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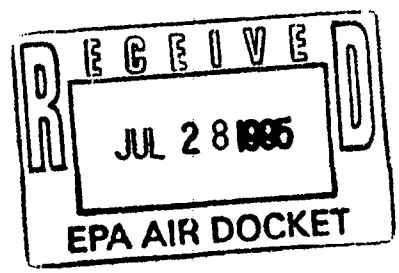
Transoft U.S., Inc.
818 Reedy Creek Road
Cary, North Carolina 27513

July 25, 1995

Mr. Joe Moeltner
OAR Regulatory Docket
Mailstop 6102
U.S. Environmental Protection Agency
401 M Street, SW
Washington, D.C. 20460



Dear Mr. Moeltner:

Please place this letter and the attached summary pages (two copies enclosed) of our Fluidyn-PANACHE model into docket AQM-95-01, Category C: Technical Material for Review and Comment. This model is being submitted for consideration for a future proposal that would adopt it as an Appendix B model in the Guideline on Air Quality Models. This model will be discussed at the Sixth Conference on Air Quality Modeling for which this docket has been established.

Fluidyn-PANACHE is a self-contained, 3-dimensional high precision fluid mechanics computer code which is designed to simulate pollution dispersion under different conditions. This easy-to-use software employs an automatic mesh generator and deterministic simulation system that enables the user to investigate accurately continuous and short term pollution dispersion in a wide range of conditions (e.g., complex terrain, and any number of obstacles and pollutant sources). A built-in chemistry module enhances the computer code for studies evaluating chemically active primary and secondary pollutant studies.

Readers of the public are encouraged to submit written comments to the docket. If members of the public have technical or availability related questions, they can contact Henley Jones at Transoft U.S., Inc. by calling (919) 380-7500.

Sincerely,

Henley Jones

Henley Jones
Manager, Business Development
Transoft U.S., Inc.

Fluidyn-PANACHE

Reference: Transoft Group, 1994. User's Guide of Fluidyn-PANACHE for a Three-Dimensional Deterministic Simulation of Pollutants Dispersion Model for Complex Terrain, Cary, North Carolina.

Availability: This computer code is available from: Transoft US, Inc.,
818, Reedy Creek Road
Cary North Carolina 27513-3307
Tel: (919) 380-7500 Fax: (919) 380-7592

Abstract: Fluidyn-PANACHE is an Eulerian (and Lagrangian for particulate matter), 3D Finite Volume fluid mechanics code designed to simulate continuous and short-term pollution dispersion in the atmosphere, in simple or complex terrain. Pollutants can be emitted from stack, point, area, volume or general sources. Emissions can also be emitted by distant sources, entering into the domain with wind. The modeling code automatically treats obstacles, single or multiple sources, the effects of vertical temperature stratification on the wind and diffusion fields, and turbulent shear flows caused by atmospheric boundary layer or terrain effects. It solves Navier Stokes equations in a curvilinear mesh espousing the terrain and obstacles. A 2nd order resolution helps keep the number of cells limited in case of shearing flow. The mesh generator, the solver and the numerical schemes have been adopted for atmospheric flows with or without chemical reactions. The modeling code operates on any workstation or any PC 486 computer.

a. Recommendations for Regulatory Use

Panache is appropriate for the following types of situations:

1. industrial or urban zone on a flat or complex terrain, with or without obstacles;
2. transport distance from a few meters to 50 kilometers;
3. continuous releases with hourly, monthly or annual averaging times;
4. calm stratified or turbulent weather;
5. chemically reactive or non-reactive gases or particulate emissions;
6. emergency planning and management for episodic emissions.

Various options can be selected for regulatory applications: stack, point, general, volume or area sources; buoyancy induced dispersion (BID) with either full gravity, Boussinesq approximation or no gravity. For highway pollutant dispersion, a special module is available taking into account the heat and turbulence due to vehicular movement.

Following modules enhance the applicability of the model into multiple areas:

1. Scavenging, Acid Rain: A built-in absorption module for water droplets traveling through a plume considers the absorption and de-absorption effects of the pollutants by the droplet. Evaporation and chemical reactions with gases are also taken into account;
2. Visibility: Predicts plume visibility and surface deposition of aerosol;
3. Particulate matter: A module with a stochastic distribution of particle diameters calculates settling and dry deposition of particles. The exchange of mass, momentum and heat between particles and gas is treated with implicit coupling procedures.

4. Ozone formation: For street level ozone formation in the presence of sunlight, a special photochemical module is available.

b. Input Requirements

Data may be input directly from an external source (e.g., GIS file) or interactively. The model provides the option to use default values when input parameters are unavailable.

PANACHE user environment integrates the pre- and post-processor with the solver. The calculations can be done interactively or in batch mode. An inverse scheme is provided to estimate missing data from a few measured values of the wind.

Terrain data requirements:
1. Location, surface roughness estimates, and altitude contours;
2. Location and dimensions of obstacles, forests, fields, and water bodies.

Source data requirements:
1. For stack, point, area, general (e.g., reservoirs and pipes), and volume sources: dimensions;
2. For all types of sources, the exit temperature and plume mass flow rates and concentration of each of the pollutants are required. External sources require mass flow rate;
3. For roadways: estimated traffic and emissions for cars and trucks.

Meteorological data requirements:
Hourly stability class, wind direction, wind speed, temperature, cloud cover, humidity, and mixing height data with lapse rate below and above it.
Primary meteorological variables available from the National Weather Service can be prepared using the PCRAMMET pre-processor, to form an array for later use.

Data required at the domain boundary:
Wind profile (uniform, log or power law); depending on the terrain conditions (e.g., residential area, forest, and sea, etc.)

Chemical source data requirements:
A database of selected species with specific heats and molecular weights can be extended by the user. For heavy gases the database includes a compressibility coefficients table.

Solar reflection:
For an accurate transient calculation of natural convection on a sunny day, approximate values of temperature for fields, forests, water bodies, shadows and their variations with the time of the day are determined automatically.

c. Output

Printed output option: pollutant concentration at receptor points, and listing of input data (terrain, chemical, weather, and source data) with turbulence and precision control data.

Graphical output includes:
In 3D perspective or in any crosswind, downwind or horizontal plane: wind velocity, pollutant

concentration, 3D isosurface. The profile of concentration can be obtained along any line on the terrain. The concentration contours can be either instantaneous or time integrated for the emission from a source or a source combination. A special utility is included to help prepare a report or a video animation. The user can select images, put in annotations, or do animation.

d. Type of Model

It uses an Eulerian (and Lagrangian for particulate matter) 3D Finite Volume model solving full Navier-Stokes equations. The numerical diffusion is low with appropriate turbulence models for building wakes. A second order resolution may be sought to limit the diffusion. The numerical scheme is self adaptive for the following situations:

1. A curvilinear mesh or a chopped Cartesian mesh is generated automatically or manually;
2. Thermal and gravity effects are simulated by full gravity (heavy gases) besides no gravity (well mixed light gases at ambient temperature) methods or Boussinesq approximation methods;
3. K-diff, K-e or a boundary layer turbulence models are used for turbulence calculations. The flow behind obstacles such as buildings, is calculated by using a modified K-e.

For heavy gases, a 3D heat conduction from the ground and a stratification model for heat exchange from the atmosphere are used (with anisotropic turbulence).

e. Pollutant Types

All kinds of gases, particulate matter, droplets or heavy gases from fixed or mobile sources.

f. Source-Receptor Relationship

Simultaneous use of multiple kinds of sources at user defined locations. Any number of user defined receptors can identify pollutants from each source individually.

g. Plume Behavior

The options influencing the behavior are full gravity, Boussinesq approximation or no gravity.

h. Horizontal Winds

Horizontal wind speed approximations are made only at the boundaries based on National Weather Service data. Inside the domain of interest, full Navier-Stokes resolution with natural viscosity is used for 3D terrain and temperature dependent wind field calculation.

i. Vertical Wind Speed

Vertical wind speed approximations are made only at the boundaries based on National Weather Service data. The domain of interest is treated as for horizontal winds.

j. Horizontal Dispersion

Diffusion is calculated using appropriate turbulence models. A 2nd order solution for shearing flow can be sought when the number of meshes is limited between obstacles.

k. Vertical Dispersion

Dispersion by full gravity unless Boussinesq approximation or no gravity requested. Vertical dispersion is treated as above for horizontal dispersion.

l. Chemical Transformation

Fluidyn-PANCHEM, an atmospheric chemistry module for chemical reactions, is available. Photochemical reactions are used for tropospheric ozone calculations.

m. Physical Removal

Physical removal is treated using dry deposition coefficients

n. Evaluation Studies

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Tripathi, Sharad, 1994. Evaluation of Fluidyn-PANACHE on Heavy Gas Dispersion Test Case. Seminar on Evaluation of Models of Heavy Gas Dispersion Organized by European Commission, Mol, Belgium.