Second-order Closure Integrated PUFF Model (SCIPUFF)

Reference

Sykes, R.I., S.F. Parker, D.S. Henn, C.P. Cerasoli and L.P. Santos, 1998. PC-SCIPUFF Version 1.2PD Technical Documentation. ARAP Report No. 718. Titan Corporation, Titan Research & Technology Division, ARAP Group, P.O. Box 2229, Princeton, NJ, 08543-2229.

Availability

SCIPUFF Version 1.2PD and its technical documentation are available for downloading from the the model developer's website (*www.titan.com/systems/prod.htm*) or by contacting: Dr. R. Ian Sykes, Titan Research & Technology, ARAP Group, P.O. Box 2229, Princeton, NJ 08543-2229. Phone: (609) 452-2950.

Abstract

SCIPUFF is a Lagrangian puff dispersion model that uses a collection of Gaussian puffs to represent an arbitrary, three-dimensional, time-dependent concentration field. The turbulent diffusion parameterization is based on modern turbulence closure theory, specifically the second-order closure model of Donaldson (1973) and Lewellen (1977), which provides a direct relationship between the predicted dispersion rates and the measurable turbulent velocity statistics of the wind field. In addition to the average concentration value, the closure model also provides a prediction of the statistical variance in the concentration field resulting from the random fluctuations in the wind field. The closure approach also provides a direct representation for the effect of averaging time (Sykes and Gabruk, 1997).

Shear distortion is accurately represented using the full Gaussian spatial moment tensor, rather than simply the diagonal moments, and an efficient puff splitting/merging algorithm minimizes the number of puffs required for a calculation. In order to increase calculation efficiency, SCIPUFF uses a multi-level time-stepping scheme with an appropriately sized time-step for each puff. An adaptive multi-grid is used to identify neighboring puffs in the spatial domain, which greatly reduces the search time for overlapping puffs in the interaction calculation and puff-merging algorithm. Static puffs are used to represent the steady-state phase of the plume near the source and are updated only with the meteorology, also decreasing the number of puffs needed for the calculation.

SCIPUFF can model many types of source geometries and material properties. It can use several types of meteorological input, including surface and upper-air observations or three-dimensional gridded data. Planetary boundary layer turbulence is represented explicitly in terms of surface heat flux and shear stress using parameterized profile shapes. A Graphical User Interface (GUI) that runs on a PC is used to define the problem scenario, run the dispersion calculation and produce color contour plots of resulting concentrations. The GUI also includes an online 'Help'.

a. Recommendations for Regulatory Use

SCIPUFF is appropriate for modeling both short and long range (greater than 50km) transport, steady or non-steady state emissions of primary pollutants (gases or particles), buoyant or neutral sources using time-dependent meteorological data (surface, profile, or gridded). Shear distortion, complex terrain, linear chemical transformations, gravitational settling and deposition are treated. In addition to the mean concentration, dose and deposition, SCIPUFF provides an estimate of the probability levels of the predicted values. The model may be used on a case-by-case basis.

b. Input Requirements

Source Data:

1. Pollutant physical and chemical properties are input by the user, including the chemical decay rates and deposition velocities. Multiple pollutants may be defined for a single release and size distributions may be defined for particles.

2. Release types are specified, e.g., continuous (arbitrary duration), instantaneous, mobile, and stack sources. Input requirements for each source depend on the release type and include emission rate and duration for each material type and size group as well as source coordinates, elevation and size.

Meteorological Data (different forms of meteorological input can be used by SCIPUFF):

1. Fixed winds: Wind speed and direction is assumed constant.

2. Observational input: Time-dependent observations are combined from multiple surface stations and/or upper-air profiles. A pre-processor is available that can be used to convert input to the Industrial Source Complex Short Term (ISCST) model to SCIPUFF's input format for surface data.

3. Time-dependent 3-dimensional gridded input.

Terrain data can be included with the gridded meteorological input files or provided as a separate file for other input types.

Turbulence Data (two types of turbulence input may be specified optionally):

1. Planetary boundary layer: Vertical profiles of the boundary layer scale turbulent velocity fluctuations, heat flux and turbulence length scales can be provided as input by the user or modeled based on boundary layer characteristics. Options for treatment of the boundary layer include "calculated", "observed" or "simple diurnal". Input requirements depend on boundary layer treatment type.

2. Large scale variability: For long range transport, the mesoscale horizontal velocity fluctuations and turbulence length scale may be specified by the user, computed from a theoretical model or read from a meteorological observation file.

Other Input:

Receptor locations are provided by the user in a 'sampler' file that includes the receptor locations and heights and the name of the material to be sampled. Other data requirements include the coordinates of the domain, duration of the calculation, averaging time and user-specified model options.

c. Output

Color contour plots can be viewed upon completion of a run at user-specified times. Available plots include: horizontal instantaneous slice, vertical instantaneous slice, vertically integrated slice, integrated surface dose, and integrated surface deposition for either the mean concentration or probability levels. The user can input the desired location of the slices and view these locations one at a time after completion of the run. Plots can be animated over the simulation time based on user-specified time intervals. Tables of data (in ASCII-format) can be exported from the plots by clicking on desired locations with the mouse or a grid may be specified.

If a sampler (i.e., receptor) file was specified on input, an ASCII file of time-dependent concentrations at each sampler location is produced as output. Surface integrals of dose and deposition are stored as adaptive grid files with multiple time breaks in direct access binary format. The puff file is a binary file that contains the complete puff data at a number of time breaks.

d. Type of Model

SCIPUFF is a time-dependent Gaussian puff model that employs second-order closure turbulence modeling techniques to relate the dispersion rate to velocity fluctuation statistics.

e. Pollutant Types

SCIPUFF may be used to model the dispersion of primary pollutants (gases or particles) which are inert or undergo linear chemical reactions, e.g., CO, NO_2, SO_2, PM-10, PM-2.5.

f. Source-Receptor Relationships

The time-dependent concentrations are calculated as the sum of the contribution from all puffs. The maximum number of continuous sources is 400. The maximum number of instantaneous sources is limited by the maximum number of puffs, which is 20,000. The maximum number of discrete receptors is 200. SCIPUFF uses an adaptive grid to compute concentrations on a plane and produces color contour plots upon the completion of a run. If desired, discrete receptors or grid receptor concentration values may be exported from the contour plot to an ASCII file. To obtain the individual contribution from each source, no additional runs are necessary, however, an extra pollutant needs to be released from each source which has the same properties as the pollutant of interest but a unique name.

g. Plume Behavior

Plume rise is treated through the conservation of buoyancy and momentum. A turbulent entrainment model based on earlier work on power plant plume rise (Sykes *et al.*, 1988) relates the turbulent velocity to the vertical rise rate. Complex terrain is treated through the reflection in the local surface tangent plane. Fumigation is treated explicitly according to the modeled boundary layer behavior. Aerodynamic downwash is not treated.

h. Horizontal Winds

Horizontal winds may be specified by the user as constant, provided in a time-dependent 3-

dimensional gridded meteorological file, or in multiple surface observations and/or upper-air profiles. Surface data and vertical profiles from multiple stations are interpolated in space and time. The arbitrary spatial locations at each observation time are interpolated onto a grid using a simple inverse square weighting. Velocity (and temperature) fields are then interpolated between the grid times to provide smoothly varying meteorology for the dispersion calculation. In the surface layer, a similarity profile which accounts for surface roughness and stability is used. A 3-dimensional mass-consistent wind field may be generated optionally.

i. Vertical Wind Speed

Unless provided in a time-dependent 3-dimensional gridded meteorological file, vertical wind speed is assumed zero. A 3-dimensional mass-consistent wind field may be generated optionally.

j. Horizontal Dispersion

Puff growth is based on second-order closure turbulence modeling involving the horizontal turbulent velocity fluctuations and length scales that are either provided as input or modeled. Wind shear effects are also treated. The effect of averaging time is explicitly represented by selectively filtering the assumed turbulence spectrum.

k. Vertical Dispersion

Puff growth is based on second-order closure turbulence modeling involving the vertical turbulent velocity fluctuations and length scales that are either provided as input or modeled. Turbulent vertical drift, buoyancy-forces and wind shear effects are also treated. Perfect reflection is assumed at the ground surface and, for a convective boundary layer, at the mixing height. The effect of averaging time is explicitly represented by selectively filtering the assumed turbulence spectrum.

l. Chemical Transformation

Linear chemical transformations are treated using exponential decay (decay rate is provided by the user).

m. Physical Removal

Deposition of gases and particles, and precipitation washout and gravitational settling of particles are treated. Gaseous dry deposition effects are based on a fixed deposition velocity provided by the user. Dry deposition of particles to vegetative canopies is based on the approach of Slinn (1982) which includes determining a particle deposition efficiency. Dry deposition of particles to non-vegetative rough surfaces and water is treated according to Lewellen and Sheng (1980). Gravitational settling effects are determined by the particle fall velocity which is obtained from the balance between gravitational acceleration and the aerodynamic drag force. Precipitation washout of particles is treated through the use of a scavenging coefficient that is a function of precipitation rate and particle size following the approach of Seinfeld (1986). Precipitation washout of gases is not treated.

n. Evaluation Studies

Sykes, R.I., W.S. Lewellen, S.F. Parker and D.S. Henn, 1988. A hierarchy of dynamic plume models incorporating uncertainty, Volume 4: Second-order Closure Integrated Puff, EPRI, EPRI EA-6095 Volume 4, Project 1616-28.

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Sykes, R.I., D.S. Henn, S.F. Parker and R.S. Gabruk, 1996. SCIPUFF - A generalized hazard dispersion model. Preprint of the 76th AMS Annual Meeting, Ninth Joint Conference on the Applications of Air Pollution Meteorology with A&WMA, 184-188.

Sykes, R.I. and R.S. Gabruk, 1997. A second-order closure model for the effect of averaging time on turbulent plume dispersion. *J. Appl. Meteor.*, **36**: 165-184.

o. Literature Cited

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