8.2 SCIPUFF CAPABILITIES AND APPLICATION IN HAZARD ASSESSMENT

R. Ian Sykes *
Sage Management Enterprise, Princeton NJ

1. INTRODUCTION

SCIPUFF, Second-order Closure Integrated PUFF, is an atmospheric dispersion model using the Gaussian puff methodology to provide a three-dimensional, time-dependent Lagrangian solution to the turbulent diffusion equations. Originally developed for the prediction of power plant plume impacts under the sponsorship of EPRI (Electric Power Research Institute), SCIPUFF has been extensively enhanced under DoD (Department of Defense) funding, and now describes a wide range of phenomena beyond buoyant plume rise and turbulent diffusion.

2. LAGRANGIAN PUFF TECHNIQUE

The time-dependent concentration field is represented as a collection of overlapping Gaussian puffs, where the Gaussian shape is described by a total mass, a centroid location, and measure of the spatial spread. The puffs are transported as Lagrangian elements, providing a grid-independent description of diffusion in inhomogeneous, time-dependent meteorology. The puff methodology can also describe multiple releases of multiple materials simultaneously. with arbitrary time-dependent and spatial characteristics.

In SCIPUFF, the spatial Gaussian spread is represented in a general tensor form using the full second-moments of the concentration field, including the off-diagonal moments, so that shear distortion can be accurately described. The transport equation for the spatial moments is based on second-order turbulence closure theory, which directly relates the diffusion rates to the measurable velocity statistics. This provides a methodology that is valid over all scales, and provides a rational basis for the treatment of time averaging effects based on the assumed shape of the velocity fluctuation spectrum (Sykes and Gabruk, 1997). The closure model gives an idealized prediction that is consistent with the analytical results of Taylor (1921) for absolute dispersion, and Richardson (1926) for relative diffusion.

The evolution equation for the spatial spread moments is written as

$$\frac{d\sigma_{ij}}{dt} = \sigma_{ik}\frac{\partial \overline{u}_j}{\partial x_k} + \sigma_{jk}\frac{\partial \overline{u}_i}{\partial x_k} + \frac{\left\langle x_i'\overline{u_j'c'}\right\rangle}{Q} + \frac{\left\langle x_j'\overline{u_i'c'}\right\rangle}{Q}$$

where σ_{ij} is the moment tensor, Q is the material mass in the puff, and the angle brackets indicate an integral over the puff. The first two terms represent shear distortion, and the last two are the spatial moments of the turbulent concentration flux, which is responsible for diffusion. The flux moment equations are derived from the closure model as

$$\frac{d}{dt}\left\langle x_i'\overline{u_j'c'}\right\rangle = Q\overline{u_i'u_j'} - A\frac{q}{\Lambda}\left\langle x_i'\overline{u_j'c'}\right\rangle$$

where $q^2 = \overline{u_i'u_i'}$ is the turbulent velocity scale, Λ is the turbulent length scale, and A is a closure constant with a value of 0.75.

3. SCIPUFF MODEL CAPABILITIES

The closure model provides a natural framework for predicting the concentration fluctuation variance, since this is a second-order quantity. The concentration fluctuations are driven by the turbulent velocity fluctuations and represent a statistical uncertainty in any measured concentration value. Using an assumed probability distribution shape for the fluctuations, based on the predicted mean and variance, we can provide a quantitative probability prediction for the concentration.

Since the fluctuation variance is a nonlinear quantity, we need to extend the simple puff model, where each puff moves and evolves independently, by calculating the overlap contributions from puffs that are closely located. The variance is predominantly controlled by the turbulent dissipation, and modeling this term requires an evolution for an internal fluctuation length scale. Results for the fluctuation intensity compared with the laboratory experiments of Fackrell and Robins (1982) are shown in Figure 1.

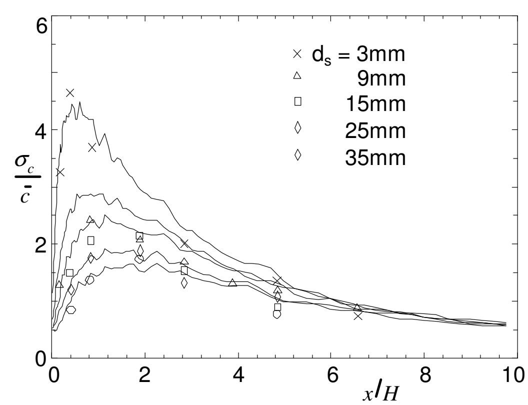

Fig. 1. SCIPUFF prediction of centerline fluctuation intensity in an elevated plume for different source sizes. Symbols are data from Fackrell and Robins (1982), model predictions are solid lines.

The implementation of the puff overlap calculations in SCIPUFF enables other nonlinear processes to be described. Specifically, some of the major dynamics processes can be represented by providing evolution

**Corresponding author address*: R. Ian Sykes, Sage Management, 15 Roszel Road, Suite 102, Princeton NJ 08540; e-mail: ian.sykes@sage-mgt.net.

equations for integrated momentum and buoyancy for each puff, and assuming simple spatial shape functions for the associated velocity fields (Sykes et al. 1999). The equations for the integrated moments are based on the Navier-Stokes conservation equations, and give a reasonable representation of buoyant jets and dense gas slumping effects. Figure 2 shows an idealized calculation of two buoyant plumes in a vertical shear environment.

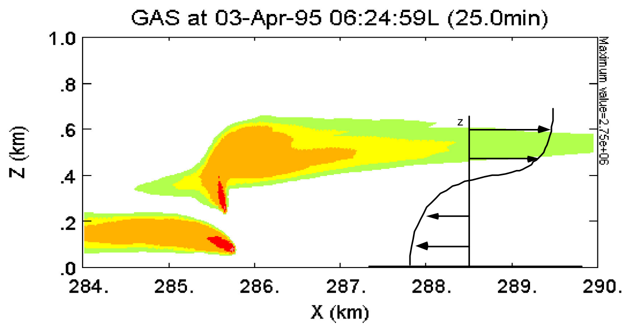

Fig. 2. SCIPUFF prediction of buoyant plumes in a simplified wind shear.

In addition to dynamics, SCIPUFF can also represent evaporating droplets and the associated thermodynamics effects. Figure 3 shows a flashing chlorine jet with initial upward momentum, but the cooling associated with the evaporation generates a cold chlorine vapor cloud which then slumps on the ground.

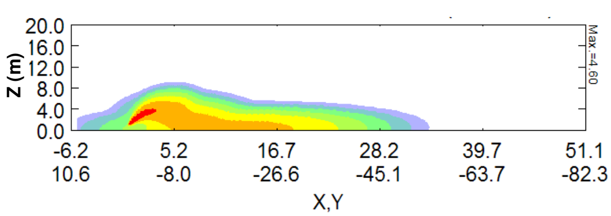

Fig. 3. SCIPUFF prediction of flashing chlorine jet.

As a final example, SCIPUFF has also been enhanced to describe nonlinear gas phase chemical reactions. The puff overlap calculations are used to estimate the total Gaussian-weighted concentration of each chemical species for each puff. The chemical reaction mechanism is used to determine the effective change in concentrations over a timestep, and the puff species masses are adjusted in proportion to their contribution to the concentration. Figure 4 shows the SCIPUF prediction of ozone depletion and subsequent formation downwind of a NOx source, using the Carbon Bond Mechanism.

4. SCIPUFF MODEL NUMERICAL FEATURES

A key feature of SCIPUFF is the splitting/merging algorithms which improve the representation of inhomogeneous meteorology. The shear and diffusion terms in the moment equations are based on local

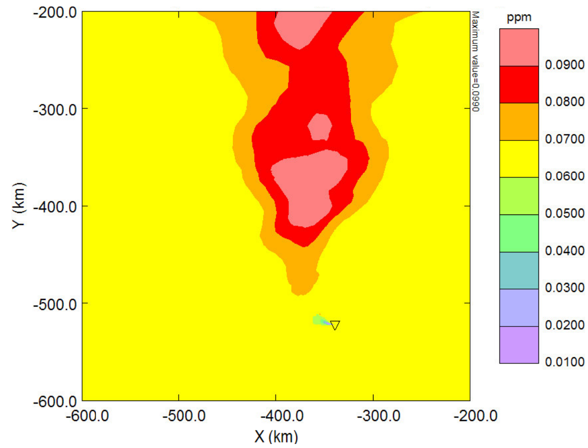

Fig. 4. SCIPUFF prediction of ozone downwind of a NOx source, shown as the small triangle in the lower half of the plot.

values of wind, wind shear and turbulence, and cannot accurately represent more complex fields. Puffs are split, conserving all the moments, when they reach a size comparable with the scale of the meteorological grid; similarly, puffs are merged when they grow large enough to overlap their neighbors sufficiently.

SCIPUFF uses adaptive timesteps and adaptive spatial grids to represent concentration, dosage, and deposition fields. These techniques are well suited to Lagrangian models, where very large ranges of scales need to be represented. Near the source, puffs may have scales of a few meters or less, but the model is required to calculate effects at ranges up to 1000's of kilometers.

SCIPUFF has been evaluated using a wide range of field experiments, ranging from the short range CONFLUX experiments with downwind range of several meters up to the ANATEX and ETEX continental scale experiments.

5. ROLE IN HAZARD MODELING SYSTEMS

SCIPUFF is the atmospheric dispersion modeling component of two US Department of Defense hazard prediction systems. The systems are HPAC, Hazard Prediction and Assessment Capability and JEM, the Joint effects Model, HPAC is developed by the Defense Threat Reduction Agency and JEM is a DoD Program of Record under the Joint Program Executive Office for Chemical and Biological Defense (JPEO CBD). The two systems are described at:

http://www.dtra.mil/rd/programs/acec/hpac.cfm, and

https://jacks.jpeocbd.army.mil/jacks/Public/FactSheetProvider.aspx?productId=335

Both of these systems comprise much more than the SCIPUFF dispersion model. They also include:

- *source term models for various incidents*
  - *weapon deployments*
  - *facilities attacks or explosive events*
- *human effects models*
  - *chemical/biological effects*
  - *nuclear radiation*
  - *global population database*
  - *casualty estimation*
- *urban dispersion nested models*
  - *building database*
- *meteorological data servers*
  - *forecast and observations*
  - *global terrain database*

These capabilities are essential for predicting hazard effects. The availability of meteorological data is crucial, and must be provided in a timely manner. Also, the prediction of human effects is an important aspect, for consequence assessment. The broad range of capabilities in SCIPUFF has been developed to provide the atmospheric dispersion calculation, linking the source term models with the human effects models. A sample output display from HPAC is shown in Figure 5.

5. REFERENCES

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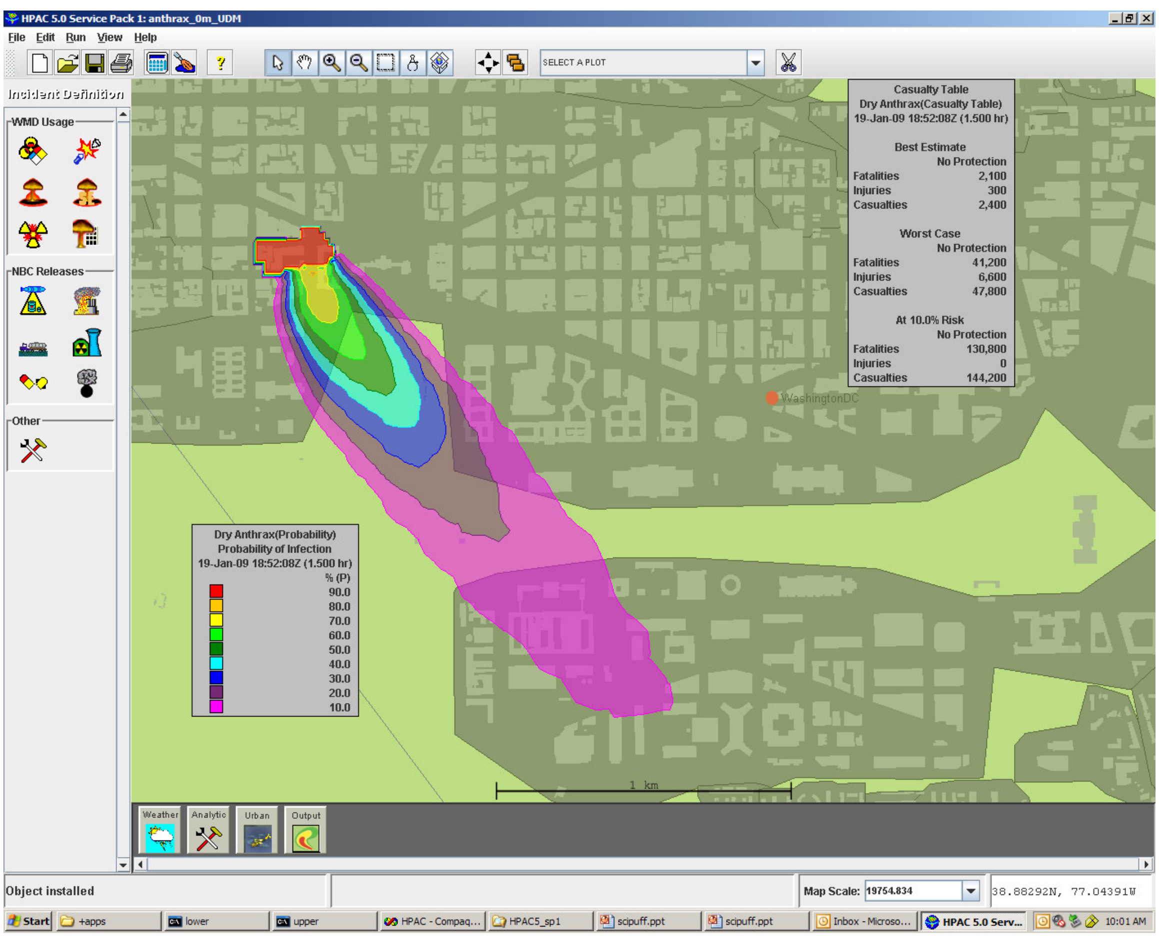

Figure 5. Sample HPAC output display illustrating the building effects submodel, building database, and human effects output with casualty estimation