for each NAICS code is assumed as a ‘year-round, full-time’ hours figure of 2,080 hours (U.S. BLS, 2016). Therefore, dividing this time by an assumed working duration of 8–12 hours/day yields a number of operating days between 174–260 days/year (U.S. EPA, 2023). In order to account for differences in operating days, EPA assumed three types of shift durations with corresponding operating days per year. These shift durations and operating days are presented in Table 3-27 below.

Table 3-27. Shift Durations and Corresponding Operating Days

Shift Duration (hrs/day)	Operating Days (days/yr)
8	260
10	208
12	174

Appendix E.7 includes the model equations and input parameters used in the Monte Carlo simulation for this COU. Table 3-28 summarizes the estimated number of sites for TCEP use in laboratory chemicals based on the two scenarios applied. The high-ends are the 95th percentile of the respective simulation output and the central tendencies are the 50th percentile.

Table 3-28. Summary of Number of Sites for the Use of TCEP as a Laboratory Chemical

Modeled Scenario	Number of Sites			
	Minimum	1st Percentile	5th Percentile	Maximum
Scenario 1: 2,500 lb annual production volume	1	13	6	511
Scenario 2: 25,000 lb annual production volume	8	126	56	3843

3.10.3 Release Assessment

3.10.3.1 Environmental Release Points

EPA expects releases to occur during the use of TCEP as a laboratory chemical. EPA estimated releases using a Monte Carlo simulation with 100,000 iterations and the Latin Hypercube sampling method using the models and approaches described in Appendix E. Input parameters and release points for the models were determined using data from literature and the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023). Specific release points considered for estimating releases are shown numbered as 1 through 8 in Figure 3-8. Per the GS, EPA expects fugitive or stack air releases from unloading containers, cleaning containers, cleaning laboratory equipment, and performing laboratory analyses. EPA expects releases in wastewater treated onsite or discharged to a POTW from cleaning containers, cleaning laboratory equipment, and disposing of residuals.

3.10.3.2 Environmental Release Assessment Results

EPA estimated releases using a Monte Carlo simulation with 100,000 iterations and the Latin Hypercube sampling method using the models and approaches described in Appendix E.7 for this COU. Input parameters for the models were determined using data from literature and the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023). EPA estimated TCEP releases by simulating two potential production volume scenarios: 1) an annual production volume of TCEP of 2,500 lb across all laboratories; and 2) an annual production volume of TCEP of 25,000 lb across all laboratories. Table 3-27 summarizes the distribution of operating days that corresponds to the number of release days per year. Table 3-29 summarizes the estimated release results for TCEP use in laboratory chemicals based on the two scenarios applied. The high-end is the 5th percentile of the respective simulation output and the central tendency is the 1st percentile.

Table 3-29. Summary of Modeled Environmental Releases for the Use of TCEP as a Laboratory Chemical

Modeled Scenario	Environmental Media	Annual Release (kg/site-yr)		Number of Release Days[a]		Daily Release (kg/site-day)	
		1st Percentile	5th Percentile	1st Percentile	5th Percentile	1st Percentile	5th Percentile
Scenario 1: 2,500 lb throughput	Fugitive or stack air[a]	1.43E–02	1.80E–02	220	214	6.47E–05	7.99E–05
	Wastewater to onsite treatment or discharge to POTW	8.72E01	1.89E02	220	214	3.96E–01	8.83E–01
Scenario 2: 25,000 lb throughput	Fugitive or stack air[a]	1.44E–02	1.79E–02	228	230	6.47E–05	7.95E–05
	Wastewater to onsite treatment or discharge to POTW	9.00E01	2.02E02	228	230	3.94E–01	8.81E–01

[a] Hours of release per day is based on typical container sizes for bottles, sampling, and cleaning. Per Table 4-11 in U.S. EPA (1991), bottle sizes range from one to five gallons, respectively. Bottles have typical unloading rates of 60 containers/hour resulting in 0.02 hr/site-day for releases per container unloaded. Sampling of liquids is expected to take one hour/site-day and equipment cleaning of multiple vessels is expected to take four hours/site-day (U.S. EPA, 1991).

3.10.3.3 Weight of Scientific Evidence for Environmental Releases

Releases to the environment are assessed using the *Draft Generic Scenario on the Use of Laboratory Chemicals* (U.S. EPA, 2023), which has a high data quality rating from the systematic review process. EPA used EPA/OPPT models combined with Monte Carlo stimulations to estimate releases to the environment, with media of release assessed using assumptions from the ESD and EPA/OPPT models. EPA believes a strength of the Monte Carlo stimulation approach is that variation in model input values and a range of potential releases values is more likely than a discrete value to capture actual releases at sites. EPA used SDSs from identified laboratory TCEP products to inform product concentration and densities. The SDSs have high data quality rating from the systematic review process. EPA believes the primary limitation to be the uncertainty in the representativeness of values toward the true distribution of potential releases. In addition, EPA lacks TCEP laboratory chemical throughput data and number of laboratories; therefore, number of laboratories and throughput estimates are based on stock solution throughputs from the *Draft Generic Scenario on the Use of Laboratory Chemicals* (U.S. EPA, 2023) and on CDR reporting thresholds. Based on this information, EPA has concluded that the WoSE for this assessment is moderate and provides a plausible estimate of releases in consideration of the strengths and limitations of reasonably available data.

3.10.4 Occupational Exposure Assessment

3.10.4.1 Workers Activities

During the use of TCEP as a laboratory chemical, workers are potentially exposed to TCEP during the following activities: transferring TCEP from transport containers to labware, laboratory sampling/analyses, and laboratory container/equipment cleaning. During these activities workers may be exposed via inhalation of vapor or dermal contact with TCEP. EPA did not find information that indicates the extent that engineering controls and worker PPE are used at laboratories that utilize TCEP. For this OES, EPA determined the ONUs from the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023) and are described in Section 3.10.4.2.

3.10.4.2 Number of Workers and Occupational Non-Users

EPA used the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023) to determine the number of workers and ONUs. The *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023) uses relevant NAICS codes and SOC codes to estimate the total number of workers and ONUs exposed to laboratory chemicals in the laboratory industry. Table 3-30 presents the total number of workers and ONUs exposed per site. On average, there are approximately three workers and three ONUs per facility that are potentially exposed to chemicals in laboratories (U.S. EPA, 2023).

Table 3-30. Number of Potentially Exposed Employees Handling TCEP as a Laboratory Chemical

NAICS Codes	SOC Codes	Exposed Workers per Site[a]	Type of Exposure
541380 – Testing laboratories 541713 – Research and development in nanotechnology 541714 – Research and development in biotechnology (except nanobiotechnology) 541715 – Research and development in the physical, engineering, and life sciences (except nanotechnology and biotechnology) 621511 – Medical Laboratories	17-2000 17-3000 51-1000	3	Worker
	19-1000 19-2000 19-4000 29-2010 51-9000	3	ONU

[a] Number of workers and ONUs associated with the relevant SOC codes under the NAICS industry sectors for laboratory chemical use. Employees with SOC codes that are unlikely to be exposed are excluded from these totals (*e.g.*, human resource workers, fundraisers, training specialists, and marketing specialists).

3.10.4.3 Occupational Inhalation Exposure Results

EPA did not identify TCEP-specific inhalation monitoring data to assess exposure during use of TCEP as a laboratory chemical. Therefore, EPA estimated inhalation exposures using a Monte Carlo simulation with 100,000 iterations and the Latin Hypercube sampling method using the models and approaches described in Appendix E. Input parameters for the models were determined using data from literature and the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023). EPA estimated inhalation exposures of TCEP by simulation two potential scenarios: 1) an annual production volume of TCEP of 2,500 lb across all laboratories; and 2) an annual production volume of TCEP of 25,000 lb across all laboratories. EPA also assumed that TCEP is imported to the site with no engineering controls present. EPA used product data from TCEP-containing laboratory products to estimate the concentration and density of TCEP used in laboratories as inputs to the Monte Carlo simulation. Actual exposures may differ based on worker activities, TCEP throughputs, and laboratory processes.

For this OES, EPA applied the EPA/OPPT Mass Balance Inhalation Model to exposures points described in the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational*

Exposures and Environmental Releases (U.S. EPA, 2023) using the vapor generation rates (G) generated from the air emission models for this OES (see Section 3.10.3) and exposure duration parameters from the 1991 CEB Manual (U.S. EPA, 1991). The EPA/OPPT Mass Balance Inhalation Model calculates the concentration of the chemical in the breathing zone of the worker for each exposure activity. The Monte Carlo stimulation then calculates a full work-shift (*i.e.*, 8-, 10-, and 12-hours) TWA by summing the contributions to exposure from each activity and averaging over the shift time, assuming no exposure occurs outside of those activities. Appendix E.7 also describes the model equations and other input parameters used in the Monte Carlo simulation for this OES.

Table 3-31 summarizes the estimated full-shift TWA exposures, AC, ADC, LADC, and $ADC_{subchronic}$ for TCEP use as a laboratory chemical based on the two production volume scenarios. The high-end values represent the 95th percentile and the central tendency values represent the 50th percentile of the simulation outputs. Equations for calculating AC, ADC, LADC, and $ADC_{subchronic}$ are presented in Appendix B.1.

The estimated exposures assume that TCEP is imported to the site with no engineering control present. Actual exposures may differ based on worker activities, TCEP throughputs, and laboratory processes.

Table 3-31. Summary of Modeled Worker Inhalation Exposures for Use of TCEP as a Laboratory Chemical

Modeled Scenario	Exposure Concentration Type	1st Percentile (mg/m^3)	5th Percentile (mg/m^3)	Data Quality Rating of Air Concentration Data
Scenario 1: 2,500 lb annual production volume	Full-shift TWA exposure concentration	5.8E–04	9.3E–04	N/A – Modeled data
	AC based on full-shift TWA	5.1E–04	7.9E–04	
	ADC based on full-shift TWA	2.7E–04	4.3E–04	
	LADC based on full-shift TWA	8.8E–05	1.5E–04	
	$ADC_{subchronic}$ based on full-shift TWA	2.9E–04	4.6E–04	
Scenario 2: 25,000 lb annual production volume	Full-shift TWA exposure concentration	5.8E–04	9.2E–04	
	AC based on full-shift TWA	5.0E–04	7.9E–04	
	ADC based on full-shift TWA	2.7E–04	4.3E–04	
	LADC based on full-shift TWA	8.7E–05	1.5E–04	
	$ADC_{subchronic}$ based on full-shift TWA	2.9E–04	4.6E–04	

AC = Acute concentration; ADC = Average daily concentration; LADC = Lifetime average daily concentration; $ADC_{subchronic}$ = Subchronic average daily concentration

3.10.4.4 Occupational Dermal Exposure Results

EPA estimated dermal exposures for this OES using the Dermal Exposure to Volatile Liquid Model described in Section 2.4.4 and a fraction absorbed value of 23.3 percent based on the dermal absorption data from (Abdallah et al., 2016) (see Section 2.4.4 and Appendix D). Table 3-32 summarizes the APDR, ARD, CRD and SCRD for TCEP use as a laboratory chemical. The high-ends are based on a higher loading rate of TCEP (2.1 mg/cm^2-event) and two-hand contact, and the central tendencies are based on a lower loading rate of TCEP (1.4 mg/cm^2-event) and one-hand contact. OES-specific parameters for dermal exposures are described in Appendix D.2.

Table 3-32. Summary of Calculated Worker Dermal Exposures for Use of TCEP as a Laboratory Chemical

Modeled Scenario	Exposure Concentration Type	Central Tendency	High-End
Average adult worker	APDR (mg/day)	175	524
	Dermal DD (mg/kg-day)	2.2	6.5
	ADD, non-cancer (mg/kg-day)	1.0	3.6
	Chronic ADD, cancer (mg/kg-day)	0.4	1.8
	Subchronic ADD (mg/kg-day)	1.6	4.8
Female of reproductive age	APDR (mg/day)	145	435
	Dermal DD (mg/kg-day)	2.0	6.0
	ADD, non-cancer (mg/kg-day)	0.9	3.3
	Chronic ADD, cancer (mg/kg-day)	0.4	1.7
	Subchronic ADD (mg/kg-day)	1.5	4.4
APDR = Acute potential dose rate; DD = Daily dose; ADD = Average daily dose			

3.10.4.5 Weight of Scientific Evidence for Occupational Exposures

EPA considered the assessment approach, the quality of the data, and uncertainties in assessment results to determine a WoSE conclusion for the full-shift TWA inhalation exposure estimates. EPA used the *Draft Generic Scenario on the Use of Laboratory Chemicals* (U.S. EPA, 2023) to assess inhalation exposures, which has a high data quality rating from the systematic review process. EPA used SDSs from identified laboratory TCEP products to inform product concentration and densities. The SDSs have high data quality rating from the systematic review process. EPA used EPA/OPPT models combined with Monte Carlo modeling to estimate inhalation exposures. A strength of the Monte Carlo stimulation approach is that variation in model input values and a range of potential exposure values is more likely than a discrete value to capture actual exposure at sites. The primary limitation is the uncertainty in the representativeness of values toward the true distribution of potential inhalation exposures. In addition, EPA lacks TCEP facility production volume data; and therefore, throughput estimates based on CDR reporting thresholds. Based on these strengths and limitations, EPA has concluded that the WoSE for this assessment is moderate and provides a plausible estimate of exposures.

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APPENDICES

Appendix A EXAMPLE OF ESTIMATING NUMBER OF WORKERS AND OCCUPATIONAL NON-USERS

Appendix A summarizes the methods that EPA used to estimate the number of workers who are potentially exposed to TCEP in each of its conditions of use. The method consists of the following steps:

1. Check relevant emission scenario documents (ESDs) and Generic Scenarios (GSs) for estimates on the number of workers potentially exposed.
2. Identify the NAICS codes for the industry sectors associated with each condition of use (COU).
3. Estimate total employment by industry/occupation combination using the Bureau of Labor Statistics' Occupational Employment Statistics data (U.S. BLS, 2016).
4. Refine the Occupational Employment Statistics estimates where they are not sufficiently granular by using the U.S. BLS (2016) Statistics of U.S. Businesses (SUSB) data on total employment by 6-digit NAICS.
5. Estimate the percentage of employees likely to be using TCEP instead of other chemicals (*i.e.*, the market penetration of TCEP in the COU).
6. Estimate the number of sites and number of potentially exposed employees per site.
7. Estimate the number of potentially exposed employees within the COU.

Step 1: Identifying Affected NAICS Codes

As a first step, EPA identified NAICS industry codes associated with each COU. EPA generally identified NAICS industry codes for a COU by:

- Querying the U.S. Census Bureau's NAICS Search tool using keywords associated with each condition of use to identify NAICS codes with descriptions that match the COU.
- Referencing EPA/OPPT Generic Scenarios (GSs) and Organisation for Economic Co-operation and Development (OECD) Emission Scenario Documents (ESDs) for a COU to identify NAICS codes cited by the GS or ESD.
- Reviewing CDR data for the chemical, identifying the industrial sector codes reported for downstream industrial uses, and matching those industrial sector codes to NAICS codes using Table D-2 provided in the CDR reporting instructions (U.S. EPA, 2020a).

Each COU section in the main body of this report identifies the NAICS codes EPA identified for the respective COU.

Step 2: Estimating Total Employment by Industry and Occupation

The U.S. BLS (2016)'s Occupational Employment Statistics data provide employment data for workers in specific industries and occupations. The industries are classified by NAICS codes (identified previously), and occupations are classified by Standard Occupational Classification (SOC) codes.

Among the relevant NAICS codes (identified previously), EPA reviewed the occupation description and identified those occupations (SOC codes) where workers are potentially exposed to TCEP. Table_Apx A-1 shows the SOC codes EPA/OPPT classified as occupations potentially exposed to TCEP. These occupations are classified as workers (W) and occupational non-users (O). All other SOC codes are assumed to represent occupations where exposure is unlikely.

Table_Apx A-1. SOCs With Worker and ONU Designation for All COUs Except Dry Cleaning

SOC	Occupation	Designation
11-9020	Construction Managers	O
17-2000	Engineers	O
17-3000	Drafters, Engineering Technicians, and Mapping Technicians	O
19-2031	Chemists	O
19-4000	Life, Physical, and Social Science Technicians	O
47-1000	Supervisors of Construction and Extraction Workers	O
47-2000	Construction Trades Workers	W
49-1000	Supervisors of Installation, Maintenance, and Repair Workers	O
49-2000	Electrical and Electronic Equipment Mechanics, Installers, and Repairers	W
49-3000	Vehicle and Mobile Equipment Mechanics, Installers, and Repairers	W
49-9010	Control and Valve Installers and Repairers	W
49-9020	Heating, Air Conditioning, and Refrigeration Mechanics and Installers	W
49-9040	Industrial Machinery Installation, Repair, and Maintenance Workers	W
49-9060	Precision Instrument and Equipment Repairers	W
49-9070	Maintenance and Repair Workers, General	W
49-9090	Miscellaneous Installation, Maintenance, and Repair Workers	W
51-1000	Supervisors of Production Workers	O
51-2000	Assemblers and Fabricators	W
51-4020	Forming Machine Setters, Operators, and Tenders, Metal and Plastic	W
51-6010	Laundry and Dry-Cleaning Workers	W
51-6020	Pressers, Textile, Garment, and Related Materials	W
51-6030	Sewing Machine Operators	O
51-6040	Shoe and Leather Workers	O
51-6050	Tailors, Dressmakers, and Sewers	O
51-6090	Miscellaneous Textile, Apparel, and Furnishings Workers	O
51-8020	Stationary Engineers and Boiler Operators	W
51-8090	Miscellaneous Plant and System Operators	W
51-9000	Other Production Occupations	W
W = Worker designation; O = ONU designation		

For dry cleaning facilities, due to the unique nature of work expected at these facilities and that different workers may be expected to share among activities with higher exposure potential (*e.g.*, unloading the dry-cleaning machine, pressing/finishing a dry-cleaned load), EPA made different SOC code worker and ONU assignments for this COU. Table_Apx A-2 summarizes the SOC codes with worker and ONU designations used for dry cleaning facilities.

Table_Apx A-2. SOCs with Worker and ONU Designations for Dry Cleaning Facilities

SOC	Occupation	Designation
41-2000	Retail Sales Workers	O

SOC	Occupation	Designation
49-9040	Industrial Machinery Installation, Repair, and Maintenance Workers	W
49-9070	Maintenance and Repair Workers, General	W
49-9090	Miscellaneous Installation, Maintenance, and Repair Workers	W
51-6010	Laundry and Dry-Cleaning Workers	W
51-6020	Pressers, Textile, Garment, and Related Materials	W
51-6030	Sewing Machine Operators	O
51-6040	Shoe and Leather Workers	O
51-6050	Tailors, Dressmakers, and Sewers	O
51-6090	Miscellaneous Textile, Apparel, and Furnishings Workers	O
W = Worker designation; O = ONU designation		

After identifying relevant NAICS and SOC codes, EPA used BLS data to determine total employment by industry and by occupation based on the NAICS and SOC combinations. For example, there are 110,640 employees associated with 4-digit NAICS 8123 (*Drycleaning and Laundry Services*) and SOC 51-6010 (*Laundry and Dry-Cleaning Workers*).

Using a combination of NAICS and SOC codes to estimate total employment provides more accurate estimates for the number of workers than using NAICS codes alone. Using only NAICS codes to estimate number of workers typically result in an overestimate, because not all workers employed in that industry sector will be exposed. However, in some cases, BLS only provide employment data at the 4-digit or 5-digit NAICS level; therefore, further refinement of this approach may be needed (see next step).

Step 3: Refining Employment Estimates to Account for lack of NAICS Granularity
The third step in EPA's methodology was to further refine the employment estimates by using total employment data in the U.S. Census Bureau (2015) SUSB. In some cases, BLS Occupational Employment Statistics' occupation-specific data are only available at the 4-digit or 5-digit NAICS level, whereas the SUSB data are available at the 6-digit level (but are not occupation-specific). Identifying specific 6-digit NAICS will ensure that only industries with potential TCEP exposure are included. As an example, OES data are available for the 4-digit NAICS 8123 *Drycleaning and Laundry Services*, which includes the following 6-digit NAICS:

- NAICS 812310 Coin-Operated Laundries and Drycleaners;
- NAICS 812320 Drycleaning and Laundry Services (except coin-operated);
- NAICS 812331 Linen Supply; and
- NAICS 812332 Industrial Launderers.

In this example, only NAICS 812320 is of interest. The Census data allow EPA to calculate employment in the specific 6-digit NAICS of interest as a percentage of employment in the BLS 4-digit NAICS.

The 6-digit NAICS 812320 comprises 46 percent of total employment under the 4-digit NAICS 8123. This percentage can be multiplied by the occupation-specific employment estimates given in the BLS OES data to further refine our estimates of the number of employees with potential exposure. Table_Apx A-3 illustrates this granularity adjustment for NAICS 812320.

Table_Apx A-3. Estimated Number of Potentially Exposed Workers and ONUs under NAICS 812320

NAICS	SOC CODE	SOC Description	Occupation Designation	Employment by SOC at 4-digit NAICS level	Percent of Total Employment	Estimated Employment by SOC at 6-digit NAICS level
8123	41-2000	Retail Sales Workers	O	44,500	46.0%	20,459
8123	49-9040	Industrial Machinery Installation, Repair, and Maintenance Workers	W	1,790	46.0%	823
8123	49-9070	Maintenance and Repair Workers, General	W	3,260	46.0%	1,499
8123	49-9090	Miscellaneous Installation, Maintenance, and Repair Workers	W	1,080	46.0%	497
8123	51-6010	Laundry and Dry-Cleaning Workers	W	110,640	46.0%	50,867
8123	51-6020	Pressers, Textile, Garment, and Related Materials	W	40,250	46.0%	18,505
8123	51-6030	Sewing Machine Operators	O	1,660	46.0%	763
8123	51-6040	Shoe and Leather Workers	O	Not reported for this NAICS code		
8123	51-6050	Tailors, Dressmakers, and Sewers	O	2,890	46.0%	1,329
8123	51-6090	Miscellaneous Textile, Apparel, and Furnishings Workers	O	0	46.0%	0
Total Potentially Exposed Employees				**206,070**		**94,740**
Total Workers						**72,190**
Total ONUs						**22,551**

W = Worker; O = ONU

Note: Numbers may not sum exactly due to rounding

Source: U.S. BLS (2016) and U.S. Census Bureau (2015)

Step 4: Estimating the Percentage of Workers Using TCEP Instead of Other Chemicals

In the final step, EPA accounted for the market share by applying a factor to the number of workers determined in Step 3. This accounts for the fact that TCEP may be only one of multiple chemicals used for the applications of interest. EPA did not identify market penetration data for any COU. In the absence of market penetration data for a given COU, EPA assumed TCEP may be used at up to all sites and by up to all workers calculated in this method as a bounding estimate. This assumes a market penetration of 100 percent. Market penetration is discussed for each COU in the main body of this report.

Step 5: Estimating the Number of Workers per Site

EPA calculated the number of workers and ONUs in each industry/occupation combination using the formula below (granularity adjustment is only applicable where SOC data are not available at the 6-digit NAICS level):

$$\begin{gathered}\text{Number of Workers or ONUs in NAICS/SOC (Step 2)} \times \text{Granularity Adjustment Percentage (Step 3)} \\ = \text{Number of Workers or ONUs in the Industry/Occupation Combination}\end{gathered}$$

EPA then estimated the total number of establishments by obtaining the number of establishments reported in the U.S. Census Bureau's SUSB (U.S. Census Bureau, 2015) data at the 6-digit NAICS level.

EPA then summed the number of workers and ONUs over all occupations within a NAICS code and divided these sums by the number of establishments in the NAICS code to calculate the average number of workers and ONUs per site.

Step 6: Estimating the Number of Workers and Sites for a COU

EPA/OPPT estimated the number of workers and ONUs potentially exposed to TCEP and the number of sites that use TCEP in a given COU through the following steps:

1. Obtaining the total number of establishments by:
    a. Obtaining the number of establishments from SUSB (U.S. Census Bureau, 2015) at the 6-digit NAICS level (Step 5) for each NAICS code in the COU and summing these values; or
    b. Obtaining the number of establishments from the Toxics Release Inventory (TRI), Discharge Monitoring Report (DMR), National Emissions Inventory (NEI), or literature for the COU.
2. Estimating the number of establishments that use TCEP by taking the total number of establishments from Step 1a and multiplying it by the market penetration factor from Step 4.
3. Estimating the number of workers and ONUs potentially exposed to TCEP by taking the number of establishments calculated in Step 1b and multiplying it by the average number of workers and ONUs per site from Step 5.

Appendix B EQUATIONS FOR CALCULATING ACUTE, SUBCHRONIC, AND CHRONIC (NON-CANCER AND CANCER) INHALATION AND DERMAL EXPOSURES

Appendix B.1 assesses TCEP inhalation exposures to workers in occupational settings, presented as 8-, 10-, or 12-hr (*i.e.*, full-shift) time weighted average (TWA). The full-shift TWA exposures are then used to calculate acute exposure concentrations (AC), subchronic average daily concentrations (SADC), average daily concentrations (ADC) for chronic, non-cancer risks, lifetime average daily concentrations (LADC) for chronic, cancer risks.

Appendix B.2 assesses TCEP dermal exposures to workers in occupational settings, presented as a dermal acute potential dose rate (APDR). The APDRs are then used to calculate acute retained doses (AD), subchronic average daily doses (SCDD), average daily doses (ADD) for chronic non-cancer risks, and lifetime average daily doses (LADD) for chronic cancer risks. This appendix presents the equations and input parameter values used to estimate each exposure metric.

B.1 Equations for Calculating Acute, Subchronic, Chronic (Non-cancer and Cancer) Inhalation Exposure

AC is used to estimate workplace inhalation exposures for acute risks (*i.e.*, risks occurring after less than one day of exposure) and are calculated using

Equation B-1.

Equation B-1

$$AC = \frac{C \times ED \times BR}{AT_{acute}}$$

Where:

AC = Acute exposure concentration
C = Contaminant concentration in air (TWA)
ED = Exposure duration (hr/day)
BR = Breathing rate ratio (unitless)
AT_{acute} = Acute averaging time (hr)

SADC is used to estimate workplace exposures for subchronic risks and are calculated using Equation B-2.

Equation B-2

$$SADC = \frac{C \times ED \times EF_{sc} \times BR}{AT_{sc}}$$

Equation B-3

$$AT_{SC} = SCD \times 24\,\frac{hr}{day}$$

Where:

$SADC$ = Subchronic average daily concentration
C = Contaminant concentration in air (TWA)
ED = Exposure duration (hr/day)
EF_{SC} = Subchronic exposure frequency
AT_{SC} = Averaging time (hr) for subchronic exposure
SCD = Days for subchronic duration (day)

ADC and LADC are used to estimate workplace exposures for non-cancer and cancer risks, respectively. These exposures are estimated as follows:

Equation B-4

$$ADC\ or\ LADC = \frac{C \times ED \times EF \times WY \times BR}{AT\ or\ AT_c}$$

Equation B-5

$$AT = WY \times 365\frac{day}{yr} \times 24\frac{hr}{day}$$

Equation B-6

$$AT_C = LT \times 365\frac{day}{yr} \times 24\frac{hr}{day}$$

Where:

ADC = Average daily concentration used for chronic non-cancer risk calculations
$LADC$ = Lifetime average daily concentration used for chronic cancer risk calculations
ED = Exposure duration (hr/day)
EF = Exposure frequency (day/yr)
WY = Working years per lifetime (yr)
BR = Breathing rate ratio (unitless)
AT = Averaging time (hr) for chronic, non-cancer risk
AT_C = Averaging time (hr) for cancer risk
LT = Lifetime years (yr) for cancer risk

B.2 Equations for Calculating Acute, Subchronic, and Chronic (Non-cancer and Cancer) Dermal Exposures

AD is used to estimate workplace dermal exposures for acute risks and are calculated using Equation B-7.

Equation B-7

$$AD = \frac{APDR}{BW}$$

Where:

AD = Acute retained dose (mg/kg-day)
$APDR$ = Acute potential dose rate (mg/day)
BW = Body weight (kg)

SCDDs is used to estimate workplace dermal exposures for subchronic risks. and is estimated using

Equation B-8.

Equation B-8

$$SCDD = \frac{APDR \times EF_{sc}}{BW \times SCD}$$

Where:

$SCDD$ = Subchronic average daily dose (mg/kg-day)
$APDR$ = Acute potential dose rate (mg/day)
EF_{SC} = Subchronic exposure frequency
BW = Body weight (kg)
SCD = Days for subchronic duration (day)

ADD and LADD are used to estimate workplace dermal exposures for non-cancer and cancer risks and are calculated using Equation B-9.

Equation B-9

$$ADD\ or\ LADD = \frac{APDR \times EF \times WY}{BW \times 365\frac{days}{yr} \times (WY\ or\ LT)}$$

Where *WY* and *LT* are used in the denominator for *ADD* and *LADD*, respectively.

B.3 Acute, Subchronic, and Chronic (Non-cancer and Cancer) Equation Inputs

The input parameter values in Table_Apx B-1 are used to calculate each of the above acute, subchronic, and chronic exposure estimates. Where exposure is calculated using probabilistic modeling, the calculations are integrated into the Monte Carlo simulation. Where multiple values are provided for ED, it indicates that EPA may have used different values for different conditions of use. The EF and EF_{SC} used for each OES can differ, and the values used are described in the appropriate sections of this report. The maximum values used in the equations as well as a general summary for these differences are described below in this section.

Table_Apx B-1. Parameter Values for Calculating Inhalation Exposure Estimates

Parameter Name	Symbol	Value	Unit
Exposure duration	ED	8, 10, or 12	hr/day
Breathing rate ratio	BR	2.04	unitless

Parameter Name	Symbol	Value	Unit
Exposure frequency	EF	Generally calculated through probabilistic modeling with a maximum of 250	days/yr
Exposure frequency, subchronic	EF_{SC}	Generally calculated through probabilistic modeling with a maximum of 22	days
Days for subchronic duration	SCD	30	days
Working years	WY	31 (50th percentile) 40 (95th percentile)	years
Lifetime years, cancer	LT	78	years
Averaging time, subchronic	AT_{SC}	720	hr
Averaging time, non-cancer	AT	271,560 (central tendency)[a] 350,400 (high-end)[b]	hr
Averaging time, cancer	AT_C	683,280	hr
Body weight	BW	80 (average adult worker) 72.4 (female of reproductive age)	kg

[a] Calculated using the 50th percentile value for working years (WY)

[b] Calculated using the 95th percentile value for working years (WY)

B.3.1 Exposure Duration (ED)

EPA generally uses an ED of eight hours per day for averaging full-shift exposures with one notable exception: Use in Laboratory Chemicals. For this OES, the full-shift duration can range from 8-hr to 12-hr shifts. EPA used a Monte Carlo model simulation to estimate exposures for the Use in Laboratory Chemicals and used a uniform distribution for ED of 8-hrs, 10-hrs, and 12-hrs. The calculated TWA from each iteration of the Monte Carlo analysis was then used to calculate a corresponding acute, subchronic, and chronic exposure values.

B.3.2 Breathing Rate Ratio (BR)

EPA uses a BR, which is the ratio between the worker breathing rate and resting breathing rate, to account for the amount of air a worker breathes during exposure. The typical worker breathes about 10 m^3 of air in eight hours, or 1.25 m^3/hr (U.S. EPA, 1991) while the resting breathing rate is 0.6125 m^3/hr (U.S. EPA, 2011b). The ratio of these two values is equivalent to 2.04.

B.3.3 Exposure Frequency (EF)

EPA generally uses a maximum EF of 250 days per year. However, in many instances for TCEP, EPA used probabilistic modeling to estimate exposures and their associated exposure frequencies, often resulting in exposure frequencies below 250 days per year. The estimation of the exposure frequency and associated distributions for each OES are described in the relevant section of this report. In general, the EF estimated for each iteration of the model is then used to calculate the corresponding chronic exposure values.

EF is expressed as the number of days per year a worker is exposed to the chemical being assessed. In some cases, it may be reasonable to assume a worker is exposed to the chemical on each working day. In other cases, it may be more appropriate to estimate a worker's exposure to the chemical that occurs during a subset of the worker's annual working days (AWD). The relationship between exposure frequency and AWD can be described mathematically as follows:

Equation B-10

$$EF = f \times AWD$$

Where:

EF = Exposure frequency, the number of days per year a worker is exposed to the chemical (day/yr)
f = Fractional number of annual working days during which a worker is exposed to the chemical (unitless)
AWD = Annual working days, the number of days per year a worker works (day/yr)

U.S. BLS (2016) provides data on the total number of hours worked and total number of employees by each industry NAICS code. These data are available from the 3- to 6-digit NAICS level (where 3-digit NAICS are less granular and 6-digit NAICS are the most granular). Dividing the total, annual hours worked by the number of employees yields the average number of hours worked per employee per year for each NAICS.

EPA has identified approximately 140 NAICS codes applicable to the multiple conditions of use for the ten chemicals undergoing risk evaluation. For each NAICS code of interest, EPA looked up the average hours worked per employee per year at the most granular NAICS level available (*i.e.*, 4-digit, 5-digit, or 6-digit). EPA converted the working hours per employee to working days per year per employee assuming employees work an average of eight hours per day. The average number of days per year worked, or AWD, ranges from 169 to 282 days per year, with a 50th percentile value of 250 days per year. EPA repeated this analysis for all NAICS codes at the 4-digit level. The average AWD for all 4-digit NAICS codes ranges from 111 to 282 days per year, with a 50th percentile value of 228 days per year. 250 days per year is approximately the 75th percentile. In the absence of industry- and TCEP-specific data, EPA assumes the parameter *f* is equal to one for all conditions of use except Use in Laboratory Chemicals. Use in Laboratory Chemicals used a discrete value of 0.962 for *f*. The 0.962 value was derived from the ratio of the number of operating days (260 days/yr) and the assumption that workers are only potentially exposed up to 250 days/yr. Therefore, the default for *f* is 0.962 day of exposure/day of operation for this OES.

B.3.4 Subchronic Exposure Frequency (EF_{SC})

For TCEP, the SCD was set at 30 days. EPA estimated the maximum number of working days within the SCD, using the following Equation B-11 and assuming five working days per week:

Equation B-11

$$EF_{SC}(max) = 5\,\frac{working\ days}{wk} \times \frac{30\ total\ days}{7\,\frac{total\ days}{wk}} = 21.4\ days, rounded\ up\ to\ 22\ days$$

However, in many instances for TCEP, EPA used probabilistic modeling to estimate exposures and their associated subchronic exposure frequencies, often resulting in subchronic exposure frequencies below 22 days. The estimation of the subchronic exposure frequency and associated distributions for each OES are described in the relevant section of this report. In general, the EF_{SC} estimated for each iteration of the model is then used to calculate the corresponding subchronic exposure values.

B.3.5 Subchronic Duration (SCD)

EPA assessed a SCD of 30 days based on the available health data.

B.3.6 Working Years (WY)

EPA has developed a triangular distribution for working years. EPA has defined the parameters of the triangular distribution as follows:

- Minimum value: BLS CPS tenure data with current employer as a low-end estimate of the number of lifetime working years: 10.4 years;
- Mode value: The 50th percentile tenure data with all employers from Survey of Income and Program Participation (SIPP) as a mode value for the number of lifetime working years: 36 years; and
- Maximum value: The maximum average tenure data with all employers from SIPP as a high-end estimate on the number of lifetime working years: 44 years.

This triangular distribution has a 50th percentile value of 31 years and 95th percentile value of 40 years. EPA uses these values for central tendency and high-end ADC and LADC calculations, respectively.

The U.S. BLS (2014) provides information on employee tenure with *current employer* obtained from the Current Population Survey (CPS). CPS is a monthly sample survey of about 60,000 households that provides information on the labor force status of the civilian non-institutional population age 16 and over; CPS data are released every two years. The data are available by demographics and by generic industry sectors but are not available by NAICS codes.

The U.S. Census Bureau (2019) SIPP provides information on *lifetime tenure with all employers*. SIPP is a household survey that collects data on income, labor force participation, social program participation and eligibility, and general demographic characteristics through a continuous series of national panel surveys of between 14,000–52,000 households (U.S. Census Bureau, 2019). EPA analyzed the 2008 SIPP Panel Wave 1, a panel that began in 2008 and covers the interview months of September 2008 through December 2008 (U.S. Census Bureau, 2019). For this panel, lifetime tenure data are available by Census Industry Codes, which can be cross-walked with NAICS codes.

SIPP data include fields for the industry in which each surveyed, employed individual works (TJBIND1), worker age (TAGE), and years of work experience *with all employers* over the surveyed individual's lifetime.[3] Census household surveys use different industry codes than the NAICS codes used in its firm surveys, so these were converted to NAICS using a published crosswalk (U.S. Census Bureau, 2012). EPA calculated the average tenure for the following age groups: 1) workers aged 50 and older; 2) workers aged 60 and older; and 3) workers of all ages employed at time of survey. EPA used tenure data for age group "50 and older" to determine the high-end lifetime working years, because the sample size in this age group is often substantially higher than the sample size for age group "60 and older". For some industries, the number of workers surveyed, or the *sample size*, was too small to provide a reliable representation of the worker tenure in that industry. Therefore, EPA excluded data where the sample size is less than five from our analysis.

Table_Apx B-2 summarizes the average tenure for workers aged 50 and older from SIPP data. Although the tenure may differ for any given industry sector, there is no significant variability between the 50th

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[3] To calculate the number of years of work experience EPA took the difference between the year first worked (TMAKMNYR) and the current data year (*i.e.*, 2008). EPA then subtracted any intervening months when not working (ETIMEOFF).

and 95th percentile values of average tenure across manufacturing and non-manufacturing sectors.

Table_Apx B-2. Overview of Average Worker Tenure from U.S. Census SIPP (Age Group 50+)

Industry Sectors	Working Years			
	Average	50th Percentile	95th Percentile	Maximum
All industry sectors relevant to the ten chemicals undergoing risk evaluation	35.9	36	39	44
Manufacturing sectors (NAICS 31–33)	35.7	36	39	40
Non-manufacturing sectors (NAICS 42–81)	36.1	36	39	44
Source: U.S. BLS (2016) Note: Industries where sample size is less than five were excluded from this analysis				

BLS CPS data provides the median years of tenure that wage and salary workers had been with their current employer. Table_Apx B-3 presents CPS data for all demographics (men and women) by age group from 2008 to 2012. To estimate the low-end value on number of working years, EPA uses the most recent (2014) CPS data for workers aged 55 to 64 years, which indicates a median tenure of 10.4 years with their current employer. The use of this low-end value represents a scenario where workers are only exposed to the chemical of interest for a portion of their lifetime working years, as they may change jobs or move from one industry to another throughout their career.

Table_Apx B-3. Median Years of Tenure with Current Employer by Age Group

Age	January 2008	January 2010	January 2012	January 2014
16 years and over	4.1	4.4	4.6	4.6
16 to 17 years	0.7	0.7	0.7	0.7
18 to 19 years	0.8	1.0	0.8	0.8
20 to 24 years	1.3	1.5	1.3	1.3
25 years and over	5.1	5.2	5.4	5.5
25 to 34 years	2.7	3.1	3.2	3.0
35 to 44 years	4.9	5.1	5.3	5.2
45 to 54 years	7.6	7.8	7.8	7.9
55 to 64 years	9.9	10.0	10.3	10.4
65 years and over	10.2	9.9	10.3	10.3
Source: U.S. BLS (2014)				

B.3.7 Lifetime Years (LT)

EPA assumes a lifetime of 78 years for all worker demographics.

B.3.8 Body Weight (BW)

EPA assumes a BW of 80 kg for average adult workers. EPA assumed a BW of 72.4 kg for females of reproductive age, pursuant to Chapter 8 of the *Exposure Factors Handbook* (U.S. EPA, 2011a).

Appendix C SAMPLE CALCULATIONS FOR CALCULATING ACUTE AND CHRONIC (NON-CANCER AND CANCER) INHALATION EXPOSURES

Sample calculations for high-end and central tendency acute and chronic (non-cancer and cancer) exposure concentrations for a COU, Processing – Incorporation – Paints & Coatings – 1-part Coatings, are provided below. The description of the equations and parameters used is provided in Appendix A.

C.1 Example High-End AC, SADC, ADC, and LADC Calculations

Calculating AC_{HE}:

$$AC_{HE} = \frac{C_{HE} \times ED \times BR}{AT_{acute}}$$

$$AC_{HE} = \frac{0.10\ mg/m^3 \times 8\ hr/day \times 2.04}{24\ hr/day} = 6.8 \times 10^{-2}\ mg/m^3$$

Calculating SADC$_{HE}$:

$$SADC = \frac{C_{HE} \times ED \times EF_{SC} \times BR}{AT_{sc}}$$

$$SADC_{HE} = \frac{0.10\ mg/m^3 \times 8\,\frac{hr}{day} \times 22\,\frac{days}{year} \times 2.04}{24\,\frac{hr}{day} \times 30\,\frac{days}{year}} = 5.0 \times 10^{-2}\ mg/m^3$$

Calculating ADC_{HE}:

$$ADC_{HE} = \frac{C_{HE} \times ED \times EF \times WY \times BR}{AT}$$

$$ADC_{HE} = \frac{0.10\ mg/m^3 \times 8\,\frac{hr}{day} \times 38\,\frac{days}{year} \times 40\ years \times 2.04}{40\ years \times 365\,\frac{days}{yr} \times 24\,\frac{hr}{day}} = 7.1 \times 10^{-3} mg/m^3$$

Calculating $LADC_{HE}$:

$$LADC_{HE} = \frac{C_{HE} \times ED \times EF \times WY \times BR}{AT_c}$$

$$LADC_{HE} = \frac{0.10\ mg/m^3 \times 8\frac{hr}{day} \times 38\frac{days}{year} \times 40\ years \times 2.04}{78\ years \times 365\frac{days}{year} \times 24\ hr/day} = 3.6 \times 10^{-3} mg/m^3$$

C.2 Example Central Tendency AC, SADC, ADC, and LADC Calculations

Calculating AC_{CT}:

$$AC_{CT} = \frac{C_{CT} \times ED \times BR}{AT_{acute}}$$

$$AC_{CT} = \frac{1.7\ \times 10^{-2}\ mg/m^3 \times 8\ hr/day \times 2.04}{24\ hr/day} = 1.2 \times 10^{-2}\ mg/m^3$$

Calculating $SADC_{CT}$:

$$SADC_{CT} = \frac{C_{CT} \times ED \times EF_{SC} \times BR}{AT_{sc}}$$

$$SADC_{CT} = \frac{1.7\ \times 10^{-2}\ mg/m^3 \times 8\frac{hr}{day} \times 6\frac{days}{year} \times 2.04}{24\frac{hr}{day} \times 30\frac{days}{year}} = 2.3 \times 10^{-3}\ mg/m^3$$

Calculating ADC_{CT}:

$$ADC_{CT} = \frac{C_{CT} \times ED \times EF \times WY \times BR}{AT}$$

$$ADC_{CT} = \frac{1.7\ \times 10^{-2}\ mg/m^3 \times 8\frac{hr}{day} \times 6\frac{days}{year} \times 31\ years \times 2.04}{31\ years \times 365\frac{days}{yr} \times 24\frac{hr}{day}} = 1.9 \times 10^{-4}\ mg/m^3$$

Calculate $LADC_{CT}$:

$$LADC_{CT} = \frac{C_{CT} \times ED \times EF \times WY \times BR}{AT_c}$$

$$LADC_{CT} = \frac{1.7\ \times 10^{-2} mg/m^3 \times 8\frac{hr}{day} \times 6\frac{days}{year} \times 31\ years \times 2.04}{78\ years \times 365\frac{days}{year} \times 24\ hr/day} = 7.6 \times 10^{-5}\ mg/m^3$$

C.3 Example High-End AD, SCDD, ADD, and LADD Calculations

Calculating AD_{HE}:

$$AD_{HE} = \frac{APDR}{BW}$$

$$AD_{HE} = \frac{524\,\frac{mg}{day}}{80\ kg} = 6.6\,\frac{mg}{kg\text{-}day}$$

Calculate $SCDD_{HE}$:

$$SCDD_{HE} = \frac{APDR \times EF_{sc}}{BW \times SCD}$$

$$SCDD_{HE} = \frac{524\,\frac{mg}{day} \times 22\,\frac{day}{yr}}{80\ kg \times 30\,\frac{day}{yr}} = 4.8\,\frac{mg}{kg\text{-}day}$$

Calculate ADD_{HE} (non-cancer):

$$ADD_{HE} = \frac{APDR \times EF \times WY}{BW \times 365\,\frac{day}{yr} \times WY}$$

$$ADD_{HE} = \frac{524\,\frac{mg}{day} \times 38\,\frac{day}{yr} \times 40\ years}{80\ kg \times 365\,\frac{day}{yr} \times 40\ years} = 0.68\,\frac{mg}{kg\text{-}day}$$

Calculate $LADD_{HE}$ (cancer):

$$LADD_{HE} = \frac{APDR \times EF \times WY}{BW \times 365\,\frac{day}{yr} \times LT}$$

$$LADD_{HE} = \frac{524\,\frac{mg}{day} \times 38\,\frac{day}{yr} \times 40\ year}{80\ kg \times 365\ \frac{day}{yr} \times 78\ yr} = 0.35\,\frac{mg}{kg\text{-}day}$$

C.4 Example Central Tendency AD, SCDD, ADD, and LADD Calculations

Calculating AD_{CT}:

$$AD_{CT} = \frac{APDR}{BW}$$

$$AD_{CT} = \frac{175\,\frac{mg}{day}}{80\,kg} = 2.2\,\frac{mg}{kg\text{-}day}$$

Calculating $SCDD_{CT}$:

$$SCDD_{CT} = \frac{APDR \times EF_{sc}}{BW \times 30\,\frac{days}{yr}}$$

$$SCDD_{CT} = \frac{175\,\frac{mg}{day} \times 6\,\frac{days}{yr}}{80\,kg \times 30\,\frac{days}{yr}} = 0.44\,\frac{mg}{kg\text{-}day}$$

Calculate ADD_{CT} (non-cancer):

$$ADD_{CT} = \frac{APDR \times EF \times WY}{BW \times AT}$$

$$ADD_{CT} = \frac{175\,\frac{mg}{day} \times 6\,\frac{days}{yr} \times 31\,years}{80\,kg \times 11{,}315\,days} = 3.6 \times 10^{-2}\,\frac{mg}{kg\text{-}day}$$

Calculate $LADD_{CT}$ (cancer):

$$LADD_{CT} = \frac{APDR \times EF \times WY}{BW \times AT_C}$$

$$LADD_{CT} = \frac{175\,\frac{mg}{day} \times 6\,\frac{days}{yr} \times 31\,years}{80\,kg \times 28{,}470\,days} = 1.4 \times 10^{-2}\,\frac{mg}{kg\text{-}day}$$

Appendix D DERMAL EXPOSURE ASSESSMENT METHOD

Appendix D presents the modeling approach and equations to estimate occupational dermal exposures. This method was developed through review of relevant literature and consideration of existing exposure models, such as EPA/OPPT models and the European Centre For Ecotoxicology and Toxicology of Chemicals' Targeted Risk Assessment model, Version 3.0 (ECETOC TRA v3).

D.1 Dermal Dose Equation

EPA used Equation D-1 to estimate the acute potential dose rate (APDR) from occupational dermal exposures.

Equation D-1

$$APDR = S \times \frac{(Q_u \times f_{abs})}{PF} \times Y_{derm} \times FT$$

Where:

S = Surface area of skin in contact with the chemical formulation (cm^2);
Q_u = Dermal load (*i.e.*, the quantity of the chemical formulation on the skin after the dermal contact event, mg/cm^2-event);
f_{abs} = Fractional absorption of the chemical formulation into the stratum corneum, accounting for evaporation of the chemical from the dermal load, Q_u (unitless, $0 \leq f_{abs} \leq 1$);
Y_{derm} = Weight fraction of the chemical of interest in the liquid (unitless, $0 \leq Y_{derm} \leq 1$);
FT = Frequency of events (integer number per day); and
PF = Glove protection factor (unitless, $PF \geq 1$)

The inputs to the dermal dose equation are described in Appendix D.2.

D.2 Model Input Parameters

Table_Apx D-1 summarizes the model parameters and their values for estimating dermal exposures. Additional explanations of EPA's selection of the inputs for each parameter are provided in the subsections after this table.

Table_Apx D-1. Summary of Model Input Values

Input Parameter	Symbol	Value	Unit	Rationale
Surface area	S	Workers: 535 (central tendency) 1,070 (high-end) Females of reproductive age: 445 (central tendency) 890 (high-end)	cm^2	See Appendix D.2.1

Input Parameter	Symbol	Value	Unit	Rationale
Dermal load	Q_u	Routine or Incidental Contact with Liquids: 1.4 (central tendency) 2.1 (high-end) Routine Immersion in Liquids: 3.8 (central tendency) 10.3 (high-end) Routine Contact with Container Surfaces (Solids): 0.84 (central tendency) 1.0 (high-end) Routine Direct Handling of Solids: 1.7 (central tendency) 2.9 (high-end)	mg/cm^2-event	See Appendix D.2.2
Fractional absorption	f_{abs}	0.233	unitless	See Appendix D.2.3
Weight fraction of chemical	Y_{derm}	OES-specific, based on maximum weight fraction expected for the OES	unitless	See Appendix D.2.4
Frequency of events	FT	1	events/day	See Appendix D.2.5
Glove protection factor	PF	1; 5; 10; or 20	unitless	See Appendix D.2.6

D.2.1 Surface Area

EPA used a high-end exposed skin surface area (S) for workers of 1,070 cm^2 based on the mean two-hand surface area for adult males ages 21 or older from Chapter 7 of EPA's *Exposure Factors Handbook* (U.S. EPA, 2011a). For females of reproductive age, EPA used a high-end exposed skin surface area of 890 cm^2 based on the mean two-hand surface area for adult females ages 21 or older from Chapter 7 of EPA's *Exposure Factors Handbook* (U.S. EPA, 2011a). For central tendency estimates, EPA assumed the exposure surface area was equivalent to only a single hand (or one side of two hands) and used half the mean values for two-hand surface areas (*i.e.*, 535 cm^2 for workers and 445 cm^2 for females of reproductive age).

It should be noted that while the surface area of exposed skin is derived from data for hand surface area, EPA did not assume that only the workers hands may be exposed to the chemical. Nor did EPA assume that the entirety of the hands is exposed for all activities. Rather, EPA assumed that dermal exposures occur to some portion of the hands plus some portion of other body parts (*e.g.*, arms) such that the total exposed surface area is approximately equal to the surface area of one or two hands for the central tendency and high-end exposure scenario, respectively.

D.2.2 Dermal Load

The dermal load (Q_u) is the quantity of chemical on the skin after the dermal contact event. This value represents the quantity remaining after the bulk chemical formulation has fallen from the hand that cannot be removed by wiping the skin (*e.g.*, the film that remains on the skin). To estimate the dermal load from each activity, EPA used data from references cited by EPA's September 2013 engineering policy memorandum, *Updating CEB's Method for Screening-Level Assessments of Dermal Exposure* (U.S. EPA, 2013). This memorandum provides for the following dermal exposure scenarios:

- Routine and incidental contact with liquids (*e.g.*, maintenance activities, manual cleaning of equipment, filling drums, connecting transfer lines, sampling, and bench-scale liquid transfers);
- Routine immersion in liquids (*e.g.*, handling of wet surfaces and spray painting);
- Routine contact with container surfaces (*e.g.*, handling closed or empty bags of solid materials); and
- Routine, direct handling of solids (*e.g.*, filling/dumping containers of powders/flakes/granules, weighing powder/scooping/mixing, handling wet or dried material in a filtration and drying process).

For liquids, the memorandum uses values of 0.7–2.1 mg/cm^2-event for routine or incidental contact with liquids and 1.3–10.3 mg/cm^2-event for routine immersion in liquids (U.S. EPA, 2013). EPA used the maximum from each range to estimate high-end dermal loads. The memorandum does not provide recommended values for a central tendency dermal loading estimate. Therefore, EPA analyzed data from EPA's technical report *A Laboratory Method to Determine the Retention of Liquids on the Surface of the Hands* (U.S. EPA, 1992b) that served as the basis for the liquid dermal loads provided in the 2013 memorandum. To estimate central tendency liquid dermal loading values, EPA used the 50th percentile of the dermal loading results from the study for each type of activity (*i.e.*, routine/incidental contact and immersion). The 50th percentile was 1.7 mg/cm^2-event for routine/incidental contact with liquids and 3.8 mg/cm^2-event for routine immersion in liquids.

For solids, the memorandum does not present dermal loads in terms of mass per unit area but rather for mass per dermal exposure event. The memorandum estimates values of up to 1,100 mg/event for routine contact with container surfaces and up to 3,100 mg/event for routine, direct handling of solids. EPA used these values as the high-end dermal loads for solids after dividing each value by the high-end dermal surface area (*i.e.*, 1,070 cm^2) to convert to units of mass per unit area. This results in a high-end dermal load of 1.0 mg/cm^2-event for routine contact with container surfaces and 2.9 mg/cm^2-event for routine, direct handling of solids.

The memorandum does not provide recommended values for central tendency dermal loading values for solids. However, the memorandum indicates the solid dermal loads are based on data reported in Lansink et al. (1996) and both the high-end and central tendency values of these data are given in Lansink et al. (1996). For routine contact with container surfaces, the central tendency dermal load is equal to 450 mg/event as reported in Lansink et al. (1996) and cited in Marquart et al. (2006). This central tendency value pertains to the gathering of closed bags of powder and is designated as the typical case exposure (Marquart et al., 2006).[4] For routine, direct handling of solids, the central tendency dermal load is equal to 900 mg/event as reported in Lansink et al. (1996) and cited in Marquart et al. (2006). This central tendency value pertains to the manual loading of mixers with dusty powder and is designated as the typical case exposure (Marquart et al., 2006).[5] EPA used these values as the central tendency dermal loads for solids after dividing each value by the central tendency dermal surface area (*i.e.*, 535 cm^2) to convert to units of mass per unit area. This results in a central tendency dermal load of 0.84 mg/cm^2-event for routine contact with container surfaces and 1.7 mg/cm^2-event for routine, direct

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[4] The high-end value of 1,100 mg/event also pertains to the gathering of closed bags of powder. This value corresponds to the value of 1,050 mg/event reported in Marquart et al. (2006) as the reasonable worst-case exposure pertaining to the gathering of closed bags of powder and obtained from Lansink et al. (1996). EPA did not directly cite Lansink et al. (1996) because, as stated in Marquart et al. (2006), this report has not been published in a scientific journal.

[5] The high-end value of 3,100 mg/event also pertains to manual loading of mixers with dusty powder. This value corresponds to the value of 3,000 mg/event reported in Marquart et al. (2006) as the reasonable worst-case exposure pertaining to loading of mixers and obtained from Lansink et al. (1996). EPA did not directly cite Lansink et al. (1996) because, as stated in Marquart et al. (2006), this report has not been published in a scientific journal.

handling of solids.

The dermal loading value EPA used for each OES depends on the specific worker activities within the OES. In some cases, workers may perform multiple activities resulting in different dermal loads for each activity. Because EPA assumed only one exposure event per day (see discussion in Appendix D.2.5), EPA presented exposures for only the activities with the highest potential dermal loads for each OES. Table_Apx D-2 summarizes the dermal loads used for each OES.

Table_Apx D-2. Summary of Dermal Loading Values by OES

OES	Activity with Highest Potential Dermal Load	Type of Dermal Exposure Scenario	Dermal Loading Values (mg/cm^2-event)
Import – Repackaging	Unloading neat liquid chemical from containers	Routine/incidental contact with liquids	1.4 (central tendency) 2.1 (high-end)
Incorporation into Paints and Coatings	Unloading neat liquid chemical from containers	Routine/incidental contact with liquids	1.4 (central tendency) 2.1 (high-end)
Use in Paints and Coatings	Application exposure	Routine/immersion with liquids	3.8 (central tendency) 10.3 (high-end)
Incorporation into Resins	Unloading neat liquid chemical from containers	Routine/incidental contact with liquids	1.4 (central tendency) 2.1 (high-end)
Incorporation into Articles	Unloading resin component from containers	Routine/incidental contact with liquids	1.4 (central tendency) 2.1 (high-end)
Use and Installation of Articles	Not assessed	Not assessed	Not assessed
Recycling	Handling of recyclables containing chemical	Routine contact with container surfaces (solids)[a]	0.8 (central tendency) 1.0 (high-end)
Waste Handling, Disposal, and Treatment	Evaluated as part of each OES as opposed to a standalone OES		
Distribution in Commerce	Distribution activities (*e.g.*, loading) considered throughout life cycle, rather than using a single distribution scenario		
Use of Laboratory Chemicals	Unloading neat liquid chemical from containers	Routine/incidental contact with liquids	1.4 (central tendency) 2.1 (high-end)

[a] Typically, EPA assumes that the chemical is entrained in the articles such that dermal exposures are negligible. However, EPA assumed that articles may abrade during transport and processing resulting in the generation of dusts that contain the chemical in solid form. EPA does not have data specific to dermal loading values for dusts generated from handling/processing of articles. Therefore, EPA assumed the dermal loads from these activities would be similar to that from handling closed/empty bags of solid materials.

D.2.3 Fractional Absorption

EPA used a single fractional absorption (f_{abs}) across all OESs of 0.233 based on data in a study (Abdallah et al., 2016). Abdallah et al. (2016) performed *in vitro* dermal absorption testing of a finite dose (*i.e.*, 500 ng/cm^2) over a 24-hr period for liquid formulations containing low concentrations of TCEP (approximately 0.001–0.005 wt% in acetone). The cumulative absorption data show 82.69 ng/cm^2 absorbed (*i.e.*, f_{abs} = 82.69/500 = 0.165) after an eight hour exposure period and the fraction remaining in the skin after 24 hours was shown to be 0.068 (Abdallah et al., 2016). EPA combined the 8-hour cumulative absorption of TCEP (0.165) from the study with the fraction of TCEP remaining in the skin after 24 hours (0.068) to estimate overall fractional absorption of 0.233 (0.165 + 0.068 = 0.233) for an 8-hour exposure. Due to a lack of dermal absorption data for the neat material, there is a high level of uncertainty with respect to modeling fractional absorption of neat TCEP. Therefore, EPA assumed that the fractional absorption of all solid and liquid TCEP-containing formulations, as well as neat TCEP, is 0.233 (Abdallah et al., 2016).

D.2.4 Weight Fraction of Chemical

The weight fraction of TCEP (Y_{derm}) refers to the concentration of TCEP in the liquid or solid formulation the worker's skin is exposed to. EPA generally assumes that this concentration will be equal to the weight fraction of TCEP in the chemical products being handled within the OES. For some OES, TCEP may be present at multiple weight fractions (*e.g.*, neat TCEP may be formulated down to lower concentrations for use in paints and coatings). In such cases, EPA estimated the dermal exposure using the maximum weight fraction of TCEP present within the OES. For example, if workers may be exposed during unloading neat TCEP into process equipment as well as loading formulated coatings containing TCEP into final packaging, EPA assessed dermal exposures to neat TCEP. Table_Apx D-3 provides a summary of the Y_{derm} values EPA used for each OES.

Table_Apx D-3. Summary of Y_{derm} Values by OES

OES	Weight Fractions of TCEP in OES	Y_{derm}
Import – Repackaging	Received as a neat liquid (weight fraction = 1) and repackaged to be formulated into coatings containing TCEP.	1
Incorporation into Paints and Coatings – 1-part coatings	Received as a neat liquid (weight fraction = 1) and formulated into coatings containing TCEP at weight fractions of 0.001–0.05.	1
Incorporation into Paints and Coatings – 2-part reactive coatings	Received as a neat liquid (weight fraction = 1) and formulated into coatings containing TCEP at weight fractions of 0.1–0.25.	1
Use in Paints and Coatings – 1-part coatings	Received as a coating and sprayed onto surfaces at weight fractions of 0.001–0.05.	0.05
Use in Paints and Coatings – 2-part reactive coatings	Received as a coating and sprayed onto surfaces at weight fractions of 0.1–0.25.	0.25
Incorporation into Resins	Received as a neat liquid (weight fraction = 1) and formulated into liquid resin containing TCEP at weight fractions of 0.01–0.4.	1
Incorporation into Articles	Received as liquid resin (weight fractions of 0.01–0.4) and cured/molded into plastic article at weight fractions of 0.01–0.4.	0.4
Use and Installation of Articles	Not assessed	Not assessed

OES	Weight Fractions of TCEP in OES	Y_{derm}
Recycling	Received as recyclable materials with literature data citing up to 1.4E–05 weight fraction	1.4E–05
Waste Handling, Disposal, and Treatment	Evaluated as part of each OES as opposed to a standalone	
Distribution in Commerce	Distribution activities (*e.g.*, loading) considered throughout life cycle, rather than using a single distribution scenario	
Use of Laboratory Chemicals	Received as a neat liquid (weight fraction = 1) and used in laboratory experiments.	1

D.2.5 Frequency of Events

The frequency of events (FT) refers to the number of dermal exposure events per day. Depending on the OES, workers may perform multiple activities throughout their shift that could potentially result in dermal exposures. Equation D-1 shows a linear relationship between FT and APDR; however, this fails to account for time between contact events. Since the chemical simultaneously evaporates from and absorbs into the skin, dermal exposure is a function of both the number of contact events per day and the time between contact events. Subsequent dermal exposure events may only meaningfully increase the dermal dose if there is sufficient time between the contact events to allow for significant evaporation/absorption of the previous exposure event. EPA did not identify information on how many contact events may occur and the time between contact events. Therefore, EPA assumes a single contact event per day for estimating dermal exposures for all OES.

D.2.6 Glove Protection Factors

Gloves may mitigate dermal exposures, if used correctly and consistently. However, data about the frequency of effective glove use – that is, the proper use of effective gloves – is very limited in industrial settings. Initial literature review suggests that there is unlikely to be sufficient data to justify a specific probability distribution for effective glove use for a chemical or industry. Instead, the impact of effective glove use should be explored by considering different percentages of effectiveness (*e.g.*, 25 percent vs. 50 percent effectiveness).

Gloves only offer barrier protection until the chemical breaks through the glove material. Using a conceptual model, Cherrie et al. (2004) proposed a glove workplace protection factor – the ratio of estimated uptake through the hands without gloves to the estimated uptake though the hands while wearing gloves; this protection factor is driven by flux, and thus varies with time. The ECETOC TRA model represents the protection factor of gloves as a fixed, APF equal to 5, 10, or 20 (Marquart et al., 2017). Where, similar to the APR for respiratory protection, the inverse of the protection factor is the fraction of the chemical that penetrates the glove.

Given the limited state of knowledge about the protection afforded by gloves in the workplace, it is reasonable to utilize the PF values of the ECETOC TRA model (Marquart et al., 2017), rather than attempt to derive new values. Table_Apx D-4 presents the PF values from ECETOC TRA v3. In the exposure data used to evaluate the ECETOC TRA model, (Marquart et al., 2017) reported that the observed glove protection factor was 34, compared to PF values of 5 or 10 used in the model.

Table_Apx D-4. Exposure Control Efficiencies and PFs for Different Dermal Protection Strategies from ECETOC TRA v3

Dermal Protection Characteristics	Affected User Group	Indicated Efficiency (%)	Protection Factor (PF)
a. Any glove/gauntlet without permeation data and without employee training	Both industrial and professional users	0	1
b. Gloves with available permeation data indicating that the material of construction offers good protection for the substance		80	5
c. Chemically resistant gloves (*i.e.*, as b above) with "basic" employee training		90	10
d. Chemically resistant gloves in combination with specific activity training (*e.g.*, procedure for glove removal and disposal) for tasks where dermal exposure can be expected to occur	Industrial users only	95	20

D.3 Potential for Occlusion

While proper use of effective gloves can effectively mitigate dermal exposures, improper use of gloves, use of damaged gloves, and/or use of the wrong glove material for the chemical being handled can result in the chemical getting trapped inside the glove. This can prevent the evaporation of volatile chemicals from the skin, resulting in occlusion. Chemicals trapped in the glove may be broadly distributed over the skin (increasing S in Equation D-1), or if not distributed within the glove, the chemical mass concentration on the skin at the site of contamination may be maintained for prolonged periods of time (increasing Q_u in Equation D-1). Conceptually, occlusion is similar to the "infinite dose" study design used in in vitro and ex vivo dermal penetration studies, in which the dermis is exposed to a large, continuous reservoir of chemical.

The impact of occlusion on dermal uptake is complex: continuous contact with the chemical may degrade skin tissues, increasing the rate of uptake, but continuous contact may also saturate the skin, slowing uptake (Guth et al., 2015). These phenomena are dependent upon the chemical, the vehicle and environmental conditions. It is probably not feasible to incorporate these sources of variability in a screening-level population model of dermal exposure without chemical-specific studies.

The dermal equation (Equation D-1) could theoretically be modified to account for the increased surface area and/or increased chemical mass in the glove. This could be achieved through a multiplicative variable or a change in the default values of S and/or Q_u. It may be reasonable to assume that the surface area of hand in contact with the chemical, S, is the area of the whole hand owing to the distribution of chemical within the glove. Since Q_u reflects the film that remains on the skin (and cannot be wiped off), a larger value should be used to reflect that the liquid volume is trapped in the glove, rather than falling from the hand. Alternatively, the product $S \times Q_u$ (cm^2 × mg/cm^2-event) could be replaced by a single variable representing the mass of chemical that deposits inside the glove per event, M (mg/event):

Equation D-2

$$APDR = M \times Y_{derm} \times FT$$

Garrod et al. (2001) surveyed contamination by involatile components of non-agricultural pesticide products inside gloves across different job tasks and found that protective gloves were nearly always contaminated inside. While the study does not describe the exact mechanism in which the contamination occurs (*e.g.*, via the cuff, permeation, or penetration through imperfections in glove materials), it quantified inner glove exposure as "amount of product per unit time," with a median value of 1.36 mg product per minute, a 75th percentile value of 4.21 mg/min, and a 95th percentile value of 71.9 mg/min. It is possible to use these values to calculate the value of M, *i.e.*, mass of chemical that deposits inside the glove, if the work activity duration is known.

Assuming an activity duration of one hour, the 50th and 95th percentile values translate to 81.6 mg and 4,314 mg of inner glove exposure. While these values may be used as defaults for M in Equation D-2, EPA notes the significant difference between the 50th and 95th percentile deposition, with the 95th percentile value being two times more conservative than the high-end values EPA used to model dermal exposures (where the product $S \times Q_u$ is 2,247 mg/event). Given the significant variability in inner glove exposure and lack of information on the specific mechanism in which the inner glove contamination occurs, EPA only addresses the occlusion scenario qualitatively, as described below.

EPA does not expect occlusion scenarios to be a reasonable occurrence for all conditions of use. Specifically, occlusion is not expected at sites using chemicals in closed systems where the only potential for dermal exposure is during the connecting/disconnecting of hoses used for unloading/loading of containers or while collecting quality control samples including repackaging sites, formulation sites, and other similar industrial sites. Occlusion is also not expected to occur at highly controlled sites, such as recycling sites, where, due to purity requirements, the use of engineering controls is expected to limit potential dermal exposures. EPA also does not expect occlusion at sites where contact with bulk liquid chemical is not expected such formulation of coatings or resins sites where workers are only expected to handle the drums or cans containing the chemical and not the actual bulk liquid chemical.

EPA expects occlusion to be a reasonable occurrence at sites where workers may come in contact with bulk liquid chemical and handle the chemical in open systems. This includes conditions of use such as the spray application of coatings where workers are expected to handle bulk chemical during the application of coatings. Similarly, occlusion may occur at coating or adhesive application sites when workers replenish application equipment with liquid coatings or adhesives.

Appendix E MODEL APPROACHES AND PARAMETERS

Appendix E presents the modeling approach and model equations used in estimating environmental releases and occupational exposures for each of the applicable OESs. The models were developed through review of the literature and consideration of existing EPA/OPPT models, ESDs, and/or GSs. An individual model input parameter could either have a discrete value or a distribution of values. EPA assigned statistical distributions based on reasonably available literature data. A Monte Carlo simulation (a type of stochastic simulation) was conducted to capture variability in the model input parameters. The simulation was conducted using the Latin Hypercube sampling method in the Palisade's @RISK software, Industrial Edition, Version 7.0.0[6]. The Latin Hypercube sampling method generates a sample of possible values from a multi-dimensional distribution and is considered a stratified method, meaning the generated samples are representative of the probability density function (variability) defined in the model. EPA performed the model at 100,000 iterations to capture a broad range of possible input values, including values with low probability of occurrence.

EPA used the 50th and 95th percentile Monte Carlo simulation result values for assessment. The 50th percentile value represents the typical release amount or exposure level, whereas the 95th percentile value represents the high-end release amount or exposure level. The following subsections detail the model design equations and parameters for each of the OESs.

E.1 EPA/OPPT Standard Models

Appendix E.1 discusses the standard models used by EPA to estimate environmental releases of chemicals and occupational inhalation exposures. All the models presented in this section are models that were previously developed by EPA and are not the result of any new model development work for this risk evaluation. Therefore, this appendix does not provide the details of the derivation of the model equations which have been provided in other documents such as the *Chemical Screening Tool for Exposures and Environmental Releases* (*ChemSTEER) User Guide* (U.S. EPA, 2015) (hereinafter referred to as the "ChemSTEER User Guide"), *Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Volume 1* (U.S. EPA, 1991) (hereinafter referred to as the "1991 CEB Manual"), *Evaporation of pure liquids from open surfaces* (Arnold and Engel, 2001), *Evaluation of the Mass Balance Model Used by the References Environmental Protection Agency for Estimating Inhalation Exposure to New Chemical Substances* (Fehrenbacher and Hummel, 1996), and *Releases During Cleaning of Equipment* (PEI Associates, 1988, 8731013}. The models include loss fraction models as well as models for estimating chemical vapor generation rates used in subsequent model equations to estimate the volatile releases to air and occupational inhalation exposure concentrations. The parameters in the equations of this appendix section are specific to calculating environmental releases of TCEP.

The EPA/OPPT Penetration Model estimates releases to air from evaporation of a chemical from an open, exposed liquid surface. This model is appropriate for determining volatile releases from activities that are performed indoors or when air velocities are expected to be less than or equal to 100 feet per minute. The EPA/OPPT Penetration Model calculates the average vapor generation rate of the chemical from the exposed liquid surface using Equation E-1.

Equation E-1

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[6] See Palisade's @RISK software for additional information.

$$G_{activity} = \frac{(8.24 \times 10^{-8}) \times (MW_{TCEP}^{0.835}) \times F_{correction\_factor} \times VP \times \sqrt{Rate_{air\_speed}} \times (0.25\pi D_{opening}^{2})\sqrt[4]{\frac{1}{29} + \frac{1}{MW_{TCEP}}}}{T^{0.05} \times \sqrt{D_{opening}} \times \sqrt{P}}$$

Where:

$G_{activity}$ = Vapor generation rate for activity (g/s)
MW_{TCEP} = TCEP molecular weight (g/mol)
$F_{correction\_factor}$ = Vapor pressure correction factor (unitless)
VP = TCEP vapor pressure (torr)
$Rate_{air\_speed}$ = Air speed (cm/s)
$D_{opening}$ = Diameter of opening (cm)
T = Temperature (K)
P = Pressure (torr)

The EPA/OPPT Mass Transfer Coefficient Model estimates releases to air from the evaporation of a chemical from an open, exposed liquid surface. This model is appropriate for determining this type of volatile release from activities that are performed outdoors or when air velocities are expected to be greater than 100 feet per minute. The EPA/OPPT Mass Transfer Coefficient Model calculates the average vapor generation rate of the chemical from the exposed liquid surface using Equation E-2.

Equation E-2

$$G_{activity} = \frac{(1.93 \times 10^{-7}) \times (MW_{TCEP^{0.78}}) \times F_{correction\_factor} \times VP \times Rate_{air\_speed}^{0.78} \times (0.25\pi D_{opening}^{2})\sqrt[3]{\frac{1}{29} + \frac{1}{MW_{TCEP}}}}{T^{0.4} \times D_{opening}^{0.11} \times (\sqrt{T} - 5.87)^{2/3}}$$

Where:

$G_{activity}$ = Vapor generation rate for activity (g/s)
MW_{TCEP} = TCEP molecular weight (g/mol)
$F_{correction\_factor}$ = Vapor pressure correction factor (unitless)
VP = TCEP vapor pressure (torr)
$Rate_{air\_speed}$ = Air speed (cm/s)
$D_{opening}$ = Diameter of opening (cm)
T = Temperature (K)

The EPA's Office of Air Quality Planning and Standards (OAQPS) AP-42 Loading Model estimates releases to air from the displacement of air containing chemical vapor as a container/vessel is filled with a liquid. This model assumes that the rate of evaporation is negligible compared to the vapor loss from the displacement and is used as the default for estimating volatile air releases during both loading activities and unloading activities. This model is used for unloading activities because it is assumed while one vessel is being unloaded another is assumed to be loaded. The EPA/OAQPS AP-42 Loading Model calculates the average vapor generation rate from loading or unloading using Equation E-3.

Equation E-3

$$G_{activity} = \frac{F_{saturation\_factor} \times MW_{TCEP} \times V_{container} \times 3{,}785.4\frac{cm^{3}}{gal} \times F_{correction\_factor} \times VP \times \frac{RATE_{fill}}{3{,}600\frac{s}{hr}}}{R \times T}$$

Where:

$G_{activity}$ = Vapor generation rate for activity (g/s)
$F_{saturation\_factor}$ = Saturation factor (unitless)
MW_{TCEP} = TCEP molecular weight (g/mol)
$V_{container}$ = Volume of container (gal/container)
$F_{correction\_factor}$ = Vapor pressure correction factor (unitless)
VP = TCEP vapor pressure (torr)
$RATE_{fill}$ = Fill rate of container (containers/hr)
R = Universal gas constant (L-torr/mol-K)
T = Temperature (K)

For each of the vapor generation rate models, the vapor pressure correction factor ($F_{correction\_factor}$) can be estimated using Raoult's Law and the mole fraction of TCEP in the liquid of interest. However, in most cases, EPA did not have data on the molecular weights of other components in the liquid formulations; therefore, EPA approximated the mole fraction using the mass fraction of TCEP in the liquid of interest. Using the mass fraction of TCEP to estimate mole fraction does create uncertainty in the vapor generation rate model. If other components in the liquid of interest have similar molecular weights as TCEP, then mass fraction is a reasonable approximation of mole fraction. However, if other components in the liquid of interest have much lower molecular weights than TCEP, the mass fraction of TCEP will be an overestimate of the mole fraction. If other components in the liquid of interest have much higher molecular weights than TCEP, the mass fraction of TCEP will underestimate the mole fraction.

If calculating an environmental release, the vapor generation rate calculated from one of the above models (Equation E-1, Equation E-2, or Equation E-3) is then used along with an operating time to calculate the release amount:

Equation E-4

$$Release\_Year_{activity} = Time_{activity} \times G_{activity} \times 3{,}600\,\frac{s}{hr} \times 0.001\,\frac{kg}{g}$$

Where:

$Release\_Year_{activity}$ = TCEP released for activity per site-year (kg/site-yr)
$Time_{activity}$ = Operating time for activity (hr/site-yr)
$G_{activity}$ = Vapor generation rate for activity (g/s)

In addition to the vapor generation rate models, EPA uses various loss fraction models to calculate environmental releases, including the following:

- EPA/OPPT Small Container Residual Model
- EPA/OPPT Drum Residual Model
- EPA/OPPT Multiple Process Vessel Residual Model
- EPA/OPPT Single Process Vessel Residual Model

The loss fraction models apply a given loss fraction to the overall throughput of TCEP for the given process. The loss fraction value or distribution of values differs for each model; however, the models each follow the same general equation:

Equation E-5

$$Release\_Year_{activity} = PV \times F_{activity\_loss}$$

Where:

$Release\_Year_{activity}$ = TCEP released for activity per site-year (kg/site-yr)
PV = Production volume throughput of TCEP (kg/site-yr)
$F_{activity\_loss}$ = Loss fraction for activity (unitless)

The EPA/OPPT Mass Balance Inhalation Model estimates a worker inhalation exposure to an estimated concentration of chemical vapors within the worker's breathing zone using a one box model. The model estimates the amount of chemical inhaled by a worker during an activity in which the chemical has volatilized and the airborne concentration of the chemical vapor is estimated as a function of the source vapor generation rate or the saturation level of the chemical in air. First, the applicable vapor generation rate model (Equation E-1, Equation E-2, or Equation E-3) is used to calculate the vapor generation rate for the given activity. With this vapor generation rate, the EPA/OPPT Mass Balance Inhalation Model calculates the volumetric concentration of TCEP using Equation E-6.

Equation E-6

$$Cv_{activity} = Minimum\colon \begin{cases} \left[\dfrac{170{,}000 \times T \times G_{activity}}{MW_{TCEP} \times Q \times k}\right] \\ \left[\dfrac{1{,}000{,}000\ ppm \times F_{correction\_factor} \times VP}{P}\right] \end{cases}$$

Where:

$Cv_{activity}$ = Exposure activity volumetric concentration (ppm)
$G_{activity}$ = Exposure activity vapor generation rate (g/s)
MW_{TCEP} = TCEP molecular weight (g/mol)
Q = Ventilation rate (ft^3/min)
k = Mixing factor (unitless)
T = Temperature (K)
$F_{correction\_factor}$ = Vapor pressure correction factor (unitless)
VP = TCEP vapor pressure (torr)
P = Pressure (torr)

Mass concentration can be estimated by multiplying the volumetric concentration by the molecular weight of TCEP and dividing by molar volume at standard temperature and pressure.

EPA uses the above equations in the TCEP environmental release and occupational exposure models, and EPA references the model equations by model name and/or equation number within Appendix B.

E.2 Import – Repackaging Model Approach and Parameters

Appendix E.2 presents the modeling approach and equations used to estimate environmental releases and occupational exposures for TCEP during the Import – Repackaging OES. This approach utilizes the *Emission Scenario Document on Transport and Storage of Chemicals* (OECD, 2009c) combined with Monte Carlo simulation (a type of stochastic simulation).

Based on the ESD, EPA identified the following release points from repackaging operations:

- Release Point 1: Transfer operation losses to air from emptying drum;
- Release Point 2: Transfer operation losses to air from filling small containers;
- Release Point 3: Releases during storage (not assessed);
- Release Point 4: Open surface losses to air during drum cleaning; and
- Release Point 5: Drum cleaning releases to water.

Based on the ESD, EPA also identified the following inhalation exposure points:

- Exposure Point A: Transfer operation exposures from emptying drum;
- Exposure Point B: Transfer operation exposures from filling small containers; and
- Exposure Point C: Exposures during drum cleaning.

Environmental releases and occupational exposures for TCEP during Import – Repackaging are a function of TCEP's physical properties, container size, mass fractions, and other model parameters. While physical properties are fixed, some model parameters are expected to vary. As described in Section 3.1, EPA used a Monte Carlo simulation to capture variability in the following model input parameters: ventilation rate, mixing factor, air speed, saturation factor, loss factor, container sizes, working years, and drum fill rates. EPA used the outputs from a Monte Carlo simulation with 100,000 iterations and the Latin Hypercube sampling method in @RISK to calculate release amounts and exposure concentrations for this OES.

E.2.1 Model Equations

Table_Apx E-1 provides the models and associated variables used to calculate environmental releases for each release point within each iteration of the Monte Carlo simulation. EPA used these environmental releases to develop a distribution of release outputs for the Import – Repackaging OES. The variables used to calculate each of the following values include deterministic or variable input parameters, known constants, physical properties, conversion factors, and other parameters. The values for these variables are provided in Appendices E.2.2 and E.2.3. The Monte Carlo simulation calculated the total TCEP release (by environmental media) across all release points during each iteration of the simulation. EPA then selected 50th and 95th percentile values to estimate the central tendency and high-end releases, respectively.

Table_Apx E-1. Models and Variables Applied for Release Points in the Import – Repackaging OES

Release Point	Model(s) Applied	Variables Used
Release Point 1: Transfer operation losses to air from emptying drum	EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP}; VP; $F_{saturation\_unloading}$; MW_{TCEP}; V_{import_cont}; R; T; $RATE_{fill\_drum}$

Release Point	Model(s) Applied	Variables Used
		Operating Time: $RATE_{fill\_drum}$
Release Point 2: Transfer operation losses to air from filling small containers	EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP}; VP; $F_{saturation\_loading}$; MW_{TCEP}; V_{fill_cont}; R; T; $RATE_{fill\_smallcont}$ Operating Time: $RATE_{fill\_smallcont}$
Release Point 3: Releases during storage (not assessed)	Not assessed; release is not expected to lead to significant losses to the environment unless there is an accident	Not applicable
Release Point 4: Open surface losses to air during drum cleaning	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_cont-cleaning}$; T; P Operating Time: $RATE_{fill\_drum}$
Release Point 5: Drum cleaning releases to water	EPA/OPPT Drum Residual Model (Appendix E.1)	PV; F_{loss_cont}

Appendix E.2.6 provides equations and discussion for release point operating times used to calculate releases to air as provided in Equation E-4.

Table_Apx E-2 provides the models and associated variables used to calculate occupational exposures for each exposure point within each iteration of the Monte Carlo simulation. EPA used these occupational exposures to develop a distribution of exposure outputs for the import–repackaging OES. EPA assumed that the same worker performed each exposure activity resulting in a total exposure duration of up to eight hours per day. The variables used to calculate each of the following exposure concentrations and durations include deterministic or variable input parameters, known constants, physical properties, conversion factors, and other parameters. The values for these variables are provided in Appendices E.2.2 and E.2.3. The Monte Carlo simulation calculated an 8-hr TWA exposure concentration for each iteration using the exposure concentration and duration associated with each activity and assuming exposures outside the exposure activities were zero. EPA then selected 50th and 95th percentile values to estimate the central tendency and high-end exposure concentrations, respectively.

Table_Apx E-2. Models and Variables Applied for Exposure Points in the Import – Repackaging OES

Exposure Point	Model(s) Applied	Variables Used
Exposure Point A: Transfer operation exposures from emptying drum	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP}; VP; $F_{saturation\_unloading}$; MW_{TCEP}; V_{import_cont}; R; T; $RATE_{fill\_drum}$; Q; k; Vm

Exposure Point	Model(s) Applied	Variables Used
		Exposure Duration: $RATE_{fill\_drum}$
Exposure Point B: Transfer operation exposure from filling small containers	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP}; VP; $F_{saturation\_loading}$; MW_{TCEP}; V_{small_cont}; R; T; $RATE_{fill\_smallcont}$; Q; k; Vm Exposure Duration: V_{import_cont}; V_{fill_cont}; $RATE_{fill\_drum}$
Exposure Point C: Exposures during drum cleaning	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_cont-cleaning}$; T; P; Q; k; Vm Exposure Duration: $RATE_{fill\_drum}$

Appendix E.2.6 provides equations and discussion for exposure durations used for each exposure activity. Note that the number of exposure days is set equal to the number of operating days per year up to a maximum of 250 days per year. If the number of operating days is greater than 250 days per year, EPA assumed that a single worker would not work more than 250 days per year such that the maximum exposure days per year was still 250.

E.2.2 Model Input Parameters

Table_Apx E-3 summarizes the model parameters and their values for the Import – Repackaging Monte Carlo simulation. Additional explanations of EPA's selection of the distributions for each parameter are provided in the following subsections.

Table_Apx E-3. Summary of Parameter Values and Distributions Used in the Import – Repackaging Models

Input Parameter	Symbol	Unit	Deterministic Values	Uncertainty Analysis Distribution Parameters				Rationale/Basis
			Value	Lower Bound	Upper Bound	Mode	Distribution Type	
Air speed	$RATE_{air\_speed}$	cm/s	10	1.3	202.2	—	Lognormal	See Appendix E.2.7
Container loss fraction	F_{loss_cont}	kg/kg	0.025	0.017	0.03	0.025	Triangular	See Appendix E.2.8
Saturation factor unloading	$F_{saturation\_unloading}$	unitless	0.5	0.5	1.45	0.5	Triangular	See Appendix E.2.10
Saturation factor loading	$F_{saturation\_loading}$	unitless	0.5	0.5	1.45	0.5	Triangular	See Appendix E.2.10
Import container volume	V_{import_cont}	gal/container	55	20	100	55	Triangular	See Appendix E.2.11
Small container volume	V_{prod_cont}	gal/container	5	5	20	5	Triangular	See Appendix E.2.11
Number of sites	N_s	sites	1	—	—	—	—	"What-if" scenario input
Production volume assessed	PV_lbs	lbs/year	2,500 or 25,000	—	—	—	—	"What-if" scenario input
Production volume	PV	kg/yr	Unit conversion	—	—	—	—	PV input converted to kilograms
Import concentration	F_{TCEP_import}	kg/kg	1.0	—	—	—	—	Assumed pure TCEP imported for Import – Repackaging
Temperature	T	K	298	—	—	—	—	Process parameter
Pressure	P	torr	760	—	—	—	—	Process parameter
Gas constant	R	L-torr/mol-K	62.36367	—	—	—	—	Universal constant
TCEP vapor pressure	VP	torr	0.0613	—	—	—	—	Physical property

Input Parameter	Symbol	Unit	Deterministic Values	Uncertainty Analysis Distribution Parameters				Rationale/Basis
			Value	Lower Bound	Upper Bound	Mode	Distribution Type	
TCEP density	ρ_{TCEP}	kg/m^3	1,390	—	—	—	—	Physical property
TCEP molecular weight	MW_{TCEP}	g/mol	285.49	—	—	—	—	Physical property
Fill rate of drum	$RATE_{fill\_drum}$	containers/hr	20	—	—	—	—	See Appendix E.2.12
Fill rate of small container	$RATE_{fill\_small}$	containers/hr	60	—	—	—	—	See Appendix E.2.12
Diameter of opening for container cleaning	$D_{opening\_cont-cleaning}$	cm	5.08	—	—	—	—	See Appendix E.2.9
Ventilation rate	Q	ft^3/min	3,000	500	10,000	3,000	Triangular	See Appendix E.2.13
Mixing factor	k	unitless	0.5	0.1	1	0.5	Triangular	See Appendix E.2.14

E.2.3 Throughput Parameters

The facility production rate is calculated as an input value to be used in the model equations during each iteration. The facility production rate is calculated using Equation E-7.

Equation E-7

$$PV_{site} = \frac{PV}{N_s}$$

Where:

PV = Production volume (kg/yr)
N_s = Number of sites (sites)
PV_{site} = Facility production rate (kg/site-yr)

EPA assumed the number of release days in a single year is also equivalent to the number of import containers received in a single year. This is a result of the production volume of TCEP selected only allows for the number of containers received in a single year to be between 4 to 40 containers per year. The number of release days in a single year is calculated using Equation E-8.

E.2.4 Number of Containers per Year

EPA assumed that facilities unloaded one imported drum in a single day. EPA assumes TCEP is imported in its pure form at 100 percent concentration. Based on the two production volumes and import container sizes shown in Table_Apx E-3, this only allows for the number of containers received in a single year to be between 4 to 40 containers per year. By assuming only one imported drum is unloaded and repackaged in a single day, the number of containers unloaded per year is equivalent to the number of release days per year. The equation to calculate the number of import containers is in Appendix E.2.5.

E.2.5 Release Days per Year

EPA calculated the number of release days in a single year using Equation E-8.

Equation E-8

$$RD = \frac{PV_{site}}{\rho_{TCEP} \times (0.00378541\,\frac{m^3}{gal}) \times V_{import\_cont}}$$

Where:

RD = Release days or number of import containers (days/site-yr or containers/site-yr)
PV_{site} = Facility production rate (kg/site-yr)
ρ_{TCEP} = TCEP density (kg/m^3)
V_{import_cont} = Import container volume (gal/container)

As described in Appendix E.2.4, EPA assumed that the number of import containers unloaded in a single operating day was one. Therefore, the number of release days is equivalent to the number of import containers, with a range of 4 to 40 days release days.

E.2.6 Operating Hours and Exposure Durations

EPA estimated operating hours and exposure durations using calculations and parameters provided by the *Emission Scenario Document on Transport and Storage of Chemicals* (OECD, 2009c) and ChemSTEER User Guide (U.S. EPA, 2015). The operating time for release and exposure activities associated with unloading (Release Points 1 and 4; Exposure Points A and C) are calculated using Equation E-9.

Equation E-9

$$Time_{RP1/RP4} = \frac{1}{RATE_{fill_{drum}}}$$

Where:

$Time_{RP1/RP4}$ = Operating time for Release Points 1 and 4 (hrs/container)
$RATE_{fill_{drum}}$ = Fill rate of drum (container/hr)

For the emptying of drums, the ChemSTEER User Guide (U.S. EPA, 2015) indicates a drum fill rate of 20 drums per hour based on the 1991 CEB Manual (U.S. EPA, 1991). EPA assumed that one drum is imported and repackaged in a single operating day therefore equating the number of import containers received in a single year to the number of release days per year. For the cleaning of drums, the ChemSTEER User Guide (U.S. EPA, 2015) uses the same drum fill rate as emptying drums to estimate an exposure duration. EPA did not identify any other information on drum fill rates; therefore, EPA used a single deterministic value for fill rate.

The operating hours for both Release Point 2 and Exposure Point B are calculated using Equation E-10.

Equation E-10

$$Time_{RP2} = \frac{V_{import\_cont}}{V_{fill\_cont} \times RATE_{fill\_smallcont} \times RD}$$

Where:

$Time_{RP2}$ = Operating time for Release Point 2 (hrs/site-day)
V_{import_cont} = Import container volume (gal/container)
V_{fill_cont} = Small container volume (gal/container)
$RATE_{fill\_smallcont}$ = Fill rate of small container (containers/hr)
RD = Release days or number of import containers (days/site-yr or containers/site-yr)

For filling small containers, see Appendix E.2.11 for details on the distribution of small container volume and Appendix E.2.12 for details on the small container fill rate. Generally, EPA calculated the duration of filling small containers using the container volume and fill rate from the ChemSTEER User Guide (U.S. EPA, 2015). The calculated small container fill duration was used for both Release Point (operating hours rate for Release Point 2) and Exposure Point (exposure duration for Exposure Point B).

E.2.7 Air Speed

Baldwin and Maynard (1998) measured indoor air speed across a variety of occupational settings in the United Kingdom, specifically 55 work areas were surveyed. EPA analyzed the air speed data from

Baldwin and Maynard (1998) and categorized the air speed surveys into settings representative of industrial facilities and representative of commercial facilities. EPA fit separate distributions for these industrial and commercial settings and used the industrial distribution for this OES.

EPA fit a lognormal distribution for the data set as consistent with the authors' observations that the air speed measurements within a surveyed location were lognormally distributed and the population of the mean air speeds among all surveys were lognormally distributed (Baldwin and Maynard, 1998). Since lognormal distributions are bound by zero and positive infinity, EPA truncated the distribution at the largest observed value among all of the survey mean air speeds.

EPA fit the air speed surveys representative of industrial facilities to a lognormal distribution with the following parameter values: mean of 22.414 cm/s and standard deviation of 19.958 cm/s. In the model, the lognormal distribution is truncated at a minimum allowed value of 1.3 cm/s and a maximum allowed value of 202.2 cm/s (largest surveyed mean air speed observed in Baldwin and Maynard (1998)) to prevent the model from sampling values that approach infinity or are otherwise unrealistically small or large.

Baldwin and Maynard (1998) presented only the mean air speed of each survey. The authors did not present the individual measurements within each survey. Therefore, these distributions represent a distribution of mean air speeds and not a distribution of spatially variable air speeds within a single workplace setting. However, a mean air speed (averaged over a work area) is the required input for the model. EPA converted the units to ft/min prior to use within the model equations.

E.2.8 Container Residue Loss Fraction

EPA previously contracted PEI Associates, Inc. (hereinafter referred to as "PEI") to conduct a study to provide estimates of potential chemical releases during cleaning of process equipment and shipping containers (PEI Associates, 1988). The study used both a literature review of cleaning practices and release data as well as a pilot-scale experiment to determine the amount of residual material left in vessels. The data from literature and pilot-scale experiments addressed different conditions for the emptying of containers and tanks, including various bulk liquid materials, different container constructions (*e.g.*, lined steel drums or plastic drums), and either a pump or pour/gravity-drain method for emptying. EPA reviewed the pilot-scale data from PEI and determined a range and average percentage of residual material remaining in vessels following emptying from drums by either pumping or pouring as well as tanks by gravity-drain (PEI Associates, 1988).

EPA previously used the study results to generate default central tendency and high end-loss fraction values for the residual models (*e.g.*, EPA/OPPT Small Container Residual Model, EPA/OPPT Drum Residual Model) provided in the ChemSTEER User Guide (U.S. EPA, 2015). Previously, EPA adjusted the default loss fraction values based on rounding the PEI study results or due to policy decisions. EPA used a combination of the PEI study results (PEI Associates, 1988) and the *ChemSTEER User Guide* (U.S. EPA, 2015) default loss fraction values to develop probability distributions for various container sizes.

Specifically, EPA paired the data from the PEI study (PEI Associates, 1988) such that the residuals data for emptying drums by pouring was aligned with the default central tendency and high-end values from the EPA/OPPT Small Container Residual Model, and the residuals data for emptying drums by pumping was aligned with the default central tendency and high-end values from the EPA/OPPT Drum Residual Model. EPA applied the EPA/OPPT Small Container Residual Model to containers with capacities less than 20 gallons, and the EPA/OPPT Drum Residual Model to containers with capacities between 20–100 gallons (U.S. EPA, 2015).

For unloading drums via pouring, the PEI study experiments showed average container residuals in the range of 0.03–0.79 percent with a total average of 0.32 percent (PEI Associates, 1988). The EPA/OPPT Small Container Residual Model recommends a default central tendency loss fraction of 0.3 percent and a high-end loss fraction of 0.6 percent (U.S. EPA, 2015). For unloading drums by pumping, the PEI study experiments showed average container residuals in the range of 1.7–4.7 percent with a total average of 2.6 percent (PEI Associates, 1988).

The EPA/OPPT Drum Residual Model from the ChemSTEER User Guide recommends a default central tendency loss fraction of 2.5 percent and a high-end loss fraction of 3.0 percent (U.S. EPA, 2015). The underlying distribution of the loss fraction parameter for small containers or drums is not known; therefore, EPA assigned a triangular distribution defined by the estimated lower bound, upper bound, and mode of the parameter values. EPA assigned the mode and upper bound values for the loss fraction triangular distributions using the central tendency and high-end values from the respective ChemSTEER model. EPA assigned the lower-bound values for the triangular distributions using the minimum average percent residual measured in the PEI study for the respective drum emptying technique (pouring or pumping) (PEI Associates, 1988).

E.2.9 Diameters of Opening

The ChemSTEER User Guide (U.S. EPA, 2015) indicates diameters for the openings for various vessels that may hold liquids in order to calculate vapor generation rates during different activities. In the simulation developed for the Import – Repackaging OES based on the *Emission Scenario Document for Transport and Storage of Chemicals* (OECD, 2009c), EPA used the default diameters of vessels from the ChemSTEER User Guide (U.S. EPA, 2015) for container cleaning.

For container cleaning activities, ChemSTEER User Guide indicates a single default value of 5.08 cm (U.S. EPA, 2015). Therefore, EPA could not develop a distribution of values for this parameter and used the single value 5.08 cm from the ChemSTEER User Guide (U.S. EPA, 2015).

E.2.10 Saturation Factor

The 1991 CEB Manual indicated that during splash filling, the saturation concentration was reached or exceeded by misting with a maximum saturation factor of 1.45 (U.S. EPA, 1991). The 1991 CEB Manual also indicated that saturation concentration for bottom filling was expected to be about 0.5 (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the lower bound, upper bound, and mode of the parameter. Because a mode was not provided for this parameter, EPA assigned a mode value of 0.5 for bottom filling as bottom filling minimizes volatilization. This value also corresponds to the typical value provided in the ChemSTEER User Guide for the EPA/OAQPS AP-42 Loading Model (U.S. EPA, 2015).

E.2.11 Container Size

EPA assumed facilities receive TCEP in drums based on a prior triphosphates chemical assessment report from Australia's NICNAS stating that TCEP is imported in 200 liter drums (NICNAS, 2001). The ChemSTEER User Guide (U.S. EPA, 2015) recommends a range of 20 to less than 100 gallons for the volume capacity of drums modeled in container-related activities, and the *Emission Scenario Document for Transport and Storage of Chemicals* (OECD, 2009c) suggests nearly 80 percent of all steel drums in the United States have a capacity of 55 gallons. The underlying distribution import drum sizes is not known; therefore, EPA assigned a lower bound of 20 gallons, an upper bound of 100 gallons, and a mode of 55 gallons for the import container volume distribution.

The ChemSTEER User Guide (U.S. EPA, 2015) recommends a range of 5 to less than 20 gallons for the volume capacity of small containers modeled in container-related activities with 5 gallons as the default volume size. Therefore, EPA assigned a lower bound of 5 gallons, an upper bound of 20 gallons, and a mode of 5 gallons for the small container volume distribution.

E.2.12 Container Fill Rate

The ChemSTEER User Guide (U.S. EPA, 2015) provides a typical fill rate of 20 containers per hour for containers with 20–100 gallons of liquid and a typical fill rate of 60 containers per hour for containers with less than 20 gallons of liquid.

E.2.13 Ventilation Rate

The 1991 CEB Manual indicates general ventilation rates in industry range from 500 to 10,000 ft^3/min, with a typical value of 3,000 ft^3/min (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on an estimated lower bound, upper bound, and mode of the parameter. EPA assumed the lower and upper bound using the industry range of 500–10,000 ft^3/min and the mode using the 3,000 ft^3/min typical value (U.S. EPA, 1991).

E.2.14 Mixing Factor

The 1991 CEB Manual indicates mixing factors may range from 0.1 to 1, with 1 representing ideal mixing (U.S. EPA, 1991). The 1991 CEB Manual references the *1988 ACGIH Ventilation Handbook*, which suggests the following factors and descriptions: 0.67–1 for best mixing; 0.5–0.67 for good mixing; 0.2–0.5 for fair mixing; and 0.1–0.2 for poor mixing (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the defined lower and upper bound and estimated mode of the parameter. The mode for this distribution was not provided; therefore, EPA assigned a mode value of 0.5 based on the typical value provided in the ChemSTEER User Guide for the EPA/OPPT Mass Balance Inhalation Model (U.S. EPA, 2015).

E.3 Incorporation into Paints and Coatings Model Approach and Parameters

Appendix E.3 presents the modeling approach and equations used to estimate environmental releases and occupational exposures for TCEP during the Incorporation into Paints and Coatings OES. EPA assessed two independent scenarios based on the type of TCEP-containing coating products, including: 1) incorporation of TCEP into 2-part reactive formulations using the *Emission Scenario Document for Adhesive Formulations* (OECD, 2009a) (hereinafter referred to as the "ESD for Adhesive Formulations"); and 2) 1-part formulations using the *Draft Formulation of Waterborne Coatings – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2014a) (hereinafter referred to as the "GS for Formulation of Waterborne Coatings").

TCEP-containing resin-based paints and coatings are similar to reactive adhesive end uses based on available TDSs. The resin-based coatings react upon application to the respective substrate to protect surfaces (FCC, 2016a). This is similar to the description of reactive adhesives described in the ESD for Adhesive Formulations as "unreacted prepolymers, oligomers, or monomers that react to form a crosslinked polymer at the point of application" (OECD, 2009a). Therefore, EPA assessed releases and exposures for these products following the approach in the ESD for Adhesive Formulation (OECD, 2009a). EPA used the information and data for a "Sealed Process (Organic Solvent-Based, Reactive Adhesives)" from the ESD for Adhesive Formulations (OECD, 2009a) to inform the release and exposure assessment for resin-based paints and coatings. EPA used the GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) to assess releases and exposures for any 1-part coating product as determined by the product.

Both the ESD for Adhesive Formulations (OECD, 2009a) and GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) identify release and exposure points that are generally the same to one another. Therefore, most of the release and exposure points are the same for 2-part reactive and 1-part coatings, with some distinctions specific to the type of coating. These distinctions are noted below.

Based on the ESD and GS, EPA identified the following release points:

- Release Point 1: Transfer operation losses to air from unloading the coating component;
- Release Point 2: Dust generation from transfer operations released to air, or collected and released to water, incineration, or landfill (not assessed);
- Release Point 3: Coating component container residue released to water, incineration, or landfill (assessed release to wastewater);
- Release Point 4: Open surface losses to air during container cleaning;
- Release Point 5: Vented losses to air during dispersion and blending/process operations;
- Release Point 6: Product sampling wastes disposed to water, incineration, or landfill (not assessed);
- Release Point 7: Open surface losses to air during product sampling;
- Release Point 8: Equipment cleaning releases to water, incineration, or landfill (assessed release to waste disposal for 2-part reactive coatings, and water for 1-part coatings);
- Release Point 9: Open surface losses to air during equipment cleaning;
- Release Point 10: Filter waste releases to incineration or landfill during filter media changeout (not assessed for resin-based formulations);
- Release Point 11: Open surface losses to air during filter media changeout (not assessed for resin-based coatings);
- Release Point 12: Transfer operation losses to air from packaging coating into transport containers; and
- Release Point 13: Off-specification and other waste coatings to water, incineration, or landfill (assessed release to waste disposal for 2-part reactive coatings, and water for 1-part coatings).

Based on the ESD and GS, EPA also identified the following inhalation exposure points:

- Exposure Point A: Transfer operation exposures from unloading the coating component;
- Exposure Point B: Container cleaning exposures after unloading the coating component;
- Exposure Point C: Open surface exposures during product sampling;
- Exposure Point D: Exposures from equipment/container cleaning;
- Exposure Point E: Exposures from filter media changeout (not assessed for resin-based formulations); and
- Exposure Point F: Transfer operation exposures from packaging coating into transport containers.

Environmental releases and occupational exposures for TCEP during Incorporation into Paints and Coatings are a function of TCEP's physical properties, container size, mass fractions, and other model parameters. While some parameters are fixed, some model parameters are expected to vary. As described in Section 3.2, EPA used a Monte Carlo simulation to capture variability in the following model input parameters: ventilation rate, mixing factor, air speed, saturation factor, container sizes, opening diameters (*e.g.*, mixing tanks, containers), batch size, time per batch, TCEP product concentration, product density, working years, and operating hours. EPA used the outputs from a Monte Carlo simulation with 100,000 iterations and the Latin Hypercube sampling method in @RISK to calculate release amounts and exposure concentrations for this OES.

E.3.1 Model Equations

Table_Apx E-4 provides the models and associated variables used to calculate environmental releases for each release point within each iteration of the Monte Carlo simulation. Additional equations not based on generic models are provided below the table. EPA used these environmental releases to develop a distribution of release outputs for the incorporation into paints and coatings OES. The variables used to calculate each of the following values include deterministic or variable input parameters, known constants, physical properties, TCEP concentrations, conversion factors, and other parameters. The values for these variables are provided in Appendices E.3.2 and E.3.3. The Monte Carlo simulation calculated the total TCEP release (by environmental media) across all release points during each iteration of the simulation. EPA then selected 50th and 95th percentile values to estimate the central tendency and high-end releases for each media, respectively.

Table_Apx E-4. Models and Variables Applied for Release Points in the Incorporation into Paints and Coatings OES

Release Point	Model(s) Applied	Variables Used
Release Point 1: Transfer operation losses to air from unloading the coating component	EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP_import}; VP; $F_{saturation\_unloading}$; MW_{TCEP}; V_{import_cont}; R; T; $RATE_{fill\_drum}$ Operating Time: N_{cont_yr}; $RATE_{fill\_drum}$
Release Point 2: Dust generation from transfer operations released to air, or collected and released to water, incineration, or landfill (not assessed)	Not assessed; release point not applicable for liquid formulations	Not applicable
Release Point 3: Coating component container residue released to water, incineration, or landfill (assessed release to wastewater)	EPA/OPPT Drum Residual Model (Appendix E.1)	PV; $F_{loss\_cont-residue}$
Release Point 4: Open Surface losses to air during container cleaning	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_import}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_cont-cleaning}$; T; P Operating Time: N_{cont_yr}; $RATE_{fill\_drum}$

Release Point	Model(s) Applied	Variables Used
Release Point 5: Vented losses to air during dispersion and blending/process operations	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_blending}$; T; P Operating Time: OH_{batch}; N_{batch_yr}
Release Point 6: Product sampling wastes disposed to water, incineration, or landfill (not assessed)	Not assessed; release expected to occur but not quantified in ESD	Not applicable
Release Point 7: Open surface losses to air during product sampling	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_sampling}$; T; P Operating Time: OH_{RP7}; N_{batch_yr}
Release Point 8: Equipment cleaning releases to water, incineration, or landfill (assessed release to waste disposal)	EPA/OPPT Multiple Process Vessel Residual Model (Appendix E.1)	PV; $F_{loss\_equip-cleaning}$
Release Point 9: Open surface losses to air during equipment cleaning	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_equip-cleaning}$; T; P Operating Time: OH_{RP9}; N_{batch_yr}
Release Point 10: Filter waste releases to incineration or landfill during filter media changeout (not assessed for resin-based formulations)	See Equation E-11	PV; F_{loss_filter}
Release Point 11: Open surface losses to air during filter media changeout (not assessed for resin-based formulations)	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_filter-changeout}$; T; P Operating Time: OH_{RP11}; N_{batch_yr}
Release Point 12: Transfer operation losses to air from packaging coatings into transport containers	EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; VP; $F_{saturation\_loading}$; MW_{TCEP}; V_{prod_cont}; R; T; $RATE_{fill\_drum}$; $RATE_{fill\_small}$ Operating Time: $N_{prodcont\_yr}$; $RATE_{fill\_drum}$; $RATE_{fill\_small}$

Release Point	Model(s) Applied	Variables Used
Release Point 13: Off-specification and other waste coatings to water, incineration, or landfill (assessed release to waste disposal)	See Equation E-12	PV; $F_{loss\_off-spec}$

Appendix E.5 provides equations and discussion for release point operating times used to calculate releases to air as provided in Equation E-4.

Release Point 10 annual release (filter waste releases during filter media changeout) is calculated using Equation E-11.

Equation E-11

$$Release\_Year_{RP10} = PV \times F_{loss\_filter}$$

Where:

$Release\_Year_{RP10}$ = TCEP released for Release Point 10 (kg/site-yr)
PV = Product volume throughput of TCEP (kg/site-yr)
F_{loss_filter} = Loss fraction for filter changeout (unitless)

Release Point 13 annual release (off-specification and other waste) is calculated using Equation E-12.

Equation E-12

$$Release\_Year_{RP13} = PV \times F_{loss\_off-spec}$$

Where:

$Release\_Year_{RP13}$ = TCEP released for Release Point 13 (kg/site-yr)
PV = Product volume throughput of TCEP (kg/site-yr)
$F_{loss\_off-spec}$ = Loss fraction for off-specification wastes (unitless)

Table_Apx E-5 provides the models and associated variables used to calculate occupational inhalation exposure concentrations for each exposure point within each iteration of the Monte Carlo simulation. EPA used these occupational exposure concentrations in order to develop a distribution of exposure outputs for the incorporation into paints and coatings OES. EPA assumed that the same worker performed each exposure activity resulting in a total exposure duration of up to eight hours per day. The variables used to calculate each of the following exposure concentrations and durations include deterministic or variable input parameters, known constants, physical properties, TCEP concentrations, conversion factors, and other parameters. The values for these variables are provided in Appendices E.3.2 and E.3.3. The Monte Carlo simulation calculated an 8-hr TWA exposure concentration for each iteration using the exposure concentration and duration associated with each activity and assuming exposures outside the exposure activities were zero. EPA then selected 50th and 95th percentile values to estimate the central tendency and high-end exposure concentrations, respectively.

Table_Apx E-5. Models and Variables Applied for Exposure Points in the Incorporation into Paints and Coatings OES

Exposure Point	Model(s) Applied	Variables Used
Exposure Point A: Transfer operation exposures from unloading the coating component.	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP_import}; VP; $F_{saturation\_unloading}$; MW_{TCEP}; V_{import_cont}; R; T; $RATE_{fill\_drum}$; Q; k; Vm Exposure Duration: N_{cont_yr}; $RATE_{fill\_drum}$; OD
Exposure Point B: Container cleaning exposures after unloading the resin component.	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_import}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_cont-cleaning}$; T; P; Q; k; Vm Exposure Duration: N_{cont_yr}; $RATE_{fill\_drum}$; OD
Exposure Point C: Open surface exposures during product sampling.	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_sampling}$; T; P; Q; k; Vm Exposure Duration: h_C
Exposure Point D: Exposures from equipment/container cleaning.	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_equip-cleaning}$; T; P; Q; k; Vm Operating Time: h_D
Exposure Point E: Exposure from filter media changeout (not assessed for resin-based formulations)	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_filter-changeout}$; T; P; Q; k; Vm Operating Time: h_E
Exposure Point F: Transfer operation exposures from packaging resin into transport containers.	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; VP; $F_{saturation\_loading}$; MW_{TCEP}; V_{prod_cont}; R; T; $RATE_{fill\_drum}$; $RATE_{fill\_small}$; Q; k; Vm Exposure Duration: $N_{prodcont\_yr}$; $RATE_{fill\_drum}$; $RATE_{fill\_small}$; OD

Appendix E.5 provides equations and discussion for exposure durations used for each exposure activity. Note that the number of exposure days is set equal to the number of operating days per year up to a maximum of 250 days per year. If the number of operating days is greater than 250 days per year, EPA assumed that a single worker would not work more than 250 day per year such that the maximum exposure days per year was still 250.

E.3.2 Model Input Parameters

Table_Apx E-6 summarizes the model parameters and their values for the Incorporation into Paints and Coatings Monte Carlo simulation. Additional explanations of EPA's selection of the distributions for each parameter are provided in the following subsections.

Table_Apx E-6. Summary of Parameter Values and Distributions Used in the Incorporation into Paints and Coatings Models

Input Parameter	Symbol	Unit	Deterministic Values	Uncertainty Analysis Distribution Parameters				Rationale/Basis
			Value	Lower Bound	Upper Bound	Mode	Distribution Type	
Air speed	$RATE_{air\_speed}$	cm/s	10	1.3	202.2	—	Lognormal	See Appendix E.3.6
Loss fraction for containers	$F_{loss\_cont\text{-}residue}$	kg/kg	0.025	0.017	0.03	0.025	Triangular	See Appendix E.3.7
Product container volume	V_{prod_cont}	gal/container	5	0.25	100	5	Triangular	See Appendix E.3.10
Import container volume	V_{import_cont}	gal/container	55	20	100	55	Triangular	See Appendix E.3.10
Saturation factor unloading	$F_{saturation\_unloading}$	unitless	0.5	0.5	1.45	0.5	Triangular	See Appendix E.3.9
Saturation factor loading	$F_{saturation\_loading}$	unitless	0.5	0.5	1.45	0.5	Triangular	See Appendix E.3.9
Loss fraction for equipment cleaning	$F_{loss\_equipment}$	kg/kg	0.02	0.013	0.03	0.02	Triangular	See Appendix E.3.14
Loss fraction for filter changeout	F_{loss_filter}	kg/kg	0.01	0	0.02	—	Uniform	See Appendix E.3.16
Off-specification loss fraction	$F_{loss\_off\text{-}spec}$	kg/kg	0.01025	0.0085	0.012	—	Uniform	See Appendix E.3.15
Diameter of opening for blending/process operations	$D_{opening\_blending}$	cm	10	10	Calculated	10	Triangular	See Appendix E.3.8
Diameter of opening for equipment cleaning	$D_{opening\_equip\text{-}cleaning}$	cm	92	92	Calculated	92	Triangular	See Appendix E.3.8
Diameter of opening for sampling	$D_{opening\_sampling}$	cm	2.5	2.5	10	2.5	Triangular	See Appendix E.3.8
Batch volume	V_{batch}	gal/batch	1000	1000	5000	1000	Triangular	See Appendix E.3.11
			1000	300	5000	1000		
Hours per batch	OH_{batch}	hr/batch	7	7	72	7	Triangular	See Appendix E.3.12
			8	8	24	8		

Input Parameter	Symbol	Unit	Deterministic Values	Uncertainty Analysis Distribution Parameters				Rationale/Basis
			Value	Lower Bound	Upper Bound	Mode	Distribution Type	
Number of sites	N_s	sites	1	—	—	—	—	"What-if" scenario input
Production volume assessed	PV_lbs	lbs/yr	2,500 or 25,000	—	—	—	—	"What-if" scenario input
Production volume	PV	kg/yr	1,134 or 11,340	—	—	—	—	PV input converted to kilograms
Import concentration	F_{TCEP_import}	kg/kg	1.0	—	—	—	—	Assumed pure TCEP imported for Import – Repackaging
TCEP density	ρ_{TCEP}	kg/m^3	1,390	—	—	—	—	Physical property
Temperature	T	K	298	—	—	—	—	Process parameter
Pressure	P	torr	760	—	—	—	—	Process parameter
Gas constant	R	L-torr/mol-K	62.36367	—	—	—	—	Universal constant
TCEP vapor pressure	VP	torr	0.0613	—	—	—	—	Physical property
TCEP molecular weight	MW_{TCEP}	g/mol	285.49	—	—	—	—	Physical property
Fill rate of drum	$RATE_{fill\_drum}$	containers/hr	20	—	—	—	—	See Appendix E.3.13
Fill rate of small container	$RATE_{fill\_smallcont}$	containers/hr	60	—	—	—	—	See Appendix E.3.13
Operating hours for product sampling	OH_{RP7}	hr/batch	1	—	—	—	—	See Appendix E.3.5
Operating hours for equipment cleaning	OH_{RP9}	hr/batch	4	—	—	—	—	See Appendix E.3.5
Operating hours for filter changeout	OH_{RP11}	hr/batch	0.25	—	—	—	—	See Appendix E.3.5
Diameter of opening for filter	$D_{opening\_filter-changeout}$	cm	15	—	—	—	—	See Appendix E.3.8
Diameter of opening for container cleaning	$D_{opening\_cont-cleaning}$	cm	5.08	—	—	—	—	See Appendix E.3.8

Input Parameter	Symbol	Unit	Deterministic Values	Uncertainty Analysis Distribution Parameters				Rationale/Basis
			Value	Lower Bound	Upper Bound	Mode	Distribution Type	
Product density	$\rho_{product}$	kg/m^3	—	Multiple distributions depending on product data			Uniform	See Appendix E.3.17
Product concentration	F_{TCEP_prod}	kg/kg	—	Multiple distributions depending on product data			Uniform	
Ventilation rate	Q	ft^3/min	3,000	500	10,000	3,000	Triangular	See Appendix E.3.19
Mixing factor	k	unitless	0.5	0.1	1	0.5	Triangular	See Appendix E.3.20

E.3.3 Throughput Parameters

The facility production rate is calculated as an input value to be used in the model equations during each iteration. The facility production rate is calculated using Equation E-13.

Equation E-13

$$Q_{product} = \frac{PV}{F_{TCEP\_prod} \times N_s}$$

Where:

$Q_{product}$ = Facility production rate (kg/site-yr)
PV = Production volume (kg/yr)
F_{TCEP_prod} = Product concentration (kg/kg)
N_s = Number of sites (sites)

E.3.4 Operating Days per Year

The number of operating days was set to a maximum of 365 days per year, consistent with the maximum number of days in a typical year. If the calculated value of operating days exceeds 365 days in a given iteration, then the number is set to 365 days per year. See Equation E-14 for calculating operating days per year:

Equation E-14

$$OD = \frac{Q_{product}}{m_{batch}} \times \frac{OH_{batch}}{24\,\frac{hr}{day}}$$

Where:

OD = Operating days (days/site-yr)
$Q_{product}$ = Facility production rate (kg/site-yr)
m_{batch} = Batch size (kg/batch)
OH_{batch} = Operating hours per batch (hr/batch)

E.3.5 Operating Hours and Exposure Durations

EPA estimated operating hours or hours of duration using data provided from the ESD for Adhesive Formulation (OECD, 2009a), GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) and/or through calculation from other parameters. Worker activities with operating hours and hours of duration provided from the ESD for Adhesive Formulation (OECD, 2009a) and GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) include product sampling, equipment cleaning, and filter changeout.

For product sampling, both the ESD for Adhesive Formulation (OECD, 2009a) and GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) indicates a single value of one hour per batch based on the 1991 CEB Manual (U.S. EPA, 1991). Therefore, the total duration of sampling activities is calculated using Equation E-15.

Equation E-15

$$Time_{RP7} = \frac{OH_{RP7} \times N_{batch_{yr}}}{OD}$$

Where:

$Time_{RP7}$ = Operating time for Release Point 7 (hrs/site-day)
OH_{RP7} = Operating hours per sampling (hrs/sample)
N_{batch_yr} = Annual number of batches (batches/site-yr)
OD = Operating days (days/site-yr)

For equipment cleaning of 1-part coatings, the GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) provides an estimate of four hours per batch based on the value for cleaning multiple vessels from the ChemSTEER User Guide (U.S. EPA, 2015).

For equipment cleaning of resin coatings, the ESD for Adhesive Formulation (OECD, 2009a) provides an estimate of four hours per batch based on the value for cleaning multiple vessels from the ChemSTEER User Guide (U.S. EPA, 2015). The ESD for Adhesive Formulation (OECD, 2009a) also states that a case study conducted by the Pollution Prevention Assistance Division indicated a range of equipment cleaning times between one and three hours per batch. The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on a lower bound, upper bound, and mode for equipment cleaning operating hours. EPA assigned the lower bound as one hour based on the lower end cleaning time observed in the case study (OECD, 2009a) and the upper bound as four hours based on the ChemSTEER User Guide (U.S. EPA, 2015), which was the default value for this worker activity. For the mode, EPA assigned four hours because, in the absence of site-specific information, the ESD for Adhesive Formulation (OECD, 2009a) recommends using four hours. EPA calculated the equipment cleaning operating hours using Equation E-16.

Equation E-16

$$Time_{RP9} = \frac{OH_{RP9} \times N_{batch_{yr}}}{OD}$$

Where:

$Time_{RP9}$ = Operating time for Release Point 9 (hrs/site-day)
OH_{RP9} = Operating hours per equipment cleaning (hrs/cleaning)
N_{batch_yr} = Annual number of batches (batches/site-yr)
OD = Operating days (days/site-yr)

The GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) estimates a value of 0.25 hours per batch for filter media changeout based on engineering judgement. The operating time per day is further calculated based on the number of batches per year using Equation E-17.

Equation E-17

$$Time_{RP11} = \frac{OH_{RP11} \times N_{batch_{yr}}}{OD}$$

Where:

$Time_{RP11}$ = Operating time for Release Point 11 (hrs/site-day)
OH_{RP11} = Operating hours per filter changeout (hrs/batch)
N_{batch_yr} = Annual number of batches (batches/site-yr)
OD = Operating days (days/site-yr)

The operating hours for Release Points 1 and 4 are calculated based on the number of containers received at the site and the fill rate using Equation E-18.

Equation E-18

$$Time_{RP1/RP4} = \frac{N_{cont\_yr}}{RATE_{fill\_drum} \times OD}$$

Where:

$Time_{RP1/RP4}$ = Operating time for Release Points 1 and 4 (hrs/site-day)
$RATE_{fill\_drum}$ = Fill rate of drum (containers/hr)
N_{cont_yr} = Annual number of import containers (containers/site-yr)
OD = Operating days (days/site-yr)

The operating hours for Release Point 5 are calculated based on the operating hours per batch and the number of batches per year using Equation E-19.

Equation E-19

$$Time_{RP5} = \frac{OH_{batch} \times N_{batch\_yr}}{OD}$$

Where:

$Time_{RP5}$ = Operating time for Release Point 5 (hrs/site-day)
OH_{batch} = Operating hours per batch (hrs/batch)
N_{batch_yr} = Annual number of batches (batches/site-yr)
OD = Operating days (days/site-yr)

The operating hours for Release Point 12 are calculated based on the number of product containers filled at the site and the fill rate using Equation E-20.

Equation E-20

$$Time_{RP12} = \frac{N_{prodcont\_yr}}{RATE_{fill\_drum/small} \times OD}$$

Where:

$Time_{RP12}$ = Operating time for Release Point 12 (hrs/site-day)
$N_{prodcont\_yr}$ = Annual number of product containers (containers/site-yr)
$RATE_{fill\_drum/small}$ = Fill rate of container, dependent on volume (containers/hr)
OD = Operating days (days/site-yr)

Exposure durations for Exposure Points A and B are calculated based on fill rate for the containers holding TCEP. The fill rate for drums used in this equation uses the deterministic value described in Appendix E.3.13 when the total calculated exposure duration across exposure activities is less than or equal to eight hours per day. However, if using this fill rate results in the total exposure duration across all the exposure points being greater than eight hours, the model adjusts the fill rate to give an exposure duration of exposure point A and B that results in a total exposure duration of eight hours. The exposure durations are calculated using Equation E-21.

Equation E-21

$$h_{A/B} = \frac{N_{cont\_yr}}{RATE_{fill\_drum} \times OD}$$

Where:

$h_{A/B}$ = Exposure durations for Exposure Points A and B (hrs/day)
N_{cont_yr} = Annual number of import containers (containers/site-yr)
$RATE_{fill\_drum}$ = Fill rate of drum (containers/hr)
OD = Operating days (days/site-yr)

The exposure duration for Exposure Point F is calculated based on number of product containers filled per year, or on remaining work-shift time after accounting for other exposure points. Since EPA assumes a single worker with total maximum exposure duration of eight hours per working day, the 8-hour TWA is estimated using the exposure activities with fixed durations or those with the largest contributions to total exposure. The fill rate for product containers used in this equation for each iteration may be either the default fill rate for drums (if product container ≥ 20 gal) or the default fill rate for small containers (if product container < 20 gal). The exposure duration is calculated using Equation E-22.

Equation E-22

$$h_F = \begin{cases} \dfrac{N_{prodcont\_yr}}{RATE_{fill\_drum/small} \times OD}, & 8 \geq \left[h_A + h_B + h_C + h_D + h_E + \dfrac{N_{prodcont\_yr}}{RATE_{fill\_drum/small} \times OD} \right] \\ 8 - (h_A + h_B + h_C + h_D + h_E), & 8 < \left[h_A + h_B + h_C + h_D + h_E + \dfrac{N_{prodcont\_yr}}{RATE_{fill\_drum/small} \times OD} \right] \end{cases}$$

Where:

h_n = Exposure duration for Exposure Point "n" (hrs/day)
$N_{prodcont\_yr}$ = Annual number of product containers (containers/site-yr)
$RATE_{fill\_drum/small}$ = Fill rate of container, dependent on volume (containers/hr)
OD = Operating days (days/site-yr)

E.3.6 Air Speed

Baldwin and Maynard (1998) measured indoor air speeds across a variety of occupational settings in the United Kingdom. A total of 55 work areas were surveyed across a variety of workplaces. EPA analyzed the air speed data from Baldwin and Maynard (1998) and categorized the air speed surveys into settings representative of industrial facilities and representative of commercial facilities. EPA fit separate distributions for these industrial and commercial settings and used the industrial distribution for this OES.

EPA fit a lognormal distribution for the data set as consistent with the authors' observations that the air speed measurements within a surveyed location were lognormally distributed and the population of the mean air speeds among all surveys were lognormally distributed (Baldwin and Maynard, 1998). Since lognormal distributions are bound by zero and positive infinity, EPA truncated the distribution at the largest observed value among all of the survey mean air speeds.

EPA fit the air speed surveys representative of industrial facilities to a lognormal distribution with the following parameter values: mean of 22.414 cm/s and standard deviation of 19.958 cm/s. In the model, the lognormal distribution is truncated at a minimum allowed value of 1.3 cm/s and a maximum allowed value of 202.2 cm/s (largest surveyed mean air speed observed in Baldwin and Maynard (1998)) to prevent the model from sampling values that approach infinity or are otherwise unrealistically small or large (Baldwin and Maynard, 1998).

Baldwin and Maynard (1998) only presented the mean air speed of each survey. The authors did not present the individual measurements within each survey. Therefore, these distributions represent a distribution of mean air speeds and not a distribution of spatially variable air speeds within a single workplace setting. However, a mean air speed (averaged over a work area) is the required input for the model. EPA converted the units to ft/min prior to use within the model equations.

E.3.7 Container Residue Loss Fraction

EPA previously contracted PEI to conduct a study to provide estimates of potential chemical releases during cleaning of process equipment and shipping containers (PEI Associates, 1988). The study used both a literature review of cleaning practices and release data as well as a pilot-scale experiment to determine the amount of residual material left in vessels. The data from literature and pilot-scale experiments addressed different conditions for the emptying of containers and tanks, including various bulk liquid materials, different container constructions (*e.g.*, lined steel drums or plastic drums), and either a pump or pour/gravity-drain method for emptying. EPA reviewed the pilot-scale data from PEI and determined a range and average percentage of residual material remaining in vessels following emptying from drums by either pumping or pouring as well as tanks by gravity-drain (PEI Associates, 1988).

EPA previously used the study results to generate default central tendency and high end-loss fraction values for the residual models (*e.g.*, EPA/OPPT Small Container Residual Model, EPA/OPPT Drum Residual Model) provided in the ChemSTEER User Guide (U.S. EPA, 2015). Previously, EPA adjusted the default loss fraction values based on rounding the PEI study results or due to policy decisions. EPA used a combination of the PEI study results (PEI Associates, 1988) and the *ChemSTEER User Guide* (U.S. EPA, 2015) default loss fraction values to develop probability distributions for various container sizes.

Specifically, EPA paired the data from the PEI study (PEI Associates, 1988) such that the residuals data for emptying drums by pouring was aligned with the default central tendency and high-end values from the EPA/OPPT Small Container Residual Model, and the residuals data for emptying drums by pumping was aligned with the default central tendency and high-end values from the EPA/OPPT Drum Residual Model. EPA applied the EPA/OPPT Small Container Residual Model to containers with capacities less than 20 gallons, and the EPA/OPPT Drum Residual Model to containers with capacities between 20–100 gallons (U.S. EPA, 2015).

For unloading drums via pouring, the PEI study experiments showed average container residuals in the range of 0.03–0.79 percent with a total average of 0.32 percent (PEI Associates, 1988). The EPA/OPPT Small Container Residual Model recommends a default central tendency loss fraction of 0.3 percent and a high-end loss fraction of 0.6 percent (U.S. EPA, 2015). For unloading drums by pumping, the PEI study experiments showed average container residuals in the range of 1.7–4.7 percent with a total average of 2.6 percent (PEI Associates, 1988).

The EPA/OPPT Drum Residual Model from the ChemSTEER User Guide recommends a default central tendency loss fraction of 2.5 percent and a high-end loss fraction of 3.0 percent (U.S. EPA, 2015). The underlying distribution of the loss fraction parameter for small containers or drums is not known; therefore, EPA assigned a triangular distribution defined by the estimated lower bound, upper bound, and mode of the parameter values. EPA assigned the mode and upper bound values for the loss fraction triangular distributions using the central tendency and high-end values from the respective ChemSTEER model. EPA assigned the lower-bound values for the triangular distributions using the minimum average percent residual measured in the PEI study for the respective drum emptying technique (pouring or pumping) (PEI Associates, 1988).

E.3.8 Diameters of Opening

The ChemSTEER User Guide (U.S. EPA, 2015) indicates diameters for the openings for various vessels that may hold liquids in order to calculate vapor generation rates during different activities. For container cleaning activities, ChemSTEER User Guide indicates a single default value of 5.08 cm (U.S. EPA, 2015).

For blending operations, the ESD for Adhesive Formulation (OECD, 2009a) and GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) assumes a closed vessel with a 4-inch diameter process vent, corresponding to 10 cm in diameter. In addition, EPA considered the potential for open process vessels used for blending as mentioned in both the ESD for Adhesive Formulation (OECD, 2009a) and GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a), with diameters of the open vessel calculated based on the batch volume for the simulation iteration and the assumption in the ESD and GS of a one-to-one height to diameter ratio for the process vessel. The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution defined by an estimated lower bound, upper bound, and mode of the parameter. EPA assigned the value of 10 cm for both the lower bound and mode of the triangular distribution as the recommended value by the ESD for Adhesive Formulation (OECD, 2009a) and GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a). For the upper bound value of the triangular distribution, EPA assigned an equation calculating the diameter of an open process vessel with a one-to-one height to diameter ratio and fixed volume from the batch volume input parameter (Equation E-23).

Equation E-23

$$D_{blending\_max} = \left[\frac{4 \times V_{batch} * 3{,}785.41\,\frac{cm^3}{gal}}{\pi}\right]^{1/3}$$

For equipment cleaning operations, the ChemSTEER User Guide indicates a single default value of 92 cm (U.S. EPA, 2015). EPA also considered open process vessels during cleaning, with diameters of the open vessel calculated based on the batch volume for the simulation iteration and an assumption of a one-to-one height to diameter ratio for the process vessel. The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the estimated lower bound, upper bound, and mode of the parameter. EPA assigned the value of 92 cm for both the lower bound and mode of the triangular distribution as the recommended value by the ChemSTEER User Guide (U.S. EPA, 2015). For the upper bound value of the triangular distribution, EPA assigned an equation calculating the diameter of an open process vessel with a one-to-one height to diameter ratio and fixed volume from the batch volume input parameter; this is the same equation (Equation E-23) used for the open process vessel diameter during blending.

For sampling liquid product, sampling liquid raw material, or general liquid sampling, the ChemSTEER User Guide indicates that the typical diameter of opening for vaporization of the liquid is 2.5 cm (U.S. EPA, 2015). Additionally, the ChemSTEER User Guide provides 10 cm as a high-end value for the diameter of opening during sampling (U.S. EPA, 2015). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the estimated lower bound, upper bound, and mode of the parameter. EPA assigned the value of 2.5 cm as a lower bound for the parameter and 10 cm as the upper bound based on the values provided in the ChemSTEER User Guide (U.S. EPA, 2015). EPA also assigned 2.5 cm as the mode diameter value for sampling liquids based on the typical value described in ChemSTEER User Guide (U.S. EPA, 2015).

E.3.9 Saturation Factor

The 1991 CEB Manual indicated that during splash filling, the saturation concentration was reached or exceeded by misting with a maximum saturation factor of 1.45 (U.S. EPA, 1991). The 1991 CEB Manual also indicated that saturation concentration for bottom filling was expected to be about 0.5 (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the lower bound, upper bound, and mode of the parameter. Because a mode was not provided for this parameter, EPA assigned a mode value of 0.5 for bottom filling as bottom filling minimizes volatilization. This value also corresponds to the typical value provided in the ChemSTEER User Guide for the EPA/OAQPS AP-42 Loading Model (U.S. EPA, 2015).

E.3.10 Container Size

EPA assumed facilities receive TCEP in drums based on a prior triphosphates chemical assessment report from Australia's NICNAS stating that TCEP is imported in 200 liter drums (NICNAS, 2001). The ChemSTEER User Guide (U.S. EPA, 2015) recommends a range of 20 to less than 100 gallons for the volume capacity of drums modeled in container-related activities, and the ESD for Adhesive Formulation (OECD, 2009a) and GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) suggests 55 gallons for an unknown container size. Therefore, EPA assigned a lower bound of 20 gallons, an upper bound of 100 gallons, and a mode of 55 gallons for the import container volume distribution.

For product containers, both the ESD for Adhesive Formulation and GS for Formulation of Waterborne Coatings recommends a range of 20 to less than 100 gallons with a default value of 55 gallons for unknown container sizes (OECD, 2009a; U.S. EPA, 2014a). EPA reviewed safety and technical data sheets for the identified paint and coating products containing TCEP to develop the minimum, maximum, and mode product container volume. Table_Apx E-7 specifies container sizes for the final coating product formulations identified in data sheets.

Table_Apx E-7. Product Container Sizes for TCEP-containing Coatings

Product	Container Size(s) Information for Product	Approximate Container Size(s) (gallons)	Source Reference
1-part Coatings			
Flame Control No. 40-40A	Container sizes are 1- and 5-gallon containers with shipping weights of 4- to 5-gallons	1–5	FCC (2016a)
Flame Control No. 5050	Container sizes are 1- and 5-gallon containers with shipping weights of 4- to 5-gallons	1–5	FCC (2016a)
CharCoat CC	Container is transported in 5-gallons	5	CharCoat (2022)
2-part Reactive Coatings			
Pitt-Char – XP EP 97-194 Component A	Overall multi-component kit packaging listed as a range of 6.2–26.75 kg with a listed density of 5.28 kg/gal when mixed	1–5	PPG (2008)
J6 Polymers – KA8860	Packaging ranges in size from half-pint to 5-gallons	0.0625–5	J6 Polymers (2021)

The paint and coating products indicate container sizes that correspond to the bottles and small container sizes described in the ChemSTEER User Guide (U.S. EPA, 2015). The small container sizes range from 1 to 20 gallons. Therefore, EPA set the lower bound product volume for 1-part paints and coatings to one gallon based on provided product values and an upper bound product volume to 100 gallons based on the GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a). For resin-based paints and coatings, EPA used an approximate lower bound product volume of 0.25 gallons based on product data and an upper bound product volume to 100 gallons based on the ESD for Adhesive Formulation (OECD, 2009a). EPA used five gallons as the product container volume mode for both paint and coating types based on the mode of the product data ranges.

E.3.11 Batch Size

The ESD for Adhesive Formulation (OECD, 2009a) includes data from a single formulator which provided batch sizes ranging from 300 to 5,000 gallons. Additionally, the ESD for Adhesive Formulation (OECD, 2009a) assumes a batch size of 1,000 gallons in cases with a known adhesive product density and unknown batch size. The underlying distribution of batch volumes is unknown; therefore, EPA assigned a triangular distribution based on the estimated lower bound, upper bound, and mode of the parameter. EPA assigned batch size lower bound of 300 gallons, upper bound of 5,000 gallons, and mode of 1,000 gallons based on the ESD for Adhesive Formulation (OECD, 2009a). EPA calculated the mass of product in each batch using the product densities from safety and technical data sheets for the TCEP-containing products.

The GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) includes data from five formulators which provided batch sizes ranging from 1,000 to 5,000 gallons. Additionally, the GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) assumes a typical batch size of 1,000 gallons. The underlying distribution of batch volumes is unknown; therefore, EPA assigned a triangular distribution based on the estimated lower bound, upper bound, and mode of the parameter. EPA assigned batch size lower bound and mode of 1,000 gallons, and upper bound of 5,000 gallons based on the GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a). EPA calculated the mass of product in each batch using the product densities from safety and technical data sheets for the TCEP-containing products.

The batch size for coating formulation is calculated using Equation E-24.

Equation E-24

$$m_{batch} = V_{batch} \times \rho_{product} \times \left(0.00378541\ \frac{m^3}{gal}\right)$$

Where:

V_{batch} = Batch volume (gal/batch)
$\rho_{product}$ = Product density (kg/m^3)
m_{batch} = Batch size (kg/batch)

The number of paint and coating formulation batches run in a single year by one site is calculated using Equation E-25.

Equation E-25

$$N_{batch\_yr} = \frac{Q_{product}}{m_{batch}}$$

Where:

$Q_{product}$ = Facility production rate (kg/site-yr)
m_{batch} = Batch size (kg/batch)
N_{batch_yr} = Number of batches (batch/site-yr)

E.3.12 Hours per Batch

The ESD for Adhesive Formulation (OECD, 2009a) recommends a default of one batch per site per day, corresponding to 24 hours per batch for a facility operating 24 hours a day, 7 days a week, with an alternative of three batches per site per day, corresponding to eight hours per batch for a facility operating 24 hours a day, 7 days a week. EPA assumed that multiple batches may be processed in a single operating day, so the recommended assumption of eight hours per batch from the ESD for Adhesive Formulation (OECD, 2009a) was considered as a typical expected value. The underlying distribution of hours per batch is unknown; therefore, EPA assigned a triangular distribution based on the estimated lower bound, upper bound, and mode of the parameter. EPA set the hours per batch upper bound to 24 hours, lower bound to eight hours, and mode to eight hours based on the ESD for Adhesive Formulation (OECD, 2009a).

The GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) states that an architectural coating formulation facility took up to seven hours to prepare a batch of coating. Additionally, an automotive coating formulation facility estimates up to 72 hours per batch. Based on this information, the GS for Formulation of Waterborne Coatings recommends assuming a batch time of seven hours per batch (U.S.

EPA, 2014a). EPA assumed that multiple batches may be processed in a single operating day, so the recommended assumption of seven hours per batch from the GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) was considered as a typical expected value. The underlying distribution of hours per batch is unknown; therefore, EPA assigned a triangular distribution based on the estimated lower bound, upper bound, and mode of the parameter. EPA set the hours per batch upper bound to 72 hours, lower bound to seven hours, and mode to seven hours (U.S. EPA, 2014a).

E.3.13 Container Fill Rate

The ChemSTEER User Guide (U.S. EPA, 2015) provides a typical fill rate of 20 containers per hour for containers with 20–100 gallons of liquid and a typical fill rate of 60 containers per hour for containers with less than 20 gallons of liquid.

E.3.14 Equipment Cleaning Loss Fraction

The ESD for Adhesive Formulation (OECD, 2009a) recommends using the EPA/OPPT Multiple Process Vessel Residual Model to estimate the releases from equipment cleaning and assuming equipment cleaning occurs following each batch of product. The EPA/OPPT Multiple Process Vessels Residual Model, as detailed in the ChemSTEER User Guide (U.S. EPA, 2015), provides an overall loss fraction of 2.0 percent from equipment cleaning.

The GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) cites data from a site visit conducted by Environment Canada that shows losses between 1.3–3.0 percent of the total annual production from equipment cleaning. The GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) also recommends estimating the amount of residual chemical remaining in the process equipment by using the EPA/OPPT Multiple Process Vessels Residual Model. This model provides an overall loss fraction of 2 percent from equipment cleaning therefore, EPA assigned a triangular distribution based on the estimated lower bound, upper bound, and mode of the parameter. EPA set the equipment cleaning loss fraction upper bound to 3.0 percent, lower bound to 1.3 percent, and mode to 2.0 percent (U.S. EPA, 2014a).

E.3.15 Off-Specification Loss Fraction

The ESD for Adhesive Formulation and GS for Formulation of Waterborne Coatings provides a loss fraction of one percent of throughput disposed from off-specification material during manufacturing (OECD, 2009a; U.S. EPA, 2014a). The one percent default loss fraction was provided as an estimate from a Source Reduction Research Partnership (SRRP) study referenced in the ESD for Adhesive Formulation (OECD, 2009a).

The GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) cites data from a site visit conducted by Environment Canada that shows losses between 0.85–1.2 percent of the total annual production from off-specification product. The underlying distribution of values is unknown; therefore, EPA used a uniform distribution of 0.85–1.2 percent based on the GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a).

E.3.16 Filter Changeout Loss Fraction

The GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) provides a loss fraction of 0.0002 kg released per kg processed for spent filter waste after the blending operation. The GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) indicates that the quantity of filter waste is minimal in comparison to the quantity of coating manufactured and the quantity of other wastes stating less than 0.02 percent of the total facility production was lost due to filter wastes at the sites visited. The underlying distribution of values is unknown; therefore, EPA used a uniform distribution of 0–0.02 percent based on the GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a).

E.3.17 TCEP Concentration and Product Density

EPA compiled TCEP concentration and product density information from various paint and coating products containing TCEP to develop distributions for each of these parameters in the simulation. Safety data sheets (SDSs) and technical data sheets (TDSs) for TCEP-containing paint and coating products provided either a range or a single value for the TCEP concentration and product density. EPA used the values from the SDSs and TDSs as single input parameters or a range of input parameters for a uniform distribution. EPA did not have information on the prevalence or market share of different coating products in commerce; therefore, EPA assumed a uniform distribution of coating products. The model uses a nested distribution that first selects a coating product for the iteration and then based on the product selected, selects a concentration and density associated with that product. Where the concentration and/or density for a product are a distribution the model selects a value based on the given distribution. Table_Apx E-8 provides the TCEP-containing paint and coating products in the "product selector" tool along with product-specific values used for the tool.

Table_Apx E-8. Product TCEP Concentrations and Densities for Incorporation into Paints and Coatings OES

Product	TCEP Concentration (Mass Fraction)	Concentration Distribution	Density (kg/m^3)	Source Reference
1-part Coatings				
Flame Control No. 40-40A	0.001–0.01	Uniform	1,000–1,100 (Specific gravity listed as 1.0–1.1)	FCC (2016a)
Flame Control No. 5050	0.01–0.05	Uniform	1,200–1,300 (Specific gravity listed as 1.2–1.3)	FCC (2016a)
CharCoat CC	0.009–0.015	Uniform	1,200 (Density listed as 1.2 g/mL)	CharCoat (2017)
Cable Coating 3i	0.009–0.015	Uniform	1,200 (Specific gravity listed as 1.2)	Vimasco (2016)
Duratec 707-062 Grey Fire Resistant Primer	0.05	Discrete (Single value)	1,300 (Specific gravity listed as 1.3)	Duratec (2018)
Resin (2-part) Coatings				
Pitt-Char – XP EP 97-194 Component A	0.10–0.25	Uniform	1,490 (Product density listed as 1.49 g/cm^3 at 20 °C)	PPG (2010)
Pitt-Char – XP PF Base Off White	0.10–0.20	Uniform	1,490 (Relative density listed as 1.49 g/cm^3)	PPG (2016)

E.3.18 Number of Containers

Based on the parameters established in the previous subsections, the number of import containers of TCEP used by a site per year is calculated using Equation E-26.

Equation E-26

$$N_{cont\_yr} = \frac{PV}{N_s \times \rho_{TCEP} \times \left(0.00378541\ \frac{m^3}{gal}\right) \times V_{import\_cont}}$$

Where:

N_{cont_yr} = Annual number of import containers (containers/site-yr)
PV = Production volume (kg/yr)
N_s = Number of sites (sites)
ρ_{TCEP} = TCEP density (kg/m^3)
V_{import_cont} = Import container volume (gal/container)

The number of TCEP-containing resin product containers filled by a site per year is calculated using Equation E-27.

Equation E-27

$$N_{productcont\_yr} = \frac{Q_{product}}{\rho_{product} \times \left(0.00378541\ \frac{m^3}{gal}\right) \times V_{prod\_cont}}$$

Where:

$N_{productcont\_yr}$ = Annual number of product containers (containers/site-yr)
$Q_{product}$ = Facility production rate (kg/site-yr)
$\rho_{product}$ = Product density (kg/m^3)
V_{prod_cont} = Product container volume (gal/container)

E.3.19 Ventilation Rate

The 1991 CEB Manual indicates general ventilation rates in industry range from 500 to 10,000 ft^3/min, with a typical value of 3,000 ft^3/min (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on an estimated lower bound, upper bound, and mode of the parameter. EPA assumed the lower and upper bound using the industry range of 500–10,000 ft^3/min and the mode using the 3,000 ft^3/min typical value (U.S. EPA, 1991).

E.3.20 Mixing Factor

The 1991 CEB Manual indicates mixing factors may range from 0.1 to 1, with 1 representing ideal mixing (U.S. EPA, 1991). The 1991 CEB Manual references the *1988 ACGIH Ventilation Handbook*, which suggests the following factors and descriptions: 0.67–1 for best mixing; 0.5–0.67 for good mixing; 0.2–0.5 for fair mixing; and 0.1–0.2 for poor mixing (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the defined lower and upper bound and estimated mode of the parameter. The mode for this distribution was not provided; therefore, EPA assigned a mode value of 0.5 based on the typical value provided in the ChemSTEER User Guide for the EPA/OPPT Mass Balance Inhalation Model (U.S. EPA, 2015).

E.4 Use in Paints and Coatings Model Approach and Parameters

Appendix E.4 presents the modeling approach and equations used to estimate environmental and occupational exposures for TCEP during the use in paints and coatings OES. This approach utilizes methods derived from the *Emission Scenario Documents on Coating Industry (Paints, Lacquers, and Varnishes)* (OECD, 2009d) (hereinafter referred to as the "ESD on Coating Industry"), *Emission Scenario Document on Coating Application via Spray-Painting in the Automotive Refinishing Industry* (OECD, 2011a) (hereinafter referred to as the "ESD on Coating Application via Spray-Painting in the Automotive Refinishing Industry"), *Draft Spray Coatings in the Furniture Industry – Generic Scenario For Estimating Occupational Exposures And Environmental Releases* (U.S. EPA, 2004) (hereinafter referred to as the "GS for Spray Coatings in the Furniture Industry"), and the *SpERC Fact Sheet: Industrial Application of Coatings by Spraying* (CEPE, 2020a) and *SpERC Fact Sheet: Professional Application of Coatings and Inks by Spraying* (CEPE, 2020b) (hereinafter referred to as the "SpERC fact sheet on professional and industrial application of coatings and inks by spraying"). Based on these sources, EPA developed release estimates for the use of TCEP-containing paints and coatings.

Based on the ESDs, GS, and SpERC factsheets, EPA identified the following release points:

- Release Point 1: Transfer operation losses to air from unloading the coating component;
- Release Point 2: Application losses;
- Release Point 3: Equipment residues;
- Release Point 4: Open surface losses to air during equipment cleaning;
- Release Point 5: Can/container residues; and
- Release Point 6: Open surface losses to air during container cleaning.

Environmental releases of TCEP during the use of paints and coatings are a function of TCEP's physical properties, container size, mass fractions, and other model parameters. While physical properties are fixed, some model parameters are expected to vary. As described in Appendix E, EPA used a Monte Carlo simulation to capture variability in the following model input parameters: ventilation rate, mixing factor, air speed, saturation factor, container sizes, opening diameters (*e.g.*, equipment, containers), days of application, transfer efficiency, product concentration, product density, working years, and operating hours. EPA used the outputs from a Monte Carlo simulation with 100,000 iterations and the Latin Hypercube sampling method in @RISK to provide estimates of TCEP release amounts for this OES.

E.4.1 Model Equations

Table_Apx E-9 provides the models and associated variables used to calculate environmental releases for each release point within each iteration of the Monte Carlo simulation. Additional equations not based on generic models are provided below the table. EPA used these environmental releases to develop a distribution of release outputs for the use in paints and coatings OES. The variables used to calculate each of the following values include deterministic or variable input parameters, known constants, physical properties, TCEP concentrations, conversion factors, and other parameters. The values for these variables are provided in Appendices E.4.2 and 0. The Monte Carlo simulation calculated the total TCEP release (by environmental media) across all release points during each iteration of the simulation. EPA then selected 50th percentile and 95th percentile values to estimate the central tendency and high-end releases for each media, respectively.

Table_Apx E-9. Models and Variables Applied for Release Points in the Use in Paints and Coatings OES

Release Point	Model(s) Applied	Variables Used
Release Point 1: Transfer operation losses to air from unloading the coating component.	EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; VP; $F_{saturation\_unloading}$; MW_{TCEP}; V_{prod_cont}; R; T; $RATE_{fill\_drum/smallcont}$ Operating Time: N_{cont_yr}; $RATE_{fill_{drum}/smallcont}$
Release Point 2: Application losses	See Equation E-28	PV; TE; N_s
Release Point 3: Equipment residues	EPA/OPPT Single Process Vessel Residual Model (Appendix E.1)	PV; $F_{loss\_equipment}$; N_s
Release Point 4: Open surface losses to air during equipment cleaning	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_equip-cleaning}$; T; P Operating Time: OH; $Days_{application}$
Release Point 5: Can/container residues	EPA/OPPT Drum/Small Container Residual Model (Appendix E.1)	PV; F_{loss_cont}; N_s
Release Point 6: Open surface losses to air during container cleaning	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_cont-cleaning}$; T; P Operating Time: N_{cont_yr}; $RATE_{fill\_drum/smallcont}$

Appendix E.1 provides equations and discussion for release point operating times used to calculate releases to air as provided in Equation E-4. Release Point 2 annual release (application losses) is calculated using Equation E-28.

Equation E-28

$$Release\_Year_{RP2} = PV \times (1 - TE)/N_s$$

Where:

$Release\_Year_{RP2}$ = TCEP released for Release Point 2 (kg/site-yr)
PV = Production volume throughput of TCEP (kg/yr)
TE = Transfer efficiency (unitless)
N_S = Number of sites (sites)

E.4.2 Model Input Parameters

Table_Apx E-10 summarizes the model parameters and their values for the use in paints and coatings Monte Carlo simulation. Additional explanations of EPA's selection of the distributions for each parameter are provided in the following subsections.

Table_Apx E-10. Summary of Parameter Values and Distributions Used in the Use in Paints and Coatings Models

Input Parameter	Symbol	Unit	Deterministic Values	Uncertainty Analysis Distribution Parameters				Rationale/Basis
			Value	Lower Bound	Upper Bound	Mode	Distribution Type	
Air speed	$RATE_{air\_speed}$	cm/s	10	1.3	202.2	—	Lognormal	See Appendix E.4.5
Days of application	$Days_{application}$	days/site-yr	1	1	2	—	Discrete	See Appendix E.4.4
Transfer efficiency	TE	unitless	0.65	0.2	0.8	0.65	Triangular	See Appendix E.4.8
Loss fraction for drum containers	F_{loss_drum}	kg/kg	0.025	0.017	0.03	0.025	Triangular	See Appendix E.4.6
Loss fraction for cans/small containers	F_{loss_can}	kg/kg	0.003	0.0003	0.006	0.003	Triangular	See Appendix E.4.6
Loss fraction for equipment cleaning	$F_{loss\_equipment}$	kg/kg	0.05	0.02	0.149	0.05	Triangular	See Appendix E.4.7
Product container volume	V_{prod_cont}	gal/container	5	0.25	100	5	Triangular	See Appendix E.4.11
Saturation factor unloading	$F_{saturation\_unloading}$	unitless	0.5	0.5	1.45	0.5	Triangular	See Appendix E.4.10
Diameter of opening for equipment cleaning	$D_{opening\_equip\text{-}cleaning}$	cm	92	—	—	—	—	See Appendix E.4.9
Diameter of opening for container cleaning	$D_{opening\_cont\text{-}cleaning}$	cm	5.08	—	—	—	—	See Appendix E.4.9
Number of sites	N_s	sites	1 or calculated	—	—	—	—	“What-if” scenario input
Production volume assessed	PV_lbs	lbs/yr	2,500 or 25,000	—	—	—	—	“What-if” scenario input
Production volume	PV	kg/yr	1,134 or 11,340	—	—	—	—	PV input converted to kilograms
Site daily use rate	DUR	kg/site-day	100 or 1,000	—	—	—	—	“What-if” scenario input
Temperature	T	K	298	—	—	—	—	Process parameter
Pressure	P	torr	760	—	—	—	—	Process parameter
Gas constant	R	L-torr/mol-K	62.36367	—	—	—	—	Universal constant

Input Parameter	Symbol	Unit	Deterministic Values	Uncertainty Analysis Distribution Parameters				Rationale/Basis
			Value	Lower Bound	Upper Bound	Mode	Distribution Type	
TCEP vapor pressure	VP	torr	0.0613	—	—	—	—	Physical property
TCEP molecular weight	MW_{TCEP}	g/mol	285.49	—	—	—	—	Physical property
Fill rate of drum	$RATE_{fill\_drum}$	containers/hr	20	—	—	—	—	See Appendix E.4.12
Fill rate of small container	$RATE_{fill\_smallcont}$	containers/hr	60	—	—	—	—	See Appendix E.4.12
Operating hours for equipment cleaning	OH_C	hr/day	0.5	—	—	—	—	See Appendix E.4.4
Product density	$\rho_{product}$	kg/m^3	—	Multiple distributions depending on product data			Uniform	See Appendix E.4.13
Product concentration	F_{TCEP_prod}	kg/kg	—	Multiple distributions depending on product data			Uniform	

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E.4.3 Throughput Parameters

Several throughput parameters are calculated as input values to be used in the model equations during each iteration. The number of sites is either a set value of one site or calculated. When the number of sites is calculated, it is calculated using Equation E-29.

Equation E-29

$$N_s = \frac{PV}{F_{TCEP\_prod} \times DUR \times Days_{application}}$$

Where:

N_s = Number of sites (sites)
PV = Production volume (kg/year)
F_{TCEP_prod} = Weight fraction of TCEP in product (unitless)
DUR = Coating site daily use rate (kg/site-day)
$Days_{application}$ = Days of application (days/site-yr)

The number of product containers used by a site per year is calculated based on whether the number of sites is fixed to one site or calculated. Equation E-30 is used when the number of sites is fixed to one site and Equation E-31 is used when the number of sites is calculated.

Equation E-30

$$N_{prodcont\_yr} = \frac{PV}{F_{TCEP\_prod} \times N_S \times \rho_{product} \times \left(0.00378541\ \frac{m^3}{gal}\right) \times V_{prod\_cont}}$$

Where:

$N_{prodcont\_yr}$ = Annual number of product containers (containers/site-yr)
PV = Production volume (kg/year)
F_{TCEP_prod} = Product concentration (kg/kg)
$\rho_{product}$ = Product density (kg/m^3)
V_{prod_cont} = Product container volume (gal/container)

Equation E-31

$$N_{prodcont\_yr} = \frac{DUR \times Days_{application}}{\rho_{product} \times \left(0.00378541\ \frac{m^3}{gal}\right) \times V_{prod\_cont}}$$

$N_{prodcont\_yr}$ = Annual number of product containers (containers/site-yr)
DUR = Site daily use rate (kg/site-day)
$Days_{application}$ = Days of application (days/site-yr)
$\rho_{product}$ = Product density (kg/m^3)
V_{prod_cont} = Product container volume (gal/container)

E.4.4 Operating Hours and Exposure Durations

EPA estimated operating hours or hours of duration by direct estimates provided from the ESD on Coating Industry (OECD, 2009d), ESD on Coating Application via Spray-Painting in the Automotive Refinishing Industry (OECD, 2011a), GS for Spray Coatings in the Furniture Industry (U.S. EPA, 2004), and SpERC factsheet on professional and industrial application of coatings and inks by spraying (CEPE, 2020a, 2020b) and/or through calculation from other parameters.

For equipment cleaning, the ESD on Coating Application via Spray-Painting in the Automotive Refinishing Industry recommends a value of 8 minutes per day based on a study of spray application and cleanup times (OECD, 2011a). Additionally, the ChemSTEER User Guide states an operating time of 0.5 hrs/site-day for equipment cleaning losses of liquids form a single, small vessel (U.S. EPA, 2015). Based on this information, EPA assumed an operating time of 0.5 hrs/site-day to assess equipment cleaning losses.

The operating hours for Release Points 1 and 6 are calculated based on the numbers of containers received at the site and the fill rate using Equation E-32.

Equation E-32

$$Time_{RP1/RP6} = \frac{N_{cont\_yr}}{RATE_{fill\_drum/smallcont} * Days_{application}}$$

Where:

$Time_{RP1/RP6}$ = Operating times for Release Points 1 and 6 (hrs/site-day)
$RATE_{fill\_drum}$ = Fill rate of drum or small container (containers/hr)
N_{cont_yr} = Annual number of import containers (containers/site-yr)
$Days_{application}$ = Days of application (days/site-yr)

E.4.5 Air Speed

Baldwin and Maynard (1998) measured indoor air speeds across a variety of occupational settings in the United Kingdom. A total of 55 work areas were surveyed across a variety of workplaces. EPA analyzed the air speed data from Baldwin and Maynard (1998) and categorized the air speed surveys into settings representative of industrial facilities and representative of commercial facilities. EPA fit separate distributions for these industrial and commercial settings and used the industrial distribution for this OES.

EPA fit a lognormal distribution for the data set as consistent with the authors' observations that the air speed measurements within a surveyed location were lognormally distributed and the population of the mean air speeds among all surveys were lognormally distributed (Baldwin and Maynard, 1998). Since lognormal distributions are bound by zero and positive infinity, EPA truncated the distribution at the largest observed value among all of the survey mean air speeds.

EPA fit the air speed surveys representative of industrial facilities to a lognormal distribution with the following parameter values: mean of 22.414 cm/s and standard deviation of 19.958 cm/s. In the model, the lognormal distribution is truncated at a minimum allowed value of 1.3 cm/s and a maximum allowed value of 202.2 cm/s (largest surveyed mean air speed observed in Baldwin and Maynard (1998)) to prevent the model from sampling values that approach infinity or are otherwise unrealistically small or large (Baldwin and Maynard, 1998).

Baldwin and Maynard (1998) only presented the mean air speed of each survey. The authors did not present the individual measurements within each survey. Therefore, these distributions represent a distribution of mean air speeds and not a distribution of spatially variable air speeds within a single workplace setting. However, a mean air speed (averaged over a work area) is the required input for the model. EPA converted the units to ft/min prior to use within the model equations.

E.4.6 Container Residue Loss Fraction

EPA previously contracted PEI to conduct a study to provide estimates of potential chemical releases during cleaning of process equipment and shipping containers (PEI Associates, 1988). The study used both a literature review of cleaning practices and release data as well as a pilot-scale experiment to determine the amount of residual material left in vessels. The data from literature and pilot-scale experiments addressed different conditions for the emptying of containers and tanks, including various bulk liquid materials, different container constructions (*e.g.*, lined steel drums or plastic drums), and either a pump or pour/gravity-drain method for emptying. EPA reviewed the pilot-scale data from PEI and determined a range and average percentage of residual material remaining in vessels following emptying from drums by either pumping or pouring as well as tanks by gravity-drain (PEI Associates, 1988).

EPA previously used the study results to generate default central tendency and high end-loss fraction values for the residual models (*e.g.*, EPA/OPPT Small Container Residual Model, EPA/OPPT Drum Residual Model) provided in the ChemSTEER User Guide (U.S. EPA, 2015). Previously, EPA adjusted the default loss fraction values based on rounding the PEI study results or due to policy decisions. EPA used a combination of the PEI study results (PEI Associates, 1988) and the *ChemSTEER User Guide* (U.S. EPA, 2015) default loss fraction values to develop probability distributions for various container sizes.

Specifically, EPA paired the data from the PEI study (PEI Associates, 1988) such that the residuals data for emptying drums by pouring was aligned with the default central tendency and high-end values from the EPA/OPPT Small Container Residual Model, and the residuals data for emptying drums by pumping was aligned with the default central tendency and high-end values from the EPA/OPPT Drum Residual Model. EPA applied the EPA/OPPT Small Container Residual Model to containers with capacities less than 20 gallons, and the EPA/OPPT Drum Residual Model to containers with capacities between 20–100 gallons (U.S. EPA, 2015).

For unloading drums via pouring, the PEI study experiments showed average container residuals in the range of 0.03–0.79 percent with a total average of 0.32 percent (PEI Associates, 1988). The EPA/OPPT Small Container Residual Model recommends a default central tendency loss fraction of 0.3 percent and a high-end loss fraction of 0.6 percent (U.S. EPA, 2015). For unloading drums by pumping, the PEI study experiments showed average container residuals in the range of 1.7–4.7 percent with a total average of 2.6 percent (PEI Associates, 1988).

The EPA/OPPT Drum Residual Model from the ChemSTEER User Guide recommends a default central tendency loss fraction of 2.5 percent and a high-end loss fraction of 3.0 percent (U.S. EPA, 2015). The underlying distribution of the loss fraction parameter for small containers or drums is not known; therefore, EPA assigned a triangular distribution defined by the estimated lower bound, upper bound, and mode of the parameter values. EPA assigned the mode and upper bound values for the loss fraction triangular distributions using the central tendency and high-end values from the respective ChemSTEER model. EPA assigned the lower-bound values for the triangular distributions using the minimum average percent residual measured in the PEI study for the respective drum emptying technique (pouring or pumping) (PEI Associates, 1988).

E.4.7 Equipment Cleaning Loss Fraction

For equipment cleaning operations, the ESD on Coating Application via Spray-Painting in the Automotive Refinishing Industry indicates a loss fraction of up to two percent based on the EPA/OPPT Multiple Process Vessel Residual Model (OECD, 2011a). Additionally, the ESD on Coating Industry indicates that losses for spraying in automotive refinishing suggest a 14.9 percent loss of coating solids are lost as equipment residues (OECD, 2009d). The ESD on Coating Industry further breaks down the release of equipment residues by stating that 9.3 percent are lost to disposal, 3.7 percent are lost to land, and 1.9 percent are lost to water (OECD, 2009d). The ESD on Coating Industry states that losses for spraying in both the aerospace industry and rail vehicle industry are five percent for coating solids and lost as equipment residues for subsequent disposal after cleaning (OECD, 2009d). The underlying distribution of the loss fractions for equipment is not known, therefore, EPA assigned a triangular distribution defined by the estimated lower bound, upper bound, and mode of the parameter values. Based on the above information, EPA assigned the equipment cleaning loss fraction lower bound to 0.02, upper bound to 0.149, and the mode to 0.05 (OECD, 2009d, 2011a).

E.4.8 Transfer Efficiency

Losses from overspray and/or process scrap are based on the transfer efficiency of the application equipment. According to the ESD on Coating Application via Spray-Painting in the Automotive Refinishing Industry (OECD, 2011a) and GS for Spray Coatings in the Furniture Industry (U.S. EPA, 2004), transfer efficiencies range from 20 to 65 percent dependent on the spraying method and equipment. Both the ESD and GS estimate a transfer efficiency of 20–40 percent for conventional spray guns, and 65 percent for high volume-low pressure (HVLP) spray guns. The ESD on Coating Industry (OECD, 2009d) estimates transfer efficiencies for HVLP spray guns of 40– 45 percent. Across all spray technologies, the ESD on Coating Industry estimates a maximum transfer efficiency of 80 percent (OECD, 2009d). The underlying distribution of the spray equipment used, and their transfer efficiencies is not known, therefore, EPA assigned a triangular distribution of the transfer efficiencies defined by the estimated lower bound, upper bound, and mode of the parameter values. EPA assigned the transfer efficiency lower bound to 0.2, upper bound to 0.8, and mode to 0.65 (U.S. EPA, 2004; OECD, 2011a).

E.4.9 Diameters of Opening

The ChemSTEER User Guide indicates diameters for the openings for various vessels that may hold liquids in order to calculate vapor generation rates during different activities (U.S. EPA, 2015). EPA used a value of 5.08 cm for container cleaning activities based on the ChemSTEER User Guide (U.S. EPA, 2015). EPA used a value of 92 cm for equipment cleaning operations based on the ChemSTEER User Guide (U.S. EPA, 2015).

E.4.10 Saturation Factor

The 1991 CEB Manual indicated that during splash filling, the saturation concentration was reached or exceeded by misting with a maximum saturation factor of 1.45 (U.S. EPA, 1991). The 1991 CEB Manual also indicated that saturation concentration for bottom filling was expected to be about 0.5 (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the lower bound, upper bound, and mode of the parameter. Because a mode was not provided for this parameter, EPA assigned a mode value of 0.5 for bottom filling as bottom filling minimizes volatilization. This value also corresponds to the typical value provided in the ChemSTEER User Guide for the EPA/OAQPS AP-42 Loading Model (U.S. EPA, 2015).

E.4.11 Container Size

EPA assumed facilities receive TCEP in drums based on a prior triphosphates chemical assessment report from Australia's NICNAS stating that TCEP is imported in 200 liter drums (NICNAS, 2001). The ChemSTEER User Guide (U.S. EPA, 2015) recommends a range of 20 to less than 100 gallons for the volume capacity of drums modeled in container-related activities, and the ESD for Adhesive Formulation (OECD, 2009a) and GS for Formulation of Waterborne Coatings (U.S. EPA, 2014a) suggests 55 gallons for an unknown container size. Therefore, EPA assigned a lower bound of 20 gallons, an upper bound of 100 gallons, and a mode of 55 gallons for the import container volume distribution.

For product containers, both the ESD for Adhesive Formulation and GS for Formulation of Waterborne Coatings recommends a range of 20 to less than 100 gallons with a default value of 55 gallons for unknown container sizes (OECD, 2009a; U.S. EPA, 2014a). EPA reviewed safety and technical data sheets for the identified paint and coating products containing TCEP to develop the minimum, maximum, and mode product container volume. Table_Apx E-11 specifies container sizes for the final coating product formulations identified in data sheets.

Table_Apx E-11. Product Container Sizes for TCEP-containing Coatings

Product	Container Size Information for Product	Approximate Container Size(s) (gallons)	Source Reference
1-part Coatings			
Flame Control No. 40-40A	Container sizes are 1- and 5-gallon containers with shipping weights of 4- to 5-gallons	1–5	FCC (2016a)
Flame Control No. 5050	Container sizes are 1- and 5-gallon containers with shipping weights of 4- to 5-gallons	1–5	FCC (2016b)
CharCoat CC	Container is transported in 5-gallons	5	CharCoat (2022)
2-part Reactive Coatings			
Pitt-Char – XP EP 97-194 Component A	Overall multi-component kit packaging listed as a range of 6.2 kg–26.75 kg with a listed density of 5.28 kg/gal when mixed	1–5	PPG (2008)
J6 Polymers – KA8860	Packaging ranges in size from half-pint to 5-gallons	0.0625–5	J6 Polymers (2021)

The paint and coating products indicate container sizes that correspond to the bottles and small container sizes described in the ChemSTEER User Guide (U.S. EPA, 2015). The small container sizes range from 1 to 20 gallons. Therefore, EPA set the lower bound product volume for both 1-part and 2-part reactive paints and coatings to 0.25 gallons based on provided product values and an upper bound product volume to 100 gallons based on the GS and ESD. EPA used the median TCEP-containing resin product container volumes of five gallons as the product container volume mode.

E.4.12 Container Fill Rate

The ChemSTEER User Guide (U.S. EPA, 2015) provides a typical fill rate of 20 containers per hour for containers with 20–100 gallons of liquid and a typical fill rate of 60 containers per hour for containers with less than 20 gallons of liquid.

E.4.13 TCEP Concentration and Product Density

EPA compiled TCEP concentration and product density information from various paint and coating products containing TCEP to develop distributions for each of these parameters in the simulation. SDS and TDS for TCEP-containing paint and coating products provided either a range or a single value for the TCEP concentration and product density. EPA used the values from the SDSs and TDSs as single input parameters or a range of input parameters for a uniform distribution. EPA did not have information on the prevalence or market share of different coating products in commerce; therefore, EPA assumed a uniform distribution of coating products. The model uses a nested distribution that first selects a coating product for the iteration and then based on the product selected, selects a concentration and density associated with that product. Where the concentration and/or density for a product are a distribution the model selects a value based on the given distribution. Table_Apx E-12 provides the TCEP-containing paint and coating products in the "product selector" tool along with product-specific values used for the tool.

Table_Apx E-12. Product TCEP Concentrations and Densities for Incorporation into Paints and Coatings OES

Product	TCEP Concentration (Mass Fraction)	Concentration Distribution	Density (kg/m^3)	Source Reference
1-part Coatings				
Flame Control No. 40-40A	0.001–0.01	Uniform	1,000–1,100 (Specific gravity listed as 1.0–1.1)	FCC (2016a)
Flame Control No. 5050	0.01–0.05	Uniform	1,200–1,300 (Specific gravity listed as 1.2–1.3)	FCC (2016b)
CharCoat CC	0.009–0.015	Uniform	1,200 (Density listed as 1.2 g/mL)	CharCoat (2022)
Cable Coating 3i	0.009–0.015	Uniform	1,200 (Specific gravity listed as 1.2)	Vimasco (2016)
Duratec 707-062 Grey Fire Resistant Primer	0.05	Discrete (Single value)	1,300 (Specific gravity listed as 1.3)	Duratec (2018)
2-part Reactive Coatings				
Pitt-Char – XP EP 97-194 Component A	0.10–0.25	Uniform	1,490 (Product density listed as 1.49 g/cm^3 at 20 °C)	PPG (2010)

Product	TCEP Concentration (Mass Fraction)	Concentration Distribution	Density (kg/m^3)	Source Reference
Pitt-Char – XP PF Base Off White	0.10–0.20	Uniform	1,490 (Relative density listed as 1.49 g/cm^3)	PPG (2016)

E.5 Incorporation into Resins Model Approach and Parameters

Appendix E.5 presents the modeling approach and equations used to estimate environmental releases and occupational exposures for TCEP during the Incorporation into Resins OES. This approach utilizes the ESD for Adhesive Formulations (OECD, 2009a) combined with Monte Carlo simulation (a type of stochastic simulation). EPA used the ESD for Adhesive Formulations (OECD, 2009a) to develop the release models due to the similarity of reactive adhesives to the end uses for TCEP-containing resins, including for polyurethanes, and the formulation characteristics of reactive adhesives as “unreacted prepolymers, oligomers, or monomers that react to form a crosslinked polymer at the point of application” (OECD, 2009a). In particular, EPA used the information and data for a “Sealed Process (Organic Solvent-Based, Reactive Adhesives)” from the ESD for Adhesive Formulations (OECD, 2009a) to inform the release assessment.

Based on the ESD, EPA identified the following release points:

- Release Point 1: Transfer operation losses to air from unloading the resin component;
- Release Point 2: Dust generation from transfer operations released to air, or collected and released to water, incineration, or landfill (not assessed);
- Release Point 3: Resin component container residue released to water, incineration, or landfill (assessed release to wastewater);
- Release Point 4: Open surface losses to air during container cleaning;
- Release Point 5: Vented losses to air during dispersion and blending/process operations;
- Release Point 6: Product sampling wastes disposed to water, incineration, or landfill (not assessed);
- Release Point 7: Open surface losses to air during product sampling;
- Release Point 8: Equipment cleaning releases to water, incineration, or landfill (assessed release to waste disposal);
- Release Point 9: Open surface losses to air during equipment cleaning;
- Release Point 10: Transfer operation losses to air from packaging resins into transport containers; and
- Release Point 11: Off-specification and other waste resins to water, incineration, or landfill (assessed release to waste disposal)

Based on the ESD, EPA identified the following inhalation exposure points:

- Exposure Point A: Transfer operation exposures from unloading the resin component;
- Exposure Point B: Container cleaning exposures after unloading the resin component;
- Exposure Point C: Open surface exposures during product sampling;
- Exposure Point D: Exposures from equipment cleaning; and
- Exposure Point E: Transfer operation exposures from packaging resin into transport containers.

Environmental releases and occupational exposures for TCEP during incorporation into resins are a function of TCEP's physical properties, container size, mass fractions, and other model parameters. While physical properties are fixed, some model parameters are expected to vary. As described in Section 3.4, EPA used a Monte Carlo simulation to capture variability in the following model input parameters: ventilation rate, mixing factor, air speed, saturation factor, container sizes, opening diameters (*e.g.*, mixing tanks, containers), batch size, time per batch, TCEP product concentration, product density, working years, and operating hours. EPA used the outputs from the Monte Carlo simulation to provide estimates of TCEP release amounts and exposure levels for this OES.

E.5.1 Model Equations

Table_Apx E-13 provides the models and associated variables used to calculate environmental releases for each release point within each iteration of the Monte Carlo simulation. Additional equations not based on generic models are provided in the following subsections. EPA used these environmental releases in order to develop a distribution of release outputs for the Incorporation into Resins OES. The variables used to calculate each of the following values include deterministic or variable input parameters, known constants, physical properties, TCEP concentrations, conversion factors, and other parameters. The values for these variables are provided in Appendix E.5.2 and E.5.3. The Monte Carlo simulation calculated the total TCEP release (by environmental media) across all release points during each iteration of the simulation. EPA then selected 50th and 95th percentile values to estimate the central tendency and high-end releases, respectively.

Table_Apx E-13. Models and Variables Applied for Release Points in the Incorporation into Resins OES

Release Point	Model(s) Applied	Variables Used
Release Point 1: Transfer operation losses to air from unloading the resin component	EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP_import}; VP; $F_{saturation\_unloading}$; MW_{TCEP}; V_{import_cont}; R; T; $RATE_{fill\_drum}$ Operating Time: N_{cont_yr}; $RATE_{fill\_drum}$
Release Point 2: Dust generation from transfer operations released to air, or collected and released to water, incineration, or landfill (not assessed)	Not assessed; release point not applicable for liquid formulations	Not applicable
Release Point 3: Resin component container residue released to water, incineration, or landfill (assessed release to wastewater)	EPA/OPPT Drum Residual Model (Appendix E.1)	PV; $F_{loss\_cont-residue}$
Release Point 4: Open surface losses to air during container cleaning	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_import}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_blending}$; T; P Operating Time: N_{cont_yr}; $RATE_{fill\_drum}$

Release Point	Model(s) Applied	Variables Used
Release Point 5: Vented losses to air during dispersion and blending/process operations	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_blending}$; T; P Operating Time: OH_{batch}; N_{batch_yr}
Release Point 6: Product sampling wastes disposed to water, incineration, or landfill (not assessed)	Not assessed; release expected to occur but not quantified in ESD	Not applicable
Release Point 7: Open surface losses to air during product sampling	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_sampling}$; T; P Operating Time: OH_{RP7}; N_{batch_yr}
Release Point 8: Equipment cleaning releases to water, incineration, or landfill (assessed release to waste disposal)	EPA/OPPT Multiple Process Vessel Residual Model (Appendix E.1)	PV; $F_{loss\_equip-cleaning}$
Release Point 9: Open surface losses to air during equipment cleaning	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_equip-cleaning}$; T; P Operating Time: OH_{RP9}; N_{batch_yr}
Release Point 10: Transfer operation losses to air from packaging resins into transport containers	EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; VP; $F_{saturation\_loading}$; MW_{TCEP}; V_{prod_cont}; R; T; $RATE_{fill\_drum}$; $RATE_{fill\_small}$ Operating Time: $N_{prodcont\_yr}$; $RATE_{fill\_drum}$; $RATE_{fill\_small}$
Release Point 11: Off-specification and other waste resins to water, incineration, or landfill (assessed release to waste disposal)	See Equation E-33	PV; $F_{loss\_off-spec}$

Appendix E.5.4 provides equations and discussion for release point operating times used to calculate releases to air as provided in Equation E-4.

Release Point 11 annual release (off-specification and other waste resins) is calculated using Equation E-33.

Equation E-33

$$Release\_Year_{RP11} = PV \times F_{loss\_off-spec}$$

Where:

$Release\_Year_{RP11}$ = TCEP released for Release Point 11 (kg/site-yr)
PV = Production volume throughput of TCEP (kg/yr)
$F_{loss\_off-spec}$ = Loss fraction for off-specification wastes (unitless)

Table_Apx E-14 provides the models and associated variables used to calculate occupational exposures for each exposure point within each iteration of the Monte Carlo simulation. EPA used these occupational exposures in order to develop a distribution of exposure outputs for the incorporation into resins OES. EPA assumed that the same worker performed exposure point activities for a total exposure duration of up to 8 hours per day, with no exposure assumed outside of the exposure points assessed. The variables used to calculate each of the following exposure concentrations and durations include deterministic or variable input parameters, known constants, physical properties, TCEP concentrations, conversion factors, and other parameters. The values for these variables are provided in Appendix E.5.2 and E.5.3. The Monte Carlo simulation calculated the TWAs and exposure concentration metrics based on calculated concentrations and exposure durations during each iteration of the simulation. EPA then selected the 50th and 95th percentile values to estimate the central tendency and high-end exposures, respectively.

Table_Apx E-14. Models and Variables Applied for Exposure Points in the Incorporation into Resins OES

Exposure Point	Model(s) Applied	Variables Used
Exposure Point A: Transfer operation exposures from unloading the resin component	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP_import}; VP; $F_{saturation\_unloading}$; MW_{TCEP}; V_{import_cont}; R; T; $RATE_{fill\_drum}$; Q; k; Vm Exposure Duration: N_{cont_yr}; $RATE_{fill\_drum}$; OD
Exposure Point B: Container cleaning exposures after unloading the resin component	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_import}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_cont-cleaning}$; T; P; Q; k; Vm Exposure Duration: N_{cont_yr}; $RATE_{fill\_drum}$; OD
Exposure Point C: Open surface exposures during product sampling	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_sampling}$; T; P; Q; k; Vm Exposure Duration: h_C
Exposure Point D: Exposures from equipment cleaning	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OPPT Penetration Model or	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$;

Exposure Point	Model(s) Applied	Variables Used
	EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	$D_{opening\_equip-cleaning}$; T; P; Q; k; Vm Operating Time: h_D
Exposure Point E: Transfer operation exposures from packaging resin into transport containers	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; VP; $F_{saturation\_loading}$; MW_{TCEP}; V_{prod_cont}; R; T; $RATE_{fill\_drum}$; $RATE_{fill\_small}$; Q; k; Vm Exposure Duration: $N_{prodcont\_yr}$; $RATE_{fill\_drum}$; $RATE_{fill\_small}$; OD

Appendix E.5.4 provides equations and discussion for exposure durations used to calculate TWAs and exposure concentration metrics for each of the exposure points. Note that the number of exposure days is set equal to the number of operating days, or it is fixed at 250 days per year if the number of operating days is greater than 250 days per year.

E.5.2 Model Input Parameters

Table_Apx E-15 summarizes the model parameters and their values for the Incorporation into Resins Monte Carlo simulation. Additional explanations of EPA's selection of the distributions for each parameter are provided in the following subsections.

Table_Apx E-15. Summary of Parameter Values and Distributions Used in the Incorporation into Resins Models

Input Parameter	Symbol	Unit	Deterministic Values	Uncertainty Analysis Distribution Parameters				Rationale/Basis
			Value	Lower Bound	Upper Bound	Mode	Distribution Type	
Air speed	$RATE_{air\_speed}$	cm/s	10	1.3	202.2	—	Lognormal	See Appendix E.5.5
Container residue loss fraction	$F_{loss\_cont\text{-}residue}$	kg/kg	0.025	0.017	0.03	0.025	Triangular	See Appendix E.5.6
Operating/exposure hours for equipment cleaning	h_D; OH_{RP9}	hr/shift; hr/batch	4	1	4	4	Triangular	See Appendix E.5.4
Diameter of opening for blending/process operations	$D_{opening\_blending}$	cm	10	10	Calculated	10	Triangular	See Appendix E.5.7
Diameter of opening for equipment cleaning	$D_{opening\_equip\text{-}cleaning}$	cm	92	92	Calculated	92	Triangular	See Appendix E.5.7
Diameter of opening for sampling	$D_{opening\_sampling}$	cm	2.5	2.5	10	2.5	Triangular	See Appendix E.5.7
Saturation factor unloading	$F_{saturation\_unloading}$	unitless	0.5	0.5	1.45	0.5	Triangular	See Appendix E.5.8
Saturation factor loading	$F_{saturation\_loading}$	unitless	0.5	0.5	1.45	0.5	Triangular	See Appendix E.5.8
Import container volume	V_{import_cont}	gal/container	55	20	100	55	Triangular	See Appendix E.5.9
Product container volume	V_{prod_cont}	gal/container	5	0.25	100	5	Triangular	See Appendix E.5.9
Batch volume	V_{batch}	gal/batch	1,000	300	5,000	1,000	Triangular	See Appendix E.5.10
Hours per batch	OH_{batch}	hr/batch	8	8	24	8	Triangular	See Appendix E.5.11
Number of sites	N_s	sites	Manual input	—	—	—	—	"What-if" scenario input
Production volume assessed	PV_lbs	lbs/yr	Manual input	—	—	—	—	"What-if" scenario input
Production volume	PV	kg/yr	Unit conversion	—	—	—	—	PV input converted to kilograms

Input Parameter	Symbol	Unit	Deterministic Values	Uncertainty Analysis Distribution Parameters				Rationale/Basis
			Value	Lower Bound	Upper Bound	Mode	Distribution Type	
Import concentration	$F_{\text{TCEP\_import}}$	kg/kg	1.0	—	—	—	—	Assumed pure TCEP imported for incorporation
Temperature	T	K	298	—	—	—	—	Process parameter
Pressure	P	torr	760	—	—	—	—	Process parameter
Gas constant	R	L-torr/mol-K	62.36367	—	—	—	—	Universal constant
TCEP vapor pressure	VP	torr	0.0613	—	—	—	—	Physical property
TCEP molecular weight	MW_{TCEP}	g/mol	285.49	—	—	—	—	Physical property
Fill rate of drum	$RATE_{\text{fill\_drum}}$	containers/hr	20	—	—	—	—	See Appendix E.5.12
Fill rate of small container	$RATE_{\text{fill\_smallcont}}$	containers/hr	60	—	—	—	—	See Appendix E.5.12
Equipment cleaning loss fraction	$F_{\text{loss\_equipment}}$	kg/kg	0.02	—	—	—	—	See Appendix E.5.13
Off-specification loss fraction	$F_{\text{loss\_off-spec}}$	kg/kg	0.01	—	—	—	—	See Appendix E.5.14
Operating/exposure hours for product sampling	h_C; OH_{RP7}	hr/shift; hr/batch	1	—	—	—	—	See Appendix E.5.4
Diameter of opening for container cleaning	$D_{\text{opening\_cont-cleaning}}$	cm	5.08	—	—	—	—	See Appendix E.5.7
Product density	ρ_{product}	kg/m^3	—	Multiple distributions depending on product data			Uniform	See Appendix E.5.15
Product concentration	$F_{\text{TCEP\_prod}}$	kg/kg	—	Multiple distributions depending on product data			Uniform	
Ventilation rate	Q	ft^3/min	—	500	10,000	3,000	Triangular	See Appendix E.5.16
Mixing factor	k	unitless	—	0.1	1	0.5	Triangular	See Appendix E.5.17

E.5.3 Throughput Parameters

Several throughput parameters are calculated as intermediate values to be used in the model equations during each iteration. The facility production rate is calculated using Equation E-34.

Equation E-34

$$Q_{product} = \frac{PV}{F_{TCEP\_prod} \times N_s}$$

Where:

$Q_{product}$ = Facility production rate (kg/site-yr)
PV = Production volume (kg/yr)
F_{TCEP_prod} = Weight fraction of TCEP in product (unitless)
N_s = Number of sites (sites)

The batch size for resin formulation is calculated using Equation E-35.

Equation E-35

$$m_{batch} = V_{batch} \times \rho_{product} \times (0.00378541\ \frac{m^3}{gal})$$

Where:

m_{batch} = Batch size (kg/batch)
V_{batch} = Batch volume (gal/batch)
$\rho_{product}$ = Product density (kg/m^3)

The number of resin formulation batches run in a single year by one site is calculated using Equation E-36.

Equation E-36

$$N_{batch\_yr} = \frac{Q_{product}}{m_{batch}}$$

Where:

N_{batch_yr} = Number of batches (batch/site-yr)
$Q_{product}$ = Facility production rate (kg/site-yr)
m_{batch} = Batch size (kg/batch)

The number of operating days was set to a maximum of 365 days per year, consistent with the maximum number of days in a typical year. If the calculated value of operating days exceeds 365 days in a given iteration, then the number is set to 365 days per year. See Equation E-37 for calculating operating days per year.

Equation E-37

$$OD = \frac{Q_{product}}{m_{batch}} \times \frac{OH_{batch}}{24\,\frac{hr}{day}} \times$$

Where:

OD = Operating days (days/site-yr)
$Q_{product}$ = Facility production rate (kg/site-yr)
m_{batch} = Batch size (kg/batch)
OH_{batch} = Operating hours per batch (hr/batch)

The number of import containers of TCEP used by a site per year is calculated using Equation E-38.

Equation E-38

$$N_{cont\_yr} = \frac{PV}{N_s \times \rho_{TCEP} \times \left(0.00378541\ \frac{m^3}{gal}\right) \times V_{import\_cont}}$$

Where:

N_{cont_yr} = Annual number of import containers (containers/site-yr)
PV = Production volume (kg/yr)
N_s = Number of sites (sites)
ρ_{TCEP} = TCEP density (kg/m^3)
V_{import_cont} = Import container volume (gal/container)

The number of TCEP-containing resin product containers filled by a site per year is calculated using Equation E-39.

Equation E-39

$$N_{productcont\_yr} = \frac{Q_{product}}{\rho_{product} \times \left(0.00378541\ \frac{m^3}{gal}\right) \times V_{prod\_cont}}$$

Where:

$N_{productcont\_yr}$ = Annual number of product containers (containers/site-yr)
$Q_{product}$ = Facility production rate (kg/site-yr)
$\rho_{product}$ = Product density (kg/m^3)
V_{prod_cont} = Product container volume (gal/container)

E.5.4 Operating Hours and Exposure Durations

EPA estimated operating hours or hours of duration by direct estimates provided from the ESD for Adhesive Formulation (OECD, 2009a) and/or through calculation from other parameters. Worker activities with operating hours and hours of duration provided from the ESD for Adhesive Formulation (OECD, 2009a) as direct estimates include product sampling and equipment cleaning.

For product sampling, the ESD for Adhesive Formulation (OECD, 2009a) indicates a single default value of one hour based on the 1991 CEB Manual (U.S. EPA, 1991). Since only one value was identified, EPA could not develop a distribution and used one hour for both release simulation (operating hours rate for Release Point 7) and exposure simulation (exposure duration for Exposure Point C). The operating time for Release Point 7 is further calculated based on the number of batches per year, with values provided in Table_Apx E-15. Equation E-40 provides the calculation.

Equation E-40

$$Time_{RP7} = OH_{RP7} \times N_{batch_{yr}}$$

Where:

$Time_{RP7}$ = Operating time for Release Point 7 (hrs/site-day)
OH_{RP7} = Operating hours per sampling (hrs/sample)
N_{batch_yr} = Annual number of batches (batches/site-yr)

For equipment cleaning, the ESD for Adhesive Formulation provides a default estimate of four hours per batch based on the default for cleaning multiple vessels from the ChemSTEER User Guide (OECD, 2009a; U.S. EPA, 2015). The ESD for Adhesive Formulation also states that a case study conducted by the Pollution Prevention Assistance Division indicated a range of equipment cleaning times between one and three hours (OECD, 2009a). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on a lower bound, upper bound, and mode for equipment cleaning operating hours. EPA assigned the lower bound as one hour based on the lower end cleaning time observed in the case study (OECD, 2009a) and the upper bound as four hours based on the ChemSTEER User Guide (U.S. EPA, 2015) default value for this worker activity. For the mode, EPA assigned 4 hours because, in the absence of site-specific information, the ESD for Adhesive Formulation recommends four hours as the default value (OECD, 2009a). EPA calculated the equipment cleaning operating hours using this triangular distribution for both the release simulation (operating hours rate for Release Point 9) and exposure simulation (exposure duration for Exposure Point D). The operating time for Release Point 9 is further calculated based on the number of batches per year, with values provided in Table_Apx E-15. Equation E-41 provides the calculation.

Equation E-41

$$Time_{RP9} = OH_{RP9} \times N_{batch_{yr}}$$

Where:

$Time_{RP9}$ = Operating time for Release Point 9 (hrs/site-day)
OH_{RP9} = Operating hours per sampling (hrs/sample)
N_{batch_yr} = Annual number of batches (batches/site-yr)

The operating hours for Release Points 1 and 4 are calculated based on the number of containers received at the site and the fill rate, which is provided in Table_Apx E-15.

Equation E-42 provides the calculation.

Equation E-42

$$Time_{RP1/RP4} = \frac{N_{cont\_yr}}{RATE_{fill\_drum}}$$

Where:

$Time_{RP1/RP4}$ = Operating time for Release Points 1 and 4 (hrs/site-day)
N_{cont_yr} = Annual number of import containers (containers/site-yr)
$RATE_{fill\_drum}$ = Fill rate of drum (containers/hr)

The operating hours for Release Point 5 is calculated based on the operating hours per batch and the number of batches per year, with values provided in Table_Apx E-15. Equation E-43 provides the calculation.

Equation E-43

$$Time_{RP5} = OH_{batch} \times N_{batch_{yr}}$$

Where:

$Time_{RP5}$ = Operating time for Release Point 5 (hrs/site-day)
OH_{batch} = Operating hours per batch (hrs/batch)
N_{batch_yr} = Annual number of batches (batches/site-yr)

The operating hours for Release Point 10 is calculated based on the number of product containers filled at the site and the fill rate, with values provided in Table_Apx E-15. Equation E-44 provides the calculation.

Equation E-44

$$Time_{RP10} = \frac{N_{prodcont\_yr}}{RATE_{fill\_drum/small}}$$

Where:

$Time_{RP10}$ = Operating time for Release Point 10 (hrs/site-day)
$N_{prodcont\_yr}$ = Annual number of product containers (containers/site-yr)
$RATE_{fill\_drum/small}$ = Fill rate of container, dependent on volume (container/hr)

Exposure durations for Exposure Points A and B are calculated based on fill rate for the containers holding the resin component. Note that the fill rate for drums used in this equation may take the default deterministic value listed as part of the model, or it may be corrected to a higher value to account for a total of eight exposure hours across all exposure points. In cases where total exposure duration across Exposure Points A, B, C, and D is greater than eight hours using the default deterministic value, the corrected fill rate calculated in Equation E-48 is used to calculate corrected Exposure Points A and B exposure durations. The exposure durations are calculated using Equation E-45.
Equation E-45

Equation E-45

$$h_{A/B} = \frac{N_{cont\_yr}}{RATE_{fill\_drum} \times OD}$$

Where:

$h_{A/B}$ = Exposure durations for Exposure Points A and B (hrs/day)
N_{cont_yr} = Annual number of import containers (containers/site-yr)
$RATE_{fill\_drum}$ = Fill rate of drum (containers/hr)
OD = Operating days (days/site-yr)

Exposure duration for Exposure Point E is calculated based on number of product containers filled per year, or on remaining work-shift time after accounting for other exposure points. Since EPA assumes a single worker with total maximum exposure duration of eight hours per working day, the 8-hour TWA is estimated using the exposure activities with fixed, default exposures or those with the largest contributions to total exposure. The fill rate for product containers used in this equation for each iteration may be either the default fill rate for drums (if product container ≥ 20 gal) or the default fill rate for small containers (if product container < 20 gal). The exposure duration is calculated using Equation E-46.

Equation E-46

$$h_F = \begin{cases} \dfrac{N_{prodcont\_yr}}{RATE_{fill\_drum/small} \times OD}, & 8 \geq \left[h_A + h_B + h_C + h_D + \dfrac{N_{prodcont\_yr}}{RATE_{fill\_drum/small} \times OD}\right] \\ 8 - (h_A + h_B + h_C + h_D), & 8 < \left[h_A + h_B + h_C + h_D + \dfrac{N_{prodcont\_yr}}{RATE_{fill\_drum/small} \times OD}\right] \end{cases}$$

Where:

h_n = Exposure duration for Exposure Point “n” (hrs/day)
$N_{prodcont\_yr}$ = Annual number of product containers (containers/site-yr)
$RATE_{fill\_drum/small}$ = Fill rate of container, dependent on volume (containers/hr)
OD = Operating days (days/site-yr)

E.5.5 Air Speed

Baldwin and Maynard (1998) measured indoor air speeds across a variety of occupational settings in the United Kingdom. A total of 55 work areas were surveyed across a variety of workplaces. EPA analyzed the air speed data from Baldwin and Maynard (1998) and categorized the air speed surveys into settings representative of industrial facilities and representative of commercial facilities. EPA fit separate distributions for these industrial and commercial settings and used the industrial distribution for this OES.

EPA fit a lognormal distribution for the data set as consistent with the authors’ observations that the air speed measurements within a surveyed location were lognormally distributed and the population of the mean air speeds among all surveys were lognormally distributed (Baldwin and Maynard, 1998). Since lognormal distributions are bound by zero and positive infinity, EPA truncated the distribution at the largest observed value among all of the survey mean air speeds.

EPA fit the air speed surveys representative of industrial facilities to a lognormal distribution with the following parameter values: mean of 22.414 cm/s and standard deviation of 19.958 cm/s. In the model, the lognormal distribution is truncated at a minimum allowed value of 1.3 cm/s and a maximum allowed value of 202.2 cm/s (largest surveyed mean air speed observed in Baldwin and Maynard (1998)) to prevent the model from sampling values that approach infinity or are otherwise unrealistically small or large (Baldwin and Maynard, 1998).

Baldwin and Maynard (1998) only presented the mean air speed of each survey. The authors did not present the individual measurements within each survey. Therefore, these distributions represent a distribution of mean air speeds and not a distribution of spatially variable air speeds within a single workplace setting. However, a mean air speed (averaged over a work area) is the required input for the model. EPA converted the units to ft/min prior to use within the model equations.

E.5.6 Container Residue Loss Fraction

EPA previously contracted PEI to conduct a study to provide estimates of potential chemical releases during cleaning of process equipment and shipping containers (PEI Associates, 1988). The study used both a literature review of cleaning practices and release data as well as a pilot-scale experiment to determine the amount of residual material left in vessels. The data from literature and pilot-scale experiments addressed different conditions for the emptying of containers and tanks, including various bulk liquid materials, different container constructions (*e.g.*, lined steel drums or plastic drums), and either a pump or pour/gravity-drain method for emptying. EPA reviewed the pilot-scale data from PEI and determined a range and average percentage of residual material remaining in vessels following emptying from drums by either pumping or pouring as well as tanks by gravity-drain (PEI Associates, 1988).

EPA previously used the study results to generate default central tendency and high end-loss fraction values for the residual models (*e.g.*, EPA/OPPT Small Container Residual Model, EPA/OPPT Drum Residual Model) provided in the ChemSTEER User Guide (U.S. EPA, 2015). Previously, EPA adjusted the default loss fraction values based on rounding the PEI study results or due to policy decisions. EPA used a combination of the PEI study results (PEI Associates, 1988) and the *ChemSTEER User Guide* (U.S. EPA, 2015) default loss fraction values to develop probability distributions for various container sizes.

Specifically, EPA paired the data from the PEI study (PEI Associates, 1988) such that the residuals data for emptying drums by pouring was aligned with the default central tendency and high-end values from the EPA/OPPT Small Container Residual Model, and the residuals data for emptying drums by pumping was aligned with the default central tendency and high-end values from the EPA/OPPT Drum Residual Model. EPA applied the EPA/OPPT Small Container Residual Model to containers with capacities less than 20 gallons, and the EPA/OPPT Drum Residual Model to containers with capacities between 20–100 gallons (U.S. EPA, 2015).

For unloading drums via pouring, the PEI study experiments showed average container residuals in the range of 0.03–0.79 percent with a total average of 0.32 percent (PEI Associates, 1988). The EPA/OPPT Small Container Residual Model recommends a default central tendency loss fraction of 0.3 percent and a high-end loss fraction of 0.6 percent (U.S. EPA, 2015). For unloading drums by pumping, the PEI study experiments showed average container residuals in the range of 1.7–4.7 percent with a total average of 2.6 percent (PEI Associates, 1988).

The EPA/OPPT Drum Residual Model from the ChemSTEER User Guide recommends a default central tendency loss fraction of 2.5 percent and a high-end loss fraction of 3.0 percent (U.S. EPA, 2015). The underlying distribution of the loss fraction parameter for small containers or drums is not known; therefore, EPA assigned a triangular distribution defined by the estimated lower bound, upper bound, and mode of the parameter values. EPA assigned the mode and upper bound values for the loss fraction triangular distributions using the central tendency and high-end values from the respective ChemSTEER model. EPA assigned the lower-bound values for the triangular distributions using the minimum average percent residual measured in the PEI study for the respective drum emptying technique (pouring or pumping) (PEI Associates, 1988).

E.5.7 Diameters of Opening

The ChemSTEER User Guide (U.S. EPA, 2015) indicates diameters for the openings for various vessels that may hold liquids in order to calculate vapor generation rates during different activities. In the simulation developed for the incorporation into resins OES based on the ESD for Adhesive Formulation (OECD, 2009a), EPA used the default diameters of vessels from the ChemSTEER User Guide (U.S. EPA, 2015) for container cleaning, blending operations, equipment cleaning, and sampling activities.

For container cleaning activities, the ChemSTEER User Guide indicates a single default value of 5.08 cm (U.S. EPA, 2015). Therefore, EPA could not develop a distribution of values for this parameter and used the single value 5.08 cm from the ChemSTEER User Guide.

For blending operations, the ESD for Adhesive Formulation assumes a closed vessel with a 4-inch diameter process vent, corresponding to 10 cm in diameter (OECD, 2009a). In addition, EPA considered the potential for open process vessels used for blending as mentioned in the ESD for Adhesive Formulation (OECD, 2009a), with diameters of the open vessel calculated based on the batch volume for the simulation iteration and an assumption of a one-to-one height to diameter ratio for the process vessel. The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution defined by an estimated lower bound, upper bound, and mode of the parameter. EPA assigned the value of 10 cm for both the lower bound and mode of the triangular distribution as the default value recommended by the ESD for Adhesive Formulation (OECD, 2009a). For the upper bound value of the triangular distribution, EPA assigned an equation calculating the diameter of an open process vessel with a one-to-one height to diameter ratio and fixed volume from the batch volume input parameter:

Equation E-47

$$D_{blending\_max} = \left[\frac{4 \times V_{batch} * 3{,}785.41\,\frac{cm^3}{gal}}{\pi}\right]^{1/3}$$

For equipment cleaning operations, the ChemSTEER User Guide indicates a single default value of 92 cm (U.S. EPA, 2015). EPA also considered open process vessels during cleaning, with diameters of the open vessel calculated based on the batch volume for the simulation iteration and an assumption of a one-to-one height to diameter ratio for the process vessel. The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the estimated lower bound, upper bound, and mode of the parameter. EPA assigned the value of 92 cm for both the lower bound and mode of the triangular distribution as the default value recommended by the ChemSTEER User Guide (U.S. EPA, 2015). For the upper bound value of the triangular distribution, EPA assigned an equation calculating the diameter of an open process vessel with a one-to-one height to diameter ratio and fixed volume from the batch volume input parameter; this is the same equation (Equation E-47) used for the open process vessel diameter during blending.

For sampling liquid product, sampling liquid raw material, or general liquid sampling, the ChemSTEER User Guide indicates that the typical diameter of opening for vaporization of the liquid is 2.5 cm (U.S. EPA, 2015). Additionally, the ChemSTEER User Guide provides 10 cm as a worst-case value for the diameter of opening during sampling (U.S. EPA, 2015). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the estimated lower bound, upper bound, and mode of the parameter. EPA assigned the value of 2.5 cm as a lower bound for the parameter and 10 cm as the upper bound based on the values provided in the ChemSTEER User Guide (U.S. EPA, 2015). EPA also assigned 2.5 cm as the mode diameter value for sampling liquids because it is provided as a typical value in the ChemSTEER User Guide (U.S. EPA, 2015).

E.5.8 Saturation Factor

The 1991 CEB Manual indicated that during splash filling, the saturation concentration was reached or exceeded by misting with a maximum saturation factor of 1.45 (U.S. EPA, 1991). The 1991 CEB Manual also indicated that saturation concentration for bottom filling was expected to be about 0.5 (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the lower bound, upper bound, and mode of the parameter. Because a mode was not provided for this parameter, EPA assigned a mode value of 0.5 for bottom filling as bottom filling minimizes volatilization. This value also corresponds to the typical value provided in the ChemSTEER User Guide for the EPA/OAQPS AP-42 Loading Model (U.S. EPA, 2015).

E.5.9 Container Size

The simulation models based on the ESD for Adhesive Formulation (OECD, 2009a) require volume inputs for import containers and product containers. The underlying distribution of each parameter is not known; therefore, EPA assigned triangular distributions based on the estimated lower bound, upper bound, and mode of each parameter.

EPA assumed facilities receive TCEP in drums based on a prior triphosphates chemical assessment report from Australia's NICNAS stating that TCEP is imported in 200 liter drums (NICNAS, 2001). The ChemSTEER User Guide (U.S. EPA, 2015) recommends a range of 20 to less than 100 gallons for the volume capacity of drums modeled in container-related activities, and the ESD for Adhesive Formulation (OECD, 2009a) suggests 55 gallons for a default container size. Therefore, EPA assigned a lower bound of 20 gallons, an upper bound of 100 gallons, and a mode of 55 gallons for the import container volume distribution.

EPA reviewed product data for identified resin products containing TCEP to develop the minimum, maximum, and mode product container volume. Table_Apx E-16 specifies container sizes for the final resin product formulations identified in data sheets or public comments.

Table_Apx E-16. Product Container Sizes for TCEP-containing Resins

Product	Container Size(s) Information for Product	Approximate Container Size(s) (gallons)	Source Reference
Pitt-Char – XP EP 97-194 Component A	Overall multi-component kit packaging listed as a range of 6.2 kg–26.75 kg with a listed density of 5.28 kg/gal when mixed	1–5	PPG (2008)
J6 Polymers – KA8860	Packaging ranges in size from half-pint to 5 gallons	0.0625–5	J6 Polymers (2021)

The ESD for Adhesive Formulation (OECD, 2009a) suggests 55 gallons for a default container size as a drum. The maximum container volume provided for drums in the ChemSTEER User Guide is 100 gallons (U.S. EPA, 2015). Therefore, EPA set the lower bound product volume to one quart (0.25 gallons) based on a reasonable lower bound approximation of provided product container size values and an upper bound product volume to 100 gallons based on the ChemSTEER User Guide maximum for drums (U.S. EPA, 2015). EPA used five gallons as the product container volume mode based on the data for approximate container sizes from TCEP-containing resin products.

E.5.10 Batch Size

The ESD for Adhesive Formulation (OECD, 2009a) includes data from a single formulator which provided batch sizes ranging from 300 to 5,000 gallons. Additionally, the ESD for Adhesive Formulation assumes a batch size of 1,000 gallons in cases with the known adhesive product density and unknown batch size (OECD, 2009a). The underlying distribution of batch volumes is unknown; therefore, EPA assigned a triangular distribution based on the estimated lower bound, upper bound, and mode of the parameter. EPA assigned batch size lower bound of 300 gallons, upper bound of 5,000 gallons, and mode of 1,000 gallons based on the ESD for Adhesive Formulation (OECD, 2009a).

E.5.11 Hours per Batch

The ESD for Adhesive Formulation (OECD, 2009a) provides default values for the number of batches per day under an assumption of a single production line operating at a facility. The ESD for Adhesive Formulation (OECD, 2009a) recommends a default of one batch per site per day, corresponding to 24 hours per batch for a facility operating 24 hours a day, 7 days a week, with an alternative default of three batches per site per day, corresponding to eight hours per batch for a facility operating 24 hours a day, 7 days a week. EPA assumed that multiple batches may be processed in a single operating day, so the recommended assumption of eight hours per batch from the ESD for Adhesive Formulation (OECD, 2009a) was considered as a typical expected value. The underlying distribution of hours per batch is unknown; therefore, EPA assigned a triangular distribution based on the estimated lower bound, upper bound, and mode of the parameter. EPA set the hours per batch upper bound to 24 hours, lower bound to 8 hours, and mode to 8 hours (OECD, 2009a).

E.5.12 Container Fill Rate

The ChemSTEER User Guide provides a typical fill rate of 20 containers per hour for containers with 20–100 gallons of liquid and a typical fill rate of 60 containers per hour for containers with less than 20 gallons of liquid. Therefore, EPA could not develop a distribution for these parameters and used the single values of 20 containers/hr (20 to 100-gallon containers) or 60 containers/hr (< 20-gallon containers) from the ChemSTEER User Guide (U.S. EPA, 2015).

To account for situations where exposure duration exceeded an 8-hour period in the exposure simulation, EPA applied an equation to determine a corrected fill rate that would replace the deterministic values provided in the ChemSTEER User Guide and included in Table_Apx E-15. The equation for the corrected fill rate in cases where total exposure hours across Exposure Points A, B, C, and D is greater than eight hours is included below. EPA only used the corrected fill rate for Exposure Points A and B in the exposure simulation and did not use it for the release simulation.

Equation E-48

$$if\ 8 < (h_A + h_B + h_C + h_D), \qquad RATE_{fill\_drum} = \frac{2 \times N_{cont\_yr}}{\big(8 - (h_C + h_D)\big) \times OD}$$

Where:

$RATE_{fill\_drum}$ = Corrected fill rate for drums (containers/hr)
N_{cont_yr} = Annual number of import containers (containers/site-year)
h_n = Exposure duration for Exposure Point "n" (hrs/day)
OD = Operating days (days/site-year)

E.5.13 Equipment Cleaning Loss Fraction

The ESD for Adhesive Formulation (OECD, 2009a) recommends using the EPA/OPPT Multiple Process Vessel Residual Model to estimate the releases from equipment cleaning, along with a conservative estimate of equipment cleaning following each batch of product. The EPA/OPPT Multiple Process Vessel Residual Model, as detailed in the ChemSTEER User Guide, provides an overall loss fraction of two percent from equipment cleaning (U.S. EPA, 2015). Therefore, EPA could not develop a distribution of values for this parameter and used a single deterministic value of 2 percent from the ChemSTEER User Guide (U.S. EPA, 2015).

E.5.14 Off-Specification Loss Fraction

The ESD for Adhesive Formulation provides a single default loss fraction of one percent of throughput disposed from off-specification material during manufacturing (OECD, 2009a). The one percent default loss fraction was provided as an estimate from a SRRP study referenced in the ESD for Adhesive Formulation (OECD, 2009a). Therefore, EPA could not develop a distribution of values for this parameter and used a single deterministic loss fraction value of one percent from the ESD for Adhesive Formulation (OECD, 2009a).

E.5.15 TCEP Concentration and Product Density

EPA compiled TCEP concentration and product density information from various resin products containing TCEP to develop distributions for each of these parameters in the simulation. Safety and technical data sheets for TCEP-containing resin products provided either a range or a single value for the TCEP concentration and product density. EPA used the values from the SDSs and TDSs as single input parameters or a range of input parameters for a uniform distribution. EPA developed a "product selector" feature in the simulation which randomly selects a TCEP-containing product for each model iteration. The "product selector" tool provides the appropriate simulation input value or distribution (range) for the TCEP concentration and product density for the selected TCEP-containing product. Product prevalence or market share data were not available, so the product selector tool was designed such that each product in the tool has an equal probability of being selected for each model iteration. Table_Apx E-17 provides the TCEP-containing resin products in the "product selector" tool along with product-specific values used for the tool.

Table_Apx E-17. Product TCEP Concentrations and Densities for Incorporation into Resins OES

Product	TCEP Concentration (Mass Fraction)	Concentration Distribution	Density (kg/m^3)	Source Reference(s)
Pitt-Char – XP PF Part A Base Off White	0.10–0.20	Uniform	1,490 (Specific gravity listed as 1.49)	PPG (2016)
Pitt-Char – XP EP 97-194 Component A	0.10–0.25	Uniform	1,490 (Product density listed as 1.49 g/cm^3 at 20 °C)	PPG (2010)

Product	TCEP Concentration (Mass Fraction)	Concentration Distribution	Density (kg/m^3)	Source Reference(s)
Normet – TamPur RBG Part B	0.01–0.05	Uniform	1,205 (Specific gravity listed as 1.205 at 20 °C)	Normet (2015)
Rampf – RC-0555 Polyurethane System	0.30–0.40	Uniform	1,100 (Specific gravity listed as 1.10)	Rampf (2017)
BJB Enterprises – TC-800 A/B Polyurethane Casting System	0.01–0.05	Uniform	1,150 (Specific gravity listed as 1.15 at 25 °C)	BJB Enterprises (2017)
J6 Polymers JFOAM 6-306-M-T	0.143[a]	Discrete (Single value)	1,220 (Specific gravity listed as 1.22 at 68 °F)	J6 Polymers (2018a) and J6 Polymers (2018c)
J6 Polymers JFOAM 6-308-M-T	0.143[a]	Discrete (Single value)	1,220 (Specific gravity listed as 1.22 at 68 °F)	J6 Polymers (2018b) and J6 Polymers (2018d)

[a] TCEP concentration in single component of 2-part resin calculated using 10 percent TCEP concentration in final resin product provided in public comment (J6 Polymers, 2021) and 70 percent mixing ratio of TCEP-containing component used in the 2-part resin provided in the TDSs (J6 Polymers, 2018c, 2018d). Therefore, EPA calculates 14.3 percent TCEP concentration ([10 TCEP percent after mixing] / [70 percent mixing ratio]) in the TCEP-containing resin component.

E.5.16 Ventilation Rate

The 1991 CEB Manual indicates general ventilation rates in industry range from 500 to 10,000 ft^3/min, with a typical value of 3,000 ft^3/min (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on an estimated lower bound, upper bound, and mode of the parameter. EPA assumed the lower and upper bound using the industry range of 500–10,000 ft^3/min and the mode using the 3,000 ft^3/min typical value (U.S. EPA, 1991).

E.5.17 Mixing Factor

The 1991 CEB Manual indicates mixing factors may range from 0.1 to 1, with 1 representing ideal mixing (U.S. EPA, 1991). The 1991 CEB Manual references the 1988 *ACGIH Ventilation Handbook*, which suggests the following factors and descriptions: 0.67–1 for best mixing; 0.5–0.67 for good mixing; 0.2–0.5 for fair mixing; and 0.1–0.2 for poor mixing (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the defined lower and upper bound and estimated mode of the parameter. The mode for this distribution was not provided; therefore, EPA assigned a mode value of 0.5 based on the typical value provided in the ChemSTEER User Guide for the EPA/OPPT Mass Balance Inhalation Model (U.S. EPA, 2015).

E.6 Incorporation into Articles Model and Approach and Parameters

Appendix E.6 presents the modeling approach and equations used to estimate environmental releases and occupational exposures for TCEP during the incorporation into articles OES. This approach utilizes the ESD on the Use of Adhesives (OECD, 2015) combined with Monte Carlo simulation (a type of stochastic simulation).

Based on the ESD, EPA identified the following release points:

- Release Point 1: Resin component container residue released to water, incineration, or landfill (assessed release to waste disposal);
- Release Point 2: Open surface losses to air during container cleaning;
- Release Point 3: Transfer operation losses to air from unloading the coating component;
- Release Point 4: Equipment cleaning releases to water, incineration, or landfill (assessed release to waste disposal);
- Release Point 5: Open surface losses to air during equipment cleaning;
- Release Point 6: Open surface losses to air during adhesive application (not assessed);
- Release Point 7: Open surface losses to air during curing/drying; and
- Release Point 8: Trimming wastes (not assessed).

Based on the ESD, EPA also identified the following inhalation exposure points:

- Exposure Point A: Transfer operation exposures from unloading the resin;
- Exposure Point B: Container cleaning exposures after unloading the resin;
- Exposure Point C: Exposures from equipment cleaning;
- Exposure Point D: Exposures during application of the resin (not assessed); and
- Exposure Point E: Exposures during curing of the resin.

Environmental releases and occupational exposures for TCEP during incorporation into articles are a function of TCEP's physical properties, container size, mass fractions, and other model parameters. While physical properties are fixed, some model parameters are expected to vary. As described in Appendix E, EPA then used a Monte Carlo simulation to capture variability in the following model input parameters: ventilation rate, mixing factor, air speed, saturation factor, container sizes, time for resin curing, concentration of TCEP in the resin, resin density, and working years. EPA used the outputs from the Monte Carlo simulation to provide estimates of TCEP release amounts and exposure levels for this OES.

E.6.1 Model Equations

Table_Apx E-18 provides the models and associated variables used to calculate environmental releases for each release point within each iteration of the Monte Carlo simulation. Additional equations not based on generic models are below the table. EPA used these environmental releases in order to develop a distribution of release outputs for the incorporation into articles OES. The variables used to calculate each of the following values include deterministic or variable input parameters, known constants, physical properties, TCEP concentrations, conversion factors, and other parameters. The values for these variables are provided in Appendices E.6.2 and E.6.3. The Monte Carlo simulation calculated the total TCEP release (by environmental media) across all release points during each iteration of the simulation. EPA then selected 50th and 95th percentile values to estimate the central tendency and high-end releases, respectively.

Table_Apx E-18. Models and Variables Applied for Release Points in the Incorporation into Articles OES

Release Point	Model(s) Applied	Variables Used
Release Point 1: Resin component container residue released to water, incineration, or landfill (assessed release to waste disposal).	EPA/OPPT Drum Residual Model or EPA/OPPT Small Container Residual Model, based on container size (Appendix E.1)	PV; F_{loss_drums}; $F_{loss\_smallcont}$
Release Point 2: Open surface losses to air during container cleaning.	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_container}$; T; P Operating Time: $N_{prodcont\_yr}$; $RATE_{fill\_drum}$; $RATE_{fill\_smallcont}$
Release Point 3: Transfer operation losses to air from unloading the coating component.	EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; VP; $F_{saturation\_unloading}$; MW_{TCEP}; V_{prod_cont}; R; T; $RATE_{fill\_drum}$; $RATE_{fill\_smallcont}$ Operating Time: $N_{prodcont\_yr}$; $RATE_{fill\_drum}$; $RATE_{fill\_smallcont}$
Release Point 4: Equipment cleaning releases to water, incineration, or landfill (assessed release to waste disposal).	EPA/OPPT Single Process Vessel Residual Model (Appendix E.1)	PV; F_{loss_equip}
Release Point 5: Open surface losses to air during equipment cleaning.	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; D_{equip_clean}; T; P Operating Time: OH_{equip_clean}; $N_{prodcont\_yr}$
Release Point 6: Open surface losses to air during adhesive application (not assessed).	Not assessed; air releases during application of the resin assessed together with releases during curing of the resin	Not applicable
Release Point 7: Open surface losses to air during curing/drying.	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_curing}$; T; P Operating Time: OH_{curing}; $N_{prodcont\_yr}$

Release Point	Model(s) Applied	Variables Used
Release Point 8: Trimming wastes (not assessed).	Not assessed; trimming waste releases for this application method are considered negligible in the ESD	Not applicable

Table_Apx E-19 provides the models and associated variables used to calculate occupational exposures for each exposure point within each iteration of the Monte Carlo simulation. EPA used these occupational exposures in order to develop a distribution of exposure outputs for the incorporation into articles OES. The variables used to calculate each of the following values include deterministic or variable input parameters, known constants, physical properties, TCEP concentrations, conversion factors, and other parameters. The values for these variables are provided in Appendices E.6.2 and E.6.3. The Monte Carlo simulation calculated the TWAs and exposure concentration metrics based on calculated concentrations and exposure durations during each iteration of the simulation, as described in Appendix E. EPA then selected 50th percentile and 95th percentile values to estimate the central tendency and high-end exposures, respectively.

Table_Apx E-19. Models and Variables Applied for Exposure Points in the Incorporation into Articles OES

Exposure Point	Model(s) Applied	Variables Used
Exposure Point A: Transfer operation exposures from unloading the resin	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OAQPS AP-42 Loading Model (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; VP; $F_{saturation\_unloading}$; MW_{TCEP}; V_{prod_cont}; R; T; $RATE_{fill\_drum}$; $RATE_{fill\_smallcont}$; Q; k; Vm Exposure Duration: $N_{prodcont\_yr}$; $RATE_{fill\_drum}$; $RATE_{fill\_smallcont}$; EF
Exposure Point B: Container cleaning exposures after unloading the resin	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_cont-cleaning}$; T; P; Q; k; Vm Exposure Duration: $N_{prodcont\_yr}$; $RATE_{fill\_drum}$; $RATE_{fill\_smallcont}$; EF
Exposure Point C: Exposures from equipment cleaning	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_equip-cleaning}$; T; P; Q; k; Vm Exposure Duration: $N_{prodcont\_yr}$; OH_{EPC}; EF

Exposure Point	Model(s) Applied	Variables Used
Exposure Point D: Exposures during application of the resin (not assessed)	Not assessed; inhalation exposures during application of the resin assessed together with exposures during curing of the resin	Not applicable
Exposure Point E: Exposures during curing of the resin	EPA/OPPT Mass Balance Inhalation Model with vapor generation rate from EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Appendix E.1)	Vapor Generation Rate: F_{TCEP_prod}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{opening\_curing}$; T; P; Q; k; Vm Exposure Duration: see other exposure points

Appendix E.6.4 provides equations and discussion for exposure durations used to calculate TWAs and exposure concentration metrics for each of the exposure points. Note that the number of exposure days is set equal to the number of operating days, or it is fixed at 250 days per year if the number of operating days is greater than 250 days per year.

E.6.2 Model Input Parameters

Table_Apx E-20 summarizes the model parameters and their values for the Incorporation into Articles Monte Carlo simulation. Additional explanations of EPA's selection of the distributions for each parameter are provided in the following subsections.

Table_Apx E-20. Summary of Parameter Values and Distributions Used in the Incorporation into Articles Models

Input Parameter	Symbol	Unit	Deterministic Values	Uncertainty Analysis Distribution Parameters				Rationale/Basis
			Value	Lower Bound	Upper Bound	Mode	Distribution Type	
Air speed	$RATE_{air\_speed}$	cm/s	10	1.3	202.2	—	Lognormal	See Appendix E.6.5
Loss fraction for drums	F_{loss_drums}	kg/kg	0.025	0.017	0.03	0.025	Triangular	See Appendix E.6.6
Loss fraction for small containers	$F_{loss\_smallcont}$	kg/kg	0.003	0.0003	0.006	0.003	Triangular	See Appendix E.6.6
Product container volume	V_{prod_cont}	gal/container	5	0.25	100	5	Triangular	See Appendix E.6.7
Saturation factor unloading	$F_{saturation\_unloading}$	unitless	0.5	0.5	1.45	0.5	Triangular	See Appendix E.6.8
Number of sites	N_s	sites	1	—	—	—	—	"What-if" scenario input
Production volume assessed	PV_lbs	lbs/yr	2,500	—	—	—	—	"What-if" scenario input
Production volume	PV	kg/yr	1,134	—	—	—	—	PV input converted to kilograms
Temperature	T	K	298	—	—	—	—	Process parameter
Pressure	P	torr	760	—	—	—	—	Process parameter
Gas constant	R	L-torr/mol-K	62.36367	—	—	—	—	Universal constant
TCEP vapor pressure	VP	torr	0.0613	—	—	—	—	Physical property
TCEP Molecular Weight	MW_{TCEP}	g/mol	285.49	—	—	—	—	Physical property
Fill rate of drum	$RATE_{fill\_drum}$	containers/hr	20	—	—	—	—	See Appendix E.6.9
Fill rate of small container	$RATE_{fill\_smallcont}$	containers/hr	60	—	—	—	—	See Appendix E.6.9
Loss fraction for equipment cleaning	F_{loss_equip}	kg/kg	0.01	—	—	—	—	See Appendix E.6.10
Hours per equipment cleaning	OH_{equip_clean}	hrs	0.5	—	—	—	—	See Appendix E.6.4

Input Parameter	Symbol	Unit	Deterministic Values	Uncertainty Analysis Distribution Parameters				Rationale/Basis
			Value	Lower Bound	Upper Bound	Mode	Distribution Type	
Diameter of opening for curing	$D_{opening\_curing}$	cm	10	—	—	—	—	See Appendix E.6.11
Diameter of opening for equipment cleaning	$D_{equip\_cleaning}$	cm	10	—	—	—	—	See Appendix E.6.11
Diameter of opening for container	$D_{opening\_container}$	cm	5.08	—	—	—	—	See Appendix E.6.11
Time for drying/curing	OH_{curing}	hr/batch	24	—	—	—	—	See Appendix E.6.12
Product density	$\rho_{product}$	kg/m³	—	Multiple distributions depending on product data			Uniform	See Appendix E.6.12
Product concentration	F_{TCEP_prod}	kg/kg	—	Multiple distributions depending on product data			Uniform	
Ventilation rate	Q	ft³/min	—	500	10,000	3,000	Triangular	See Appendix E.6.13
Mixing factor	k	unitless	—	0.1	1	0.5	Triangular	See Appendix E.6.14

E.6.3 Throughput Parameters

Several throughput parameters are calculated as intermediate values to be used in the model equations during each iteration. The facility production rate is calculated using Equation E-49.

Equation E-49

$$Q_{product} = \frac{PV}{F_{TCEP\_prod} \times N_s}$$

Where:

$Q_{product}$ = Facility production rate (kg/site-yr)
PV = Production volume (kg/yr)
F_{TCEP_prod} = Weight fraction of TCEP in product (unitless)
N_s = Number of sites (sites)

The number of product containers used by a site per year is calculated using Equation E-50.

Equation E-50

$$N_{productcont\_yr} = \frac{Q_{product}}{\rho_{product} \times \left(0.00378541\ \frac{m^3}{gal}\right) \times V_{prod\_cont}}$$

Where:

$N_{productcont\_yr}$ = Annual number of product containers (containers/site-yr)
$Q_{product}$ = Facility production rate (kg/site-yr)
$\rho_{product}$ = Product density (kg/m^3)
V_{prod_cont} = Product container volume (gal/container)

E.6.4 Operating Hours and Exposure Durations

EPA estimated operating hours or hours of duration by direct estimates provided from the ESD on the Use of Adhesives (OECD, 2015) and through calculation from other parameters. The operating times for Release Points 2 and 3 are calculated based on the number of product containers used at the site and the container fill rate, with values provided in Table_Apx E 20. Equation E-51 provides the calculation.

Equation E-51

$$Time_{RP2/3} = \frac{N_{prodcont\_yr}}{RATE_{fill\_drum/smallcont}}$$

Where:

$Time_{RP2/3}$ = Operating time for Release Points 2 and 3 (hrs/site-day)
$N_{prodcont\_yr}$ = Annual number of product containers (containers/site-yr)
$RATE_{fill\_drum/small}$ = Fill rate of container, dependent on volume (containers/hr)

For equipment cleaning, the ESD on the Use of Adhesives provides a default estimate of one hour per batch based on the default for cleaning a single, large vessel(OECD, 2015); however, EPA assumes that the aerospace and aircraft industries will use smaller-scale vessels for application in specialty articles. For cleaning a single, small vessel, the ChemSTEER User Guide provides a default value of 0.5 hours for equipment cleaning time (U.S. EPA, 2015). Therefore, EPA could not develop a distribution of values for this parameter and used the single value of 0.5 hours for operating hours for equipment cleaning. The operating time for Release Point 5 is calculated based on the operating hours per equipment cleaning and the number of product containers per year. Equation E-52 provides the calculation.

Equation E-52

$$Time_{RP5} = OH_{equip\_clean} \times N_{prodcont\_yr}$$

Where:

$Time_{RP5}$ = Operating time for Release Point 5 (hrs/site-day)
OH_{equip_clean} = Operating hours per equipment cleaning (hrs/container)
$N_{prodcont\_yr}$ = Annual number of product containers (containers/site-yr)

The operating hours for Release Point 7 are calculated based on the number of product containers used at the site and the resin curing time, as discussed in Appendix E.6.12. EPA assumes that one full product container is used per article, so the operating hours for cure time is applied for each product container. Equation E-53 provides the calculation.

Equation E-53

$$Time_{RP7} = OH_{curing} \times N_{prodcont\_yr}$$

Where:

$Time_{RP7}$ = Operating time for Release Point 7 (hrs/site-day)
OH_{equip_clean} = Operating hours per resin cure/container (hrs/container)
$N_{prodcont\_yr}$ = Annual number of product containers (containers/site-yr)

Exposure durations for Exposure Points A and B are calculated based on number of product containers used per year or limited to four hours to account for a total 8-hour work-shift across Exposure Points A and B (equivalent exposure durations). Exposure durations for these exposure points are "prioritized" over Exposure Points C and E because Exposure Points A and B contribute the most to total exposure for a single worker. The fill rate for product containers used in this equation for each iteration may be either the default fill rate for drums (if product container ≥ 20 gal) or the default fill rate for small containers (if product container < 20 gal). Exposure durations for Exposure Points A and B are calculated using Equation E-54.

Equation E-54

$$h_{A/B} = \begin{cases} \dfrac{N_{prodcont\_yr}}{RATE_{fill\_drum/small} \times EF}, & 8 > h_A + h_B \\ 4 \qquad\qquad\qquad , & 8 \leq h_A + h_B \end{cases}$$

Where:

h_n = Exposure duration for Exposure Point “n” (hrs/day)
$N_{prodcont\_yr}$ = Annual number of product containers (containers/site-yr)
$RATE_{fill\_drum/small}$ = Fill rate of container, dependent on volume (containers/hr)
EF = Exposure days (days/site-yr)

Exposure durations for Exposure Points C and E are calculated based on number of product containers filled per year and operating hours for the activity, or on remaining work-shift time after accounting for other exposure points. Since EPA assumes a single worker with total maximum exposure duration of eight hours per working day, the 8-hour TWA is estimated using the exposure activities with fixed, default exposures or those with the largest contributions to total exposure. When the total exposure duration per day exceeds eight hours, the calculated durations for Exposure Points C and E are adjusted to calculate a total exposure duration of 8 hours per day. EPA assigned 0.5 operating hours for equipment cleaning per product container (for Exposure Point C), as discussed previously. Exposure duration for Exposure Point C is calculated using Equation E-55.

Equation E-55

$$h_C = \begin{cases} \dfrac{N_{prodcont\_yr} \times OH_{EPC}}{EF}, & 8 \geq \left[h_A + h_B + \dfrac{N_{prodcont\_yr} \times OH_{EPC}}{EF}\right] \\ \left(8 - (h_A + h_B)\right), & 8 < \left[h_A + h_B + \dfrac{N_{prodcont\_yr} \times OH_{EPC}}{EF}\right] \end{cases}$$

Where:

h_n = Exposure duration for Exposure Point “n” (hrs/day)
$N_{prodcont\_yr}$ = Annual number of product containers (container/site-year)
OH_{EPC} = Operating hours for equipment cleaning (hrs/batch)
EF = Exposure days (days/site-year)

EPA determined the resin curing time exposure duration (for Exposure Point E) based on product data as discussed in Appendix E.6.12. Due to the resin curing time operating hours extending longer than the maximum exposure duration per day, the exposure duration for Exposure Point E is calculated as a remainder of the exposure day following Exposure Points A, B, and C. Exposure duration for Exposure Point E is calculated using Equation E-56.

Equation E-56

$$h_E = 8 - (h_a + h_b + h_c)$$

Where:

h_n = Exposure duration for Exposure Point “n” (hrs/day)

E.6.5 Air Speed

Baldwin and Maynard (1998) measured indoor air speeds across a variety of occupational settings in the United Kingdom. A total of 55 work areas were surveyed across a variety of workplaces. EPA analyzed the air speed data from Baldwin and Maynard (1998) and categorized the air speed surveys into settings representative of industrial facilities and representative of commercial facilities. EPA fit separate distributions for these industrial and commercial settings and used the industrial distribution for this OES.

EPA fit a lognormal distribution for the data set as consistent with the authors' observations that the air speed measurements within a surveyed location were lognormally distributed and the population of the mean air speeds among all surveys were lognormally distributed (Baldwin and Maynard, 1998). Since lognormal distributions are bound by zero and positive infinity, EPA truncated the distribution at the largest observed value among all of the survey mean air speeds.

EPA fit the air speed surveys representative of industrial facilities to a lognormal distribution with the following parameter values: mean of 22.414 cm/s and standard deviation of 19.958 cm/s. In the model, the lognormal distribution is truncated at a minimum allowed value of 1.3 cm/s and a maximum allowed value of 202.2 cm/s (largest surveyed mean air speed observed in Baldwin and Maynard (1998)) to prevent the model from sampling values that approach infinity or are otherwise unrealistically small or large (Baldwin and Maynard, 1998).

Baldwin and Maynard (1998) only presented the mean air speed of each survey. The authors did not present the individual measurements within each survey. Therefore, these distributions represent a distribution of mean air speeds and not a distribution of spatially variable air speeds within a single workplace setting. However, a mean air speed (averaged over a work area) is the required input for the model. EPA converted the units to ft/min prior to use within the model equations.

E.6.6 Container Residue Loss Fraction

EPA previously contracted PEI to conduct a study to provide estimates of potential chemical releases during cleaning of process equipment and shipping containers (PEI Associates, 1988). The study used both a literature review of cleaning practices and release data as well as a pilot-scale experiment to determine the amount of residual material left in vessels. The data from literature and pilot-scale experiments addressed different conditions for the emptying of containers and tanks, including various bulk liquid materials, different container constructions (*e.g.*, lined steel drums or plastic drums), and either a pump or pour/gravity-drain method for emptying. EPA reviewed the pilot-scale data from PEI and determined a range and average percentage of residual material remaining in vessels following emptying from drums by either pumping or pouring as well as tanks by gravity-drain (PEI Associates, 1988).

EPA previously used the study results to generate default central tendency and high end-loss fraction values for the residual models (*e.g.*, EPA/OPPT Small Container Residual Model, EPA/OPPT Drum Residual Model) provided in the ChemSTEER User Guide (U.S. EPA, 2015). Previously, EPA adjusted the default loss fraction values based on rounding the PEI study results or due to policy decisions. EPA used a combination of the PEI study results (PEI Associates, 1988) and the ChemSTEER User Guide (U.S. EPA, 2015) default loss fraction values to develop probability distributions for various container sizes.

Specifically, EPA paired the data from the PEI study (PEI Associates, 1988) such that the residuals data for emptying drums by pouring was aligned with the default central tendency and high-end values from the EPA/OPPT Small Container Residual Model, and the residuals data for emptying drums by pumping was aligned with the default central tendency and high-end values from the EPA/OPPT Drum Residual Model. EPA applied the EPA/OPPT Small Container Residual Model to containers with capacities less than 20 gallons, and the EPA/OPPT Drum Residual Model to containers with capacities between 20–100 gallons (U.S. EPA, 2015).

For unloading drums via pouring, the PEI study experiments showed average container residuals in the range of 0.03–0.79 percent with a total average of 0.32 percent (PEI Associates, 1988). The EPA/OPPT Small Container Residual Model recommends a default central tendency loss fraction of 0.3 percent and a high-end loss fraction of 0.6 percent (U.S. EPA, 2015). For unloading drums by pumping, the PEI study experiments showed average container residuals in the range of 1.7–4.7 percent with a total average of 2.6 percent (PEI Associates, 1988).

The EPA/OPPT Drum Residual Model from the ChemSTEER User Guide recommends a default central tendency loss fraction of 2.5 percent and a high-end loss fraction of 3.0 percent (U.S. EPA, 2015). The underlying distribution of the loss fraction parameter for small containers or drums is not known; therefore, EPA assigned a triangular distribution defined by the estimated lower bound, upper bound, and mode of the parameter values. EPA assigned the mode and upper bound values for the loss fraction triangular distributions using the central tendency and high-end values from the respective ChemSTEER model. EPA assigned the lower-bound values for the triangular distributions using the minimum average percent residual measured in the PEI study for the respective drum emptying technique (pouring or pumping) (PEI Associates, 1988).

E.6.7 Product Container Volume

The simulation models based on the ESD on the Use of Adhesives (OECD, 2015) requires an input for volume of resin product containers. The underlying distribution of this parameter is not known; therefore, EPA assigned triangular distributions based on the estimated lower bound, upper bound, and mode of each parameter. EPA reviewed safety and technical data sheets for identified resin products containing TCEP to develop the minimum, maximum, and mode product container volume. Table_Apx E-21 specifies container sizes for the final resin product formulations identified in data sheets.

Table_Apx E-21. Product Container Sizes for TCEP-containing Resins

Product	Container Size(s) Information for Product	Approximate Container Size(s) (gallons)	Source Reference
Pitt-Char – XP EP 97-194 Component A	Overall multi-component kit packaging listed as a range of 6.2–26.75 kg with a listed density of 5.28 kg/gal when mixed	1–5	PPG (2008)
J6 Polymers – KA8860	Packaging ranges in size from half-pint to 5 gallons	0.0625–5	J6 Polymers (2021)

The ESD on the Use of Adhesives suggests 55 gallons for a default container size as a drum (OECD, 2015). The maximum container volume provided for drums in the ChemSTEER User Guide is 100 gallons (U.S. EPA, 2015). Therefore, EPA set the lower bound product volume to one quart (0.25 gallons) based on a reasonable lower bound approximation of provided product container size values and an upper bound product volume to 100 gallons based on the ChemSTEER User Guide maximum for drums. EPA used five gallons as the product container volume mode based on the data for approximate container sizes from TCEP-containing resin products.

E.6.8 Saturation Factor

The 1991 CEB Manual indicated that during splash filling, the saturation concentration was reached or exceeded by misting with a maximum saturation factor of 1.45 (U.S. EPA, 1991). The 1991 CEB Manual also indicated that saturation concentration for bottom filling was expected to be about 0.5 (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the lower bound, upper bound, and mode of the parameter. Because a mode was not provided for this parameter, EPA assigned a mode value of 0.5 for bottom filling as bottom filling minimizes volatilization. This value also corresponds to the typical value provided in the ChemSTEER User Guide for the EPA/OAQPS AP-42 Loading Model (U.S. EPA, 2015).

E.6.9 Container Fill Rate

The ChemSTEER User Guide provides a typical fill rate of 20 containers per hour for containers with 20–100 gallons of liquid and a typical fill rate of 60 containers per hour for containers with less than 20 gallons of liquid. EPA estimates unload rates for containers as equivalent to the fill rates. Therefore, EPA could not develop a distribution for these parameters and used the single values of 20 containers per hour or 60 containers per hour from the ChemSTEER User Guide (U.S. EPA, 2015).

E.6.10 Equipment Cleaning Loss Fraction

The ESD on the Use of Adhesives recommends using the EPA/OPPT Single Process Vessel Residual Model to estimate the releases from equipment cleaning, along with a conservative estimate of equipment cleaning following each batch of resin (OECD, 2015). The EPA/OPPT Single Process Vessel Residual Model, as detailed in the ChemSTEER User Guide, provides an overall loss fraction of 1 percent from equipment cleaning (U.S. EPA, 2015). Therefore, EPA could not develop a distribution of values for this parameter and used a single deterministic value of 1 percent from the ChemSTEER User Guide (U.S. EPA, 2015).

E.6.11 Diameters of Opening

The ChemSTEER User Guide (U.S. EPA, 2015) indicates diameters for the openings for various vessels that may hold liquids in order to calculate vapor generation rates during different activities. In the simulation developed for the Incorporation into Articles OES based on the ESD on the Use of Adhesives (OECD, 2015), EPA used default diameters of vessels from the ChemSTEER User Guide for container cleaning, application equipment cleaning, and curing activities (U.S. EPA, 2015). For each of these activities, EPA assumed a single default value; therefore, EPA could not develop a distribution of values and used the single value as a deterministic parameter. For container cleaning activities, the ChemSTEER User Guide indicates a single default value of 5.08 cm (U.S. EPA, 2015). For application equipment cleaning and resin curing activities, EPA applied the EPA/OPPT Penetration Model default value of 10 cm for diameter of opening, which is based on diameter of a 4-inch beaker opening (U.S. EPA, 2015). EPA assumed the 10 cm default value to account for smaller scales of resin curing and application conditions expected for this OES, which may include blending two-part resins in a beaker or venting over smaller surface areas during curing.

E.6.12 Product Data (Concentration, Density, and Curing Time)

EPA compiled TCEP concentration and product density information from various resin products containing TCEP to develop distributions for each of these parameters in the simulation. SDSs and TDSs for TCEP-containing resin products provided either a range or a single value for the TCEP concentration and product density. EPA used the values from the SDSs and TDSs as single input parameters or a range of input parameters for a uniform distribution. EPA developed a “product selector” feature in the simulation which randomly selects a TCEP-containing product for each model iteration. The “product selector” tool provides the appropriate simulation input value or distribution (range) for the TCEP concentration, product density, and resin curing time for the selected TCEP-containing product. The tool was designed such that each product in the tool has an equal probability of being selected for each model iteration. Table_Apx E-22 below provides the TCEP-containing resin products in the "product selector" tool along with product-specific concentration and density values used for the tool.

Table_Apx E-22. Product TCEP Concentrations and Densities for Incorporation into Articles OES

Product	TCEP Concentration (Mass Fraction)	Concentration Distribution	Density (kg/m^3)	Source Reference(s)
Pitt-Char – XP PF Part A Base Off White	0.10–0.20	Uniform	1,490 (Specific gravity listed as 1.49)	PPG (2016)
Pitt-Char – XP EP 97-194 Component A	0.10–0.25	Uniform	1,490 (Product density listed as 1.49 g/cm^3 at 20 °C)	PPG (2010)
Normet – TamPur RBG Part B	0.01–0.05	Uniform	1,205 (Specific gravity listed as 1.205 at 20 °C)	Normet (2015)
Rampf – RC-0555 Polyurethane System	0.30–0.40	Uniform	1,100 (Specific gravity listed as 1.10)	Rampf (2017)
BJB Enterprises – TC-800 A/B Polyurethane Casting System	0.01–0.05	Uniform	1,150 (Specific gravity listed as 1.15 at 25 °C)	BJB Enterprises (2017)
J6 Polymers JFOAM 6-306-M-T	0.143[a]	Discrete (Single value)	1,220 (Specific gravity listed as 1.22 at 68 °F)	J6 Polymers (2018a) and J6 Polymers (2018c)
J6 Polymers JFOAM 6-308-M-T	0.143[a]	Discrete (Single value)	1,220 (Specific gravity listed as 1.22 at 68 °F)	J6 Polymers (2018b) and J6 Polymers (2018d)

[a] TCEP concentration in single component of 2-part resin calculated using 10 percent TCEP concentration in final resin product provided in public comment (J6 Polymers, 2021) and 70 percent mixing ratio of TCEP-containing component used in the 2-part resin provided in the TDSs (J6 Polymers, 2018c, 2018d). Therefore, EPA calculates 14.3 percent TCEP concentration ([10 TCEP percent after mixing] / [70 percent mixing ratio]) in the TCEP-containing resin component.

For the curing time, EPA assigned a value of 24 hours across all products based on available curing information for J6 Polymers products near room temperature (approximately 25 °C, or 298 K), with the TDSs stating, "if post-curing is not possible, allow part to remain in mold 18–24 hours" (J6 Polymers, 2018c, 2018d). EPA assumed the terms of "post-cure" used in the product data sheets more accurately represent the time for curing to a hardened resin, with significantly reduced potential for diffusion of TCEP within the resin and vaporization from the surface. While vapor generation rate may vary over the course of the cure time, EPA conservatively assumed the vapor generation rate during the cure time period is constant based on the initial liquid formulation.

E.6.13 Ventilation Rate

The 1991 CEB Manual indicates general ventilation rates in industry range from 500 to 10,000 ft^3/min, with a typical value of 3,000 ft^3/min (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on an estimated lower bound, upper bound, and mode of the parameter. EPA assumed the lower and upper bound using the industry range of 500–10,000 ft^3/min and the mode using the 3,000 ft^3/min typical value (U.S. EPA, 1991).

E.6.14 Mixing Factor

The 1991 CEB Manual indicates mixing factors may range from 0.1 to 1, with 1 representing ideal mixing (U.S. EPA, 1991). The 1991 CEB Manual references the 1988 *ACGIH Ventilation Handbook*, which suggests the following factors and descriptions: 0.67–1 for best mixing; 0.5–0.67 for good mixing; 0.2–0.5 for fair mixing; and 0.1–0.2 for poor mixing (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the defined lower and upper bound and estimated mode of the parameter. The mode for this distribution was not provided; therefore, EPA assigned a mode value of 0.5 based on the typical value provided in the ChemSTEER User Guide for the EPA/OPPT Mass Balance Inhalation Model (U.S. EPA, 2015).

E.7 Use in Laboratory Chemicals Model and Approach and Parameters

Appendix E.7 presents the modeling approach and equations used to estimate environmental releases and occupational exposures for TCEP during the Use in Laboratory Chemicals OES. This approach utilized the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023) combined with Monte Carlo simulations (a type of stochastic simulation).

Based on the GS, EPA identified the following release points from laboratory operations:

- Release Point 1: Release during unloading of liquids;
- Release Point 2: Release during unloading of solids;
- Release Point 3: Release from cleaning transport container;
- Release Point 4: Open surface losses to air during container cleaning;
- Release Point 5: Labware equipment cleaning;
- Release Point 6: Open surface losses during equipment cleaning;
- Release Point 7: Releases to air during laboratory analyses; and
- Release Point 8: Release from disposal.

Based on the GS, EPA also identified the following inhalation exposure points:

- Exposure Point A: Exposure during handling;
- Exposure Point B: Exposure from unloading;
- Exposure Point C: Exposure from container cleaning;
- Exposure Point D: Exposure from equipment cleaning;
- Exposure Point E: Exposure from laboratory analyses; and

- Exposure Point F: Exposure from disposal

Environmental releases and occupational exposure for TCEP during laboratory uses are a function of TCEP's physical properties, container size, mass fractions, and other model parameters. While some parameters are fixed, others are expected to vary. EPA used a Monte Carlo simulation to capture variability in the following model input parameters: ventilation rate, mixing factor, air speed, saturation factor, loss factor, container sizes, working years, and drum fill rates. EPA used the outputs from a Monte Carlo simulation with 100,000 iterations and the Latin Hypercube sampling method in @RISK to calculate release amounts and exposure concentrations for this OES.

E.7.1 Model Equations

Table_Apx E-23 provides the models and associated variables used to calculate environmental releases for each release point within each iteration of the Monte Carlo simulation. EPA used these environmental releases to develop a distribution of release outputs for the Use in Laboratory Chemicals OES. The variables used to calculate each of the following values include deterministic or variable input parameters. The values for these variables are provided in Appendices E.7.2 and E.7.3. The Monte Carlo simulation calculated the total TCEP release (by environmental media) across all release points during each iteration of the simulation. EPA then selected 50th and 95th percentile values to estimate the central tendency and high-end releases, respectively.

Table_Apx E-23. Models and Variables Applied for Release Points in the Use of Laboratory Chemicals OES

Release Point	Model(s) Applied	Variables Used
Release Point 1: Release during unloading of liquid	EPA/OAQPS AP-42 Loading Model (Equation E-3)	Vapor Generation Rate: F_{TCEP}; VP; $F_{saturation\_unloading}$; MW_{TCEP}; Q_{cont}; R; T; $RATE_{fill\ smallcont}$ Operating Time: $RATE_{fill\_smallcont}$; $N_{cont\ unload\ yr}$; OP_{days}
Release Point 2: Release during unloading of solids	Not assessed; release is not expected since TCEP is a liquid at room temperature	Not applicable
Release Point 3: Release from cleaning transport container	EPA/OPPT Small Container Residual Model (Equation E-5)	$Q_{chem\ site\ day\ (recalc)}$; $F_{loss\_smallcont}$; OP_{days}
Release Point 4: Open surface losses to air during container cleaning	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Equation E-1 and Equation E-2)	Vapor Generation Rate: F_{TCEP}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{container}$; T; P Operating Time: $RATE_{fill\_smallcont}$; $N_{cont\ unload\ yr}$; OP_{days}
Release Point 5: Labware equipment cleaning	EPA/OPPT Multiple Process Residual Model (Equation E-5)	$Q_{chem\ site\ day\ (recalc)}$; F_{loss_equip}; OP_{days}

Release Point	Model(s) Applied	Variables Used
Release Point 6: Open surface losses during equipment cleaning	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Equation E-1 and Equation E-2)	Vapor Generation Rate: F_{TCEP}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{container}$; T; P Operating Time: OH_{equip}
Release Point 7: Releases to air during laboratory analyses	EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Equation E-1 and Equation E-2)	Vapor Generation Rate: F_{TCEP}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{container\ lab\ analysis}$; T; P Operating Time: $OH_{sampling}$
Release Point 8: Release from disposal	No model applicable; all chemicals used in the laboratory are expected to be disposed at the end of each working day. Remaining chemical not released from the previous release points is released here	Not applicable

Table_Apx E-24 provides the models and associated variables used to calculate occupational exposures for each exposure point within each iteration of the Monte Carlo simulation. EPA used these occupational exposures to develop a distribution of exposure outputs for the Use in Laboratory Chemicals OES. EPA assumed that the same worker performed each exposure activity during a full-shift, resulting in a total exposure duration of up to 8–12 hours per day. Details about the determination of a full-shift of 8–12 hours of exposure are described in Appendix E.7.5. The variables used to calculate each of the following exposure concentrations and durations include deterministic or variable input parameters, known constants, physical properties, conversion factors, and other parameters. The values for these variables are provided in Appendices E.7.2 and E.7.3. The Monte Carlo simulation calculated a full-shift TWA exposure concentration for each iteration using the exposure concentration and duration associated with each activity and assuming exposures outside the exposure activities were zero. EPA then selected 50th and 95th percentile values to estimate the central tendency and high-end exposure concentrations, respectively.

Table_Apx E-24. Models and Variables Applied for Exposure Points in the Use of Laboratory Chemicals OES

Exposure Point	Model(s) Applied	Variables Used
Exposure Point A: Full-shift exposure for all Activities	No model applicable	This exposure is only to be assessed when evaluating exposures across all activities. EPA decided to assess exposures across individual activities, therefore this exposure point is not applicable.
Exposure Point B: Exposure from unloading	EPA/OPPT Mass Balance Inhalation Model (Equation E-6) with vapor generation rate from EPA/OAQPS AP-42 Loading Model (Equation E-3)	Vapor Generation Rate: F_{TCEP}; VP; $F_{saturation\_unloading}$; MW_{TCEP}; Q_{cont}; R; T; $RATE_{fill\ smallcont}$; Q; k; Vm

Exposure Point	Model(s) Applied	Variables Used
		Exposure Duration: $RATE_{fill\_smallcont}$; $N_{cont\ unload\ yr}$; EF_{yearly}
Exposure Point C: Exposure from container cleaning	EPA/OPPT Mass Balance Inhalation Model (Equation E-6) with vapor generation rate from EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Equation E-1 and Equation E-2)	Vapor Generation Rate: F_{TCEP}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{container}$; T; P; Q; k; Vm Exposure Duration: $RATE_{fill\_smallcont}$; $N_{cont\ unload\ yr}$; EF_{yearly}
Exposure Point D: Exposure from equipment cleaning	EPA/OPPT Mass Balance Inhalation Model (Equation E-6) with vapor generation rate from EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Equation E-1 and Equation E-2)	Vapor Generation Rate: F_{TCEP}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{container}$; T; P; Q; k; Vm Exposure Duration: OH_{equip}
Exposure Point E: Exposure from laboratory analyses	EPA/OPPT Mass Balance Inhalation Model (Equation E-6) with vapor generation rate from EPA/OPPT Penetration Model or EPA/OPPT Mass Transfer Coefficient Model, based on air speed (Equation E-1 and Equation E-2)	Vapor Generation Rate: : F_{TCEP}; MW_{TCEP}; VP; $RATE_{air\_speed}$; $D_{container\ lab\ analysis}$; T; P; Q; k; Vm Exposure Duration: $OH_{sampling}$
Exposure Point F: Exposure from disposal	No model applicable	This exposure is non-quantifiable and expected to be less than potential exposures from all other activities. Workers place waste into containers or other receptacles, where they are fully contained for disposal.

Appendix E.7.7 provides equations and discussion for exposure durations used to calculate TWAs and exposure concentration metrics for each of the exposure points.

E.7.2 Model Input Parameters

Table_Apx E-25 summarizes the model parameters and their values for the Use in Laboratory Chemicals Monte Carlo simulation. Additional explanations of EPA's selection of the distributions for each parameter are provided in the following subsections.

6472 **Table_Apx E-25. Summary of Parameter Values and Distributions Used in the Use in Laboratory Chemicals Models**

Input Parameter	Symbol	Unit	Deterministic Values	Uncertainty Analysis Distribution Parameters				Rationale/Basis
			Value	Lower Bound	Upper Bound	Mode	Distribution Type	
Air speed	$RATE_{air\_speed}$	cm/s	10	1.3	202.2	—	Lognormal	See Appendix E.7.8
Loss fraction for small containers	$F_{loss\_smallcont}$	kg/kg	0.003	0.0003	0.006	0.003	Triangular	See Appendix E.7.9
Saturation factor unloading	$F_{saturation\_unloading}$	unitless	0.5	0.5	1.45	0.5	Triangular	See Appendix E.7.11
Daily throughput of stock solutions	$Q_{stock\_site\_day}$	mL/site-day	2,000	0.5	4,000	2,000	Triangular	See Appendix E.7.3
Diameter of laboratory analysis containers	$D_{container\_lab\_analysis}$	cm	2.5	2.5	10	2.5	Triangular	See Appendix E.7.14
Operating days	$TIME_{operating\_days}$	days/yr	260	173	261	260	Triangular	See Appendix E.7.5
Number of sites	N_s	sites	Manual input	—	—	—	—	"What-if" scenario input
Production volume assessed	PV_lbs	lbs/yr	2,500 or 25,000	—	—	—	—	"What-if" scenario input
Production volume	PV	kg/yr	1,134 or 11,340	—	—	—	—	PV input converted to kilograms
Temperature	T	K	298	—	—	—	—	Process parameter
Pressure (torr)	P_torr	torr	760	—	—	—	—	Process parameter
Pressure (atm)	P_atm	atm	1	—	—	—	—	Process parameter
Gas constant	R	L-torr/mol-K	62.36367	—	—	—	—	Universal constant
TCEP vapor pressure	VP	torr	0.0613	—	—	—	—	Physical property
TCEP molecular weight	MW_{TCEP}	g/mol	285.49	—	—	—	—	Physical property
Molar volume	Vm_{TCEP}	L/mol	24.45	—	—	—	—	Physical property

Input Parameter	Symbol	Unit	Deterministic Values	Uncertainty Analysis Distribution Parameters				Rationale/Basis
			Value	Lower Bound	Upper Bound	Mode	Distribution Type	
Fill rate of small container	$RATE_{fill\_smallcont}$	containers/hr	60	—	—	—	—	See Appendix E.7.12
Container volume	Q_{cont}	gal/container	1	—	—	—	—	See Appendix E.7.10
Loss fraction for equipment cleaning	F_{loss_equip}	kg/kg	0.02	—	—	—	—	See Appendix E.7.13
Hours per equipment cleaning	OH_{equip_clean}	hrs	4	—	—	—	—	See Appendix E.7.7
Hours per analysis sampling	$OH_{sampling}$	hrs	1					See Appendix E.7.7
Diameter of opening for container	$D_{opening\_container}$	cm	5.08	—	—	—	—	See Appendix E.7.14
Product density	$\rho_{product}$	kg/m^3	—	Multiple distributions depending on product data			Uniform	See Appendix E.7.15
Product concentration	F_{TCEP_prod}	kg/kg	—	Multiple distributions depending on product data			Uniform	
Ventilation rate	Q	ft^3/min	—	500	10,000	3,000	Triangular	See Appendix E.7.16
Mixing factor	k	unitless	—	0.1	1	0.5	Triangular	See Appendix E.7.17

E.7.3 Number of Sites

The *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023) provides a method of determining the number of laboratory sites based on the total annual production volume and annual throughput per site of the chemical of interest. The total annual production volume ranges from 2,500 and 25,000 lb per year (see Section 3.10.3). The annual throughput per site of TCEP is determined according to Appendix E.7.4.

Equation E-57

$$N_s = \frac{PV_{site}}{Q_{chem\ site\ yr}}$$

Where:

N_s = Number of sites (site)
PV = Annual production volume (kg/yr)
$Q_{chem\ site\ yr}$ = Annual throughput of TCEP (kg/site-yr)

E.7.4 Throughput Parameters

The *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023) provides daily throughput of TCEP required for laboratory stock solutions. According to the GS, laboratory liquid use rate ranges from 0.5 mL up to 4 liters per day. Laboratory stock solutions are used for multiple analyses and eventually need to be replaced. The expiration or replacement times range from daily to six months (U.S. EPA, 2023). For this scenario, EPA assumes stock solutions are prepared daily. Therefore, EPA assigned a triangular distribution for the daily throughput of laboratory stock solutions with upper and lower bounds corresponding to the high and low throughputs, which are 4,000 and 0.5 mL respectively, with a mode of 2,000 mL. The daily throughput of TCEP is calculated using Equation E-58.

Equation E-58

$$Q_{chem\ site\ day} = \frac{Q_{stock\ site\ day}}{\rho_{product} \times F_{TCEP\ prod} \times 1{,}000\,\frac{L}{m^3} \times 1{,}000\,\frac{mL}{L}}$$

Where:

$Q_{chem\ site\ day}$ = Daily throughput of TCEP (kg/site-day)
$Q_{stock\ site\ day}$ = Daily throughput of stock solutions (kg/site-day)
$\rho_{product}$ = Product density (kg/m^3)
$F_{TCEP\ prod}$ = Weight fraction of TCEP in product (unitless)

The annual throughput of TCEP is calculated using Equation E-59 by multiplying the daily throughput by the number of operating days. The number of operating days is determined according to Appendix E.7.6.

Equation E-59

$$Q_{chem\ site\ yr} = Q_{chem\ site\ day} \times TIME_{operating\ days}$$

Where:

$Q_{chem\ site\ yr}$ = Annual throughput of TCEP (kg/site-yr)
$Q_{chem\ site\ day}$ = Daily throughput of TCEP (kg/site-day)
$TIME_{operating\ days}$ = Operating days (days/yr)

The annual throughput of TCEP cannot exceed the production volume limit of 2,500 or 25,000 lb per year. Therefore, in the event an iteration of the simulation does calculate an annual throughput greater than the production volume limit, EPA set the number of sites equal to one, and the annual throughput equal to the total annual production volume. The model then recalculated the number of operating days using Equation E-60 below.

Equation E-60

$$TIME_{operating\ days\ (recalc)} = \frac{PV}{N_s \times Q_{chem\ site\ day}}$$

Where:

$TIME_{operating\ days\ (recalc)}$ = Recalculated number of operating days (days/yr)
PV = Annual production volume (kg/yr)
N_s = Number of sites (site)
$Q_{chem\ site\ day}$ = Daily throughput of TCEP (kg/site-day)

E.7.5 Number of Containers Unloaded Annually per Site

EPA estimated the number of containers unloaded annually per site using the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023), as well as other parameters. The total number of containers unloaded annually per site is calculated based on the annual throughput (see Appendix E.7.4), product concentration (see Appendix E.7.15), and container volume (see Appendix E.7.10). The total number of containers unloaded annually per site is calculated using Equation E-61 below.

Equation E-61

$$N_{cont\ unload\ yr} = \frac{Q_{chem\ site\ yr}}{F_{TCEP\ prod} \times Q_{cont}}$$

Where:

$N_{cont\ unload\ yr}$ = Number of containers unloaded annually per site (containers/site-yr)
$Q_{chem\ site\ yr}$ = Annual throughput of TCEP (kg/site-yr)
$F_{TCEP\ prod}$ = Weight fraction of TCEP in product (unitless)
Q_{cont} = Container volume (gal/container)

E.7.6 Operating Days and Days Exposed per Year

The *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023), estimates the number of operating days from employment data obtained through the U.S. Bureau of Labor Statistics (BLS) Occupational Employment Statistics. The U.S. BLS assumes the operating duration per NAICS code or a ‘year-round, full-time’ hours figure, to be 2,080 hours (U.S. EPA, 2023). Using this annual duration and an assumed daily shift lengths of 8-,10-, and 12-hours per day, EPA calculated 260, 208, and 174 operating days per year, respectively.

The number of exposure days is dependent on the worker activity frequency (U.S. EPA, 2023); however, EPA did not find industry-specific information on the frequency of the worker activities. Generally, the number of exposure days is less than or equal to the number of operating days and can be estimated by multiplying the number of operating days ($TIME_{operating\ days)}$) by the fraction of operating days during which there is worker exposure ($F_{exposure}$). EPA typically assumes that workers are potentially exposed up to 250 days per year (based on working 5 days per week for 50 weeks per year). Assuming the 260 operating days per year results in a $F_{exposure}$ of 0.962 (250 exposure days divided by 260 operating days, which equals to 0.962). Exposure days are calculated using Equation E-62.

Equation E-62

$$EF_{yearly} = TIME_{operating\ days} \times F_{exposure}$$

Where:

EF_{yearly} = Number of exposure days (days/yr)
$TIME_{operating\ days}$ = Operating days (days/yr)
$F_{exposure}$ = Fraction of operating days with worker exposure (0.962 day exposure/day operation)

For the Laboratory Chemicals scenario, EPA assumes 8-, 10-, and 12-hours shifts and calculates 250, 200, and 167 days per year, respectively, using Equation E-62.

E.7.7 Operating Hours and Exposure Durations

EPA estimated operating hours or exposure duration using the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023), as well as other parameters and equations. The operating hours for Release Points 1 and 4 are calculated using the number of product containers used at the site, the container fill rate, and operating days (see Appendix E.7.5). Equation E-63 provides the calculation.

Equation E-63

$$Time_{RP1/4} = \frac{N_{cont\ unload\ yr}}{TIME_{operating\ days\ (recalc)} * RATE_{fill\_smallcont}}$$

Where:

$Time_{RP1/4}$ = Operating times for Release Points 1 and 4 (hrs/site-day)
$N_{cont\ unload\ yr}$ = Number of containers unloaded annually per site (containers/site-yr)
$TIME_{operating\ days\ (recalc)}$ = Recalculated number of operating days (days/yr)
$RATE_{fill\_smallcont}$ = Fill rate of small container (containers/hr)

For equipment cleaning, *the Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* uses the multiple vessel model with a default release and exposure duration of four hours per day (U.S. EPA, 2023). Therefore, EPA assumes four hours per day as both the release and exposure duration for Release Point 6 and Exposure Point D.

For laboratory analyses, the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* provides a default release and exposure estimate of one hour per day based on the default for sampling (U.S. EPA, 2023). EPA assumes one hour per day for Release Point 7 and Exposure Point E.

Exposure durations for Exposure Points B and C are calculated based on the number of product containers used at the site, the container fill rate, and days exposed per year. In the event the exposure duration associated with Exposure Points B and C resulted in total exposure duration that exceeds the shift duration (either 8-, 10- or 12-hrs), EPA assumed that there are multiple workers each performing a different subset of tasks during their shift. For this analysis, EPA used the full-shift TWA for a worker performing activities for Exposure Points D and E (a total of five hours) with the remainder of their day split between Exposure Points B and C (either 1.5-, 2.5-, or 3.5-hours/day per activity). The exposure duration calculation and logic for Exposure Points B and C is shown in Equation E-64. The fill rate for product containers used in this equation is 60 containers per hour (see Appendix E.7.12) based on the container size of 1 gallon (see Appendix E.7.10).

Equation E-64

$$h_{B/C} = \begin{cases} \dfrac{N_{cont\ unload\ yr}}{RATE_{fill\ smallcont} * EF_{yearly}}, & Shift\ duration - h_D - h_E > h_B + h_C \\ 1.5\,, & Shift\ duration - h_D - h_E \leq h_B + h_C;\ 8\ hour\ shift \\ 2.5, & Shift\ duration - h_D - h_E \leq h_B + h_C;\ 10\ hour\ shift \\ 3.5, & Shift\ duration - h_D - h_E \leq h_B + h_C;\ 12\ hour\ shift \end{cases}$$

Where:

$h_{B/C}$ = Exposure duration for Exposure Point B or C (hrs/day)
$N_{cont\ unload\ yr}$ = Number of containers unloaded annually per site (containers/site-yr)
$RATE_{fill\_smallcont}$ = Fill rate of small container (containers/hr)
EF_{yearly} = Number of exposure days (days/yr)

Exposure from Exposure Point F for disposal of laboratory waste are non-quantifiable and expected to be less than potential exposures from the other activities assessed by the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023). Workers are expected to place laboratory waste into containers or other receptacles, where they are fully contained for disposal to prevent volatilizations or spills/leaks of chemicals while awaiting final off-site disposal. While there may be residual chemicals in the laboratory waste that workers handle, the concentration of TCEP is expected to be lower than that in other activities because, at this point, it is mixed with other reagents and the sample material. TCEP may have also been fully consumed during the analysis. Due to the amounts of other reagents and sample volumes and potential consumption of TCEP, the TCEP exposure is non-quantifiable for this activity (U.S. EPA, 2023).

E.7.8 Air Speed

Baldwin and Maynard (1998) measured indoor air speeds across a variety of occupational settings in the United Kingdom. A total of 55 work areas were surveyed across a variety of workplaces. EPA analyzed the air speed data from Baldwin and Maynard (1998) and categorized the air speed surveys into settings representative of industrial facilities and representative of commercial facilities. EPA fit separate distributions for these industrial and commercial settings and used the industrial distribution for this OES.

EPA fit a lognormal distribution for the data set as consistent with the authors’ observations that the air speed measurements within a surveyed location were lognormally distributed and the population of the mean air speeds among all surveys were lognormally distributed (Baldwin and Maynard, 1998). Since lognormal distributions are bound by zero and positive infinity, EPA truncated the distribution at the largest observed value among all of the survey mean air speeds.

EPA fit the air speed surveys representative of industrial facilities to a lognormal distribution with the following parameter values: mean of 22.414 cm/s and standard deviation of 19.958 cm/s. In the model, the lognormal distribution is truncated at a minimum allowed value of 1.3 cm/s and a maximum allowed value of 202.2 cm/s (largest surveyed mean air speed observed in Baldwin and Maynard (1998)) to prevent the model from sampling values that approach infinity or are otherwise unrealistically small or large (Baldwin and Maynard, 1998).

Baldwin and Maynard (1998) only presented the mean air speed of each survey. The authors did not present the individual measurements within each survey. Therefore, these distributions represent a distribution of mean air speeds and not a distribution of spatially variable air speeds within a single workplace setting. However, a mean air speed (averaged over a work area) is the required input for the model. EPA converted the units to ft/min prior to use within the model equations.

E.7.9 Container Residue Loss Fraction

EPA previously contracted PEI to conduct a study to provide estimates of potential chemical releases during cleaning of process equipment and shipping containers (PEI Associates, 1988). The study used both a literature review of cleaning practices and release data as well as a pilot-scale experiment to determine the amount of residual material left in vessels. The data from literature and pilot-scale experiments addressed different conditions for the emptying of containers and tanks, including various bulk liquid materials, different container constructions (*e.g.*, lined steel drums or plastic drums), and either a pump or pour/gravity-drain method for emptying. EPA reviewed the pilot-scale data from PEI and determined a range and average percentage of residual material remaining in vessels following emptying from drums by either pumping or pouring as well as tanks by gravity-drain (PEI Associates, 1988).

EPA previously used the study results to generate default central tendency and high end-loss fraction values for the residual models (*e.g.*, EPA/OPPT Small Container Residual Model, EPA/OPPT Drum Residual Model) provided in the ChemSTEER User Guide (U.S. EPA, 2015). Previously, EPA adjusted the default loss fraction values based on rounding the PEI study results or due to policy decisions. EPA used a combination of the PEI study results (PEI Associates, 1988) and the ChemSTEER User Guide (U.S. EPA, 2015) default loss fraction values to develop probability distributions for various container sizes.

Specifically, EPA paired the data from the PEI study (PEI Associates, 1988) such that the residuals data for emptying drums by pouring was aligned with the default central tendency and high-end values from the EPA/OPPT Small Container Residual Model, and the residuals data for emptying drums by pumping was aligned with the default central tendency and high-end values from the EPA/OPPT Drum Residual Model. EPA applied the EPA/OPPT Small Container Residual Model to containers with capacities less than 20 gallons, and the EPA/OPPT Drum Residual Model to containers with capacities between 20–100 gallons (U.S. EPA, 2015).

For unloading drums via pouring, the PEI study experiments showed average container residuals in the range of 0.03–0.79 percent with a total average of 0.32 percent (PEI Associates, 1988). The EPA/OPPT Small Container Residual Model recommends a default central tendency loss fraction of 0.3 percent and a high-end loss fraction of 0.6 percent (U.S. EPA, 2015). For unloading drums by pumping, the PEI study experiments showed average container residuals in the range of 1.7–4.7 percent with a total average of 2.6 percent (PEI Associates, 1988).

The EPA/OPPT Drum Residual Model from the ChemSTEER User Guide recommends a default central tendency loss fraction of 2.5 percent and a high-end loss fraction of 3.0 percent (U.S. EPA, 2015). The underlying distribution of the loss fraction parameter for small containers or drums is not known; therefore, EPA assigned a triangular distribution defined by the estimated lower bound, upper bound, and mode of the parameter values. EPA assigned the mode and upper bound values for the loss fraction triangular distributions using the central tendency and high-end values from the respective ChemSTEER model. EPA assigned the lower-bound values for the triangular distributions using the minimum average percent residual measured in the PEI study for the respective drum emptying technique (pouring or pumping) (PEI Associates, 1988).

E.7.10 Product Container Volume

EPA did not identify container sizes for TCEP use in laboratories from available literature. Therefore, EPA assumes that TCEP is transported in one-liter containers to small vials for use per the *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023).

E.7.11 Saturation Factor

The 1991 CEB Manual indicated that during splash filling, the saturation concentration was reached or exceeded by misting with a maximum saturation factor of 1.45 (U.S. EPA, 1991). The 1991 CEB Manual also indicated that saturation concentration for bottom filling was expected to be about 0.5 (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the lower bound, upper bound, and mode of the parameter. Because a mode was not provided for this parameter, EPA assigned a mode value of 0.5 for bottom filling as bottom filling minimizes volatilization. This value also corresponds to the typical value provided in the ChemSTEER User Guide for the EPA/OAQPS AP-42 Loading Model (U.S. EPA, 2015).

E.7.12 Container Fill Rate

The ChemSTEER User Guide provides a typical fill rate of 60 containers per hour for containers with less than 20 gallons of liquid (U.S. EPA, 2015).

E.7.13 Equipment Cleaning Loss Fraction

The *Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* recommends using the EPA/OPPT Multiple Process Residual Model to estimate the releases from equipment cleaning (U.S. EPA, 2023). The EPA/OPPT Multiple Process Residual Model, as detailed in the ChemSTEER User Guide, provides an overall loss fraction of two percent from equipment cleaning (U.S. EPA, 2023).

E.7.14 Diameters of Opening

The ChemSTEER User Guide (U.S. EPA, 2015) indicates diameters for the openings for various vessels that may hold liquids in order to calculate vapor generation rates during different activities. In the simulation developed for the *Use in Laboratory Chemicals OES based on the Use of Laboratory Chemicals – Generic Scenario for Estimating Occupational Exposures and Environmental Releases* (U.S. EPA, 2023), EPA used default diameters of vessels from the ChemSTEER User Guide (U.S. EPA, 2015) for container and equipment cleaning, and laboratory analyses. For container and equipment cleaning, EPA assessed a single value of 5.08 cm (U.S. EPA, 2015). For laboratory analyses, EPA applied the EPA/OPPT Penetration Model and assumed two container sizes for sampling liquid product. For a typical release estimate, the model assumes sampling occurs from a 2.5 cm diameter bottle opening; and for a worst-case release estimate, the model assumes sampling occurs from a 10 cm diameter beaker opening. The underlying distribution for laboratory container sizes is not known, therefore, EPA assigned this parameter a triangular distribution with lower bound of 2.5 cm, upper bound or 10 cm, and mode of 2.5 cm.

E.7.15 Product Data (Concentration and Density)

EPA compiled TCEP concentration and product density information from laboratory products containing TCEP to develop distributions for concentration and density in the simulation. SDSs and TDSs for TCEP laboratory products provided a single value for the TCEP concentration and product density in each product. Therefore, EPA used the values from the SDSs and TDSs as discrete input parameters. EPA did not have information on the prevalence or market share of different laboratory products in commerce; therefore, EPA assumed a uniform distribution of laboratory products. The model first selects a laboratory product for the iteration and then based on the product selected, selects a concentration and density associated with that product. Table_Apx E-26 provides the TCEP-containing laboratory products used in the model along with product-specific concentration and density values used.

Table_Apx E-26. TCEP Concentrations and Densities for Use in Laboratory Chemicals OES

Product	TCEP Concentration (Mass Fraction)	Concentration Distribution	Density (kg/m^3)	Source Reference
Tris(2-chloroethyl) phosphate NG-13718	1.00	Discrete (Single value)	1,430 (Density listed as 1.4249 g/cm^3 at 20 °C)	Chem Service (2015)
Tris(2-chloroethyl) phosphate SC-229621	0.98	Discrete (Single value)	1,390 (Liquid density listed as 1.39 g/mL)	Santa Cruz Biotechnology (2018)
Tris(2-chloroethyl) phosphate 119660	1.00	Discrete (Single value)	1,390 (Relative density listed as 1.39 g/cm^3 at 25 °C)	Sigma-Aldrich (2019)
Tris(2-chloroethyl) phosphate P0268	0.97	Discrete (Single value)	1,430 (Relative density listed as 1.43)	TCI America (2018)

E.7.16 Ventilation Rate

The 1991 CEB Manual indicates general ventilation rates in industry range from 500 to 10,000 ft^3/min, with a typical value of 3,000 ft^3/min (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on an estimated lower bound, upper bound, and mode of the parameter. EPA assumed the lower and upper bound using the industry range of 500–10,000 ft^3/min and the mode using the 3,000 ft^3/min typical value (U.S. EPA, 1991).

E.7.17 Mixing Factor

The 1991 CEB Manual indicates mixing factors may range from 0.1 to 1, with 1 representing ideal mixing (U.S. EPA, 1991). The 1991 CEB Manual references the 1988 *ACGIH Ventilation Handbook*, which suggests the following factors and descriptions: 0.67–1 for best mixing; 0.5–0.67 for good mixing; 0.2–0.5 for fair mixing; and 0.1–0.2 for poor mixing (U.S. EPA, 1991). The underlying distribution of this parameter is not known; therefore, EPA assigned a triangular distribution based on the defined lower and upper bound and estimated mode of the parameter. The mode for this distribution was not provided; therefore, EPA assigned a mode value of 0.5 based on the typical value provided in the ChemSTEER User Guide for the EPA/OPPT Mass Balance Inhalation Model (U.S. EPA, 2015).