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SECOND ORDER CLOSURE INTEGRATED PUFF (SCIPUFF) MODEL VERIFICATION AND EVALUATION STUDY

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Executive Summary

The results of this verification and evaluation study refer to SCIPUFF as contained in HPAC version 2.0. It is noted that HPAC 3.0 was released in October 1997, and that improvements over HPAC 2.0 have been made. The summary given below is organized according to the four main tasks undertaken by the Atmospheric Turbulence and Diffusion Division (ATDD).

1. *General applicability and limitations.*

   a. Overall, the approach used by SCIPUFF to represent turbulent diffusion is physically sound. The second-order-closure approach used by the model allows estimates to be made of both mean concentration and concentration uncertainty. This ability distinguishes SCIPUFF from most other air dispersion models.

   b. The complex second-order-closure approach used in SCIPUFF is likely to be of greatest benefit when extensive field measurements are available for the winds and turbulence, such as could be expected when simulating tracer releases during a research-grade field experiment. Under more operational conditions, when SCIPUFF must rely more heavily on idealized wind and turbulence profiles, the accuracy of the second-order-closure approach may not be significantly better than simpler approaches.

   c. For long range applications and upper atmospheric conditions, the turbulence input to SCIPUFF is based on climatological information. Predictions with such data will almost certainly be less reliable than with on-site measurements. For these situations, a complex model such as SCIPUFF may not be justified. It is therefore reasonable to conclude that the benefits of using SCIPUFF will be greatest for short-range atmospheric boundary-layer scale dispersion applications.

   d. The experiences of the study team indicate that the there are deficiencies in the Technical Document manual, and that running HASCAL is not always straightforward, especially when using observed meteorological input data. Several important diagnostic quantities are available in the PUFF files; however, these are binary files that are not easily accessible to the user. We anticipate that SCIPUFF users will require extensive training in the use of the model and in properly assessing the model output. We recommend the addition of a "research switch" that would make potentially useful internal results readily available to the skilled user.

2. *The scientific basis of the model.*

a. The verification of the scientific basis of SCIPUFF was based on the Technical Documentation (Sykes *et al.*, 1996, ARAP Report 712, Titan Corp.), and other available documents. Unfortunately, this technical document is not complete and self-sufficient in the sense that it relies heavily on previous reports and papers for derivations of equations and other details of various topics. A complete and comprehensive "science" document, which explains the technical basis for the SCIPUFF model and includes derivations of equations and other details missing in the Technical Documentation, would have been very helpful, but there is no indication that such a document exists. The Technical Documentation is also not helped by the lack of a List of Symbols, since much of the notation in this report is non-standard.

b. Although the second-order turbulence closure scheme used in SCIPUFF is physically sound, the practical advantages of this approach over alternate approaches may be somewhat overstated in the SCIPUFF documentation. In Section 1 of the Technical Documentation, it is stated that the second-order-closure approach is (a) more general than alternate approaches because it is less empirical and (b) provides a fundamental relationship between turbulent diffusion and the velocity fluctuation statistics. However, a closer inspection reveals that SCIPUFF's approach also contains a significant degree of empiricism. Moreover, other approaches commonly used in puff models are also based on fundamental relationships between turbulent diffusion and the velocity fluctuation statistics. One feature of the second-order-closure approach that different from other approaches is the estimation of the concentration fluctuation variance.

3. *Verify the numerical code.*

3a. *Code verification*

a. Our examination of the SCIPUFF computer source code showed that there are 2260 subprograms in 534 source files, 76 include files, over 760,000 non-comment source lines, and over 85,000 non-empty comment lines. These lines mostly contain FORTRAN code that has been blanked from the program. Descriptive comments in the code are rare, and there is no up-to-date documentation of the code. Thus, it was not possible to do a comprehensive verification of the code in the time allotted. Instead it was decided to do a static analysis of the SCIPUFF FORTRAN code using a commercial code analyzer. The code analysis was conducted on the SCIPUFF V0.625.2R source code dated 11 March 1997. This version of the SCIPUFF source code matches the SCIPUFF runtime program included on the HPAC 2.0 distribution CD-ROM (which also contains HASCAL Ver. 2.1). NOAA/ATDD first received the v0.625.2R source files at the end of July 1997.

b. After several trials, a commercial static FORTRAN code analyzer called FORCHECK was ultimately used to investigate the SCIPUFF model code. FORCHECK is F77/F90/F95 compatible and uses compiler-specific configuration files to properly analyze FORTRAN source code. For the SCIPUFF analysis, the Absoft compiler configuration was used, which correctly dealt with nearly all of SCIPUFF's F77 extensions. The basic FORCHECK analysis and cross-reference (without calling tree) of SCIPUFF produced a 165 Mbyte analysis output file. The analysis file was carefully examined for flagged errors that might corrupt SCIPUFF simulation results.

c. The FORCHECK code analyzer indicated 47 possible sources of coding conflicts or coding errors. These mostly occurred in subroutine calling arguments, dimension statements, and type declarations. However, these inconsistencies may be resolved by the source code compiler, and so may not be a problem. Since we do not have access to the compiler, we cannot verify that this is the case.

3b. *Model sensitivity tests.*

a. Sensitivity testing provides a means of assessing the integrity of the code. In order to obtain a clear picture of how model output is affected by changes in input parameters, it is necessary to change one input variable at a time while holding the others fixed. The input variables tested for daytime and nighttime conditions were: wind speed, mixing height, surface heat flux, stability class, surface roughness, plume release height, conditional averaging time, and boundary-layer parameterization type. In all cases, SCIPUFF behaved as expected from diffusion theory; *i.e.,* there were no unexplainable or extraneous results. For daytime and nighttime conditions, the most sensitive parameter is conditional averaging time, and the least sensitive parameter is the surface roughness. The second most sensitive parameters are mixing height for the daytime case, and wind speed for the nighttime case. Mixing height in the nighttime case is not a very sensitive parameter. Heat flux and source height are about equally sensitive for both day and night conditions.

b. A possible source of user confusion appears in the vertical cross-section graphs of the plume produced by SCIPUFF. The mixing height is considered a reflecting surface, so concentration contours are not expected above that height; however, SCIPUFF concentration contours were observed to be present above the mixing height elevation. This problem was brought to the attention of the model developers, and their analysis revealed a coding error that essentially treated the atmosphere as having a uniform potential temperature when only a single temperature was specified on the surface observations file. It was reported to us that the problem has been fixed.

4. *Test the model against data.*

   a. SCIPUFF output was compared with the sulfur hexafluoride (SF_6) tracer test data taken as part of the U. S. Air Force Model Validation Program (MVP) at Cape Canaveral, Florida. The MVP tests used here were performed in November 1995, and involved continuous releases of about two hours duration. Plume sampling was done with real-time samplers in vans along roadways. Three tracer tests were selected: Test 208 on 6 November with releases from 1030 to 1312 Local Standard Time (LST); Test 209 on 6 November with releases from 1622 to 1856 LST; and Test 215 on 10 November with releases from 0800 to 1000 LST. Examination of time-averaged predicted and observed plume cross section plots indicates a tendency for SCIPUFF to underpredict by more than a factor of two during convective conditions, to overpredict by about a factor of two during transition from convective to stable conditions, and to be close to the observed values during stable conditions. However, we did not have observed mixing heights for these calculations and, as we have seen from the sensitivity tests, SCIPUFF is very sensitive to mixing heights during convective conditions. We feel that the use of observed mixing heights would improve these comparison results.

   b. The concentration maxima of 23 time-averaged observed and predicted plume cross sections along the sampler arrays were statistically compared. The range of these data was quite large, so the geometric mean bias MG and the geometric variance VG were calculated. These values were 0.69 and 4.89 respectively. A perfect model would give values of 1 for both MG and VG. An MG of 0.5 and 2.0 indicates an overprediction and an underprediction by a factor of two, respectively, and a VG of about 1.6 indicates a typical factor of two scatter between individual pairs of observed and predicted values. Thus, for these tests SCIPUFF can be said to overpredict by less than a factor of two, but the scatter between individual pairs of observed and predicted values is greater than a factor of two.

Second Order Closure Integrated Puff (SCIPUFF) Model Verification and Evaluation Study

Carmen J. Nappo, Richard M. Eckman, K. Shankar Rao,
Jerold A. Herwehe, and R. Laureen Gunter

ABSTRACT. This report summarizes a verification of the SCIPUFF model as described in the draft report "PC-SCIPUFF Version 0.2 Technical Documentation" by Sykes *et al.* (1996, ARAP Report 712, Titan Corp). The verification included a scientific review of the model physics and parameterizations described in the report, and checks for their internal usage and consistency with current practices in atmospheric dispersion modeling. This work is intended to examine the scientific basis and defensibility of the model for the intended application. A related task is an assessment of the model's general capabilities and limitations. A line-by-line verification of the computer source code was not possible; however, the code was checked with a commercial code analyzer. About 47 potential coding inconsistencies were identified. The sensitivity of SCIPUFF to changes in input parameters was examined. These tests indicated that SCIPUFF behaved in a rational way to these changes. Comparisons of SCIPUFF output with time-averaged tracer gas plumes showed that, overall, SCIPUFF can be said to overpredict by less than a factor of two, but there is a greater than factor of two scatter between individual pairs of observed and predicted values.

1. Introduction

The Defense Special Weapons Agency (DSWA) is developing technology to assist military commanders in the assessment of toxic hazards produced on the battlefield resulting from Weapons of Mass Destruction (WMD)-related engagements with enemy forces. Assessments may involve predicting the amount of WMD agent released from a damaged facility, the atmospheric transport of the released material, the spread of material throughout the commander's area of responsibility, and the number of casualties, both military and civilian. To address this military requirement, DSWA intends to adapt the Hazard Assessment System and Consequence Analysis (HASCAL) to their Hazard Prediction and Assessment Capability (HPAC), in order to estimate the potential hazards associated with conventional attacks on nuclear, biological, and chemical (NBC) facilities. HASCAL (see DNA, 1996) consists of an atmospheric dispersion model called the Second-order Closure Integrated Puff (SCIPUFF) model, and an associated mean wind field model, MINERVE. Because of their importance in safety assessment, the concentration and dose estimates from the dispersion model should be as accurate as possible, and should provide an estimate of the associated uncertainties to aid in planning and decision-making.

The Atmospheric Turbulence and Diffusion Division (ATDD) of NOAA's Air Resources Laboratory has performed a large number of studies involving the verification and evaluation of atmospheric dispersion models intended for a variety of applications. Because of this expertise and experience, ATDD was asked by DSWA to undertake a verification, sensitivity analysis, and evaluation study of the SCIPUFF model. This report presents the results of these studies.

Model verification is the process of assessing the scientific accuracy of a model. The model should be based on sound physics and give good predictions for the "right" reasons. A scientific review of the model formulations is an essential component of verification. A review of the computer code ("code verification") is also required to verify that the mathematical model is properly implemented, and to detect gross errors in the computer code. In general, the more complex a model, the greater is the likelihood for errors in logic and coding, as well as the difficulty in detecting them. Successful verification of a model provides faith in predictions beyond the range of experimental data used for testing the model, and confidence in modeling new situations with different meteorological and release conditions. It also provides insights into the limitations of the model.

A sensitivity study examines the way a particular model responds to variations in values of input variables or internal parameters. The results of such a study are not directly related to model accuracy and may not correspond to physical reality, but can identify the relative importance of the input variables. This is helpful in indicating how accurately the input variables must be measured. Sensitivity studies are also useful for checking if the model is performing as expected; otherwise, additional verification and/or development may be necessary.

Model evaluation is the process of assessing the model's performance by comparing its predictions to measured concentrations; the latter are often obtained from research-grade tracer experiments that are capable of testing key features of the atmospheric dispersion model. Over the past two decades or so, sophisticated statistical techniques have been advanced for the evaluation of air quality models from the scientific and operational viewpoints. (Tangirala *et al.*, 1992; Weil *et al.*, 1992; Rao and Hosker, 1993).

The model verification described in Section 6 of this report consists of a detailed examination of the physics and mathematical equations used by SCIPUFF to describe puff transport, diffusion, and deposition. It also includes the numerical techniques, and model input/output features such as specification of sources, meteorology, and turbulence. An effort was made to work through and independently derive as many of the equations as possible in the time available. The discrepancies, omissions, and needed revisions (both major and minor) in the documentation are listed. An interim partial list of these model corrections was earlier provided to DSWA to guide the concurrent code verification and improvement effort.

There are three important limitations to this model verification. First, the model verification was based mainly on the SCIPUFF description given in the "PC-SCIPUFF Version 0.2 Technical Documentation" by Sykes *et al.* (1996a), hereafter referred to as the Technical Document (TD). Second, this verification did not include the mean wind field model MINERVE, which has recently been modified and renamed SWIFT. Third, no detailed examination of the possible physics and chemistry of NBC sources was performed, since ATDD does not have expertise in this area, and the TD does not contain this information (except for what was included in the TD's brief Section 4 titled 'Source Specification'). It is well known that proper characterization of source emissions is critical to the satisfactory performance of a dispersion model.

Perceived problems with the model from both scientific and operational points are discussed in this report. The report mainly focuses on the discrepancies and problems of the SCIPUFF model that were discovered. For those unfamiliar with the scientific review process, this emphasis may appear to be negative in tone. However, it is noted that SCIPUFF in general has a good scientific basis, and has been described in the refereed scientific literature.

2. ATDD Work Statement

During the past several years, NOAA's Air Resources Laboratory's Atmospheric Turbulence and Diffusion Division (ATDD) has evaluated atmospheric transport and diffusion models for the U.S. Environmental Protection Agency, the U.S. Center for Disease Control, the U.S. Army Nuclear and Chemical Agency, and the U.S. Air Force. These models have application time and space scales ranging from minutes to years, and from tens of meters to hundreds of kilometers. Some of these model verification studies involved only a thorough review of the model equations and interpretations of previous studies; others involved extensive model sensitivity tests. In all cases, judgements of model performance were based not only on quantitative measures of model behavior, but also on scientific insight and experience. It is recognized that the scientific understanding of turbulent processes is still limited, and that the predictions of turbulent flows always contain an inherent uncertainty. It is generally accepted by atmospheric scientists that no one model will be applicable to all situations all the time, and that a successful model prediction in a few selected circumstances does not guarantee model performance in all circumstances. Therefore, the performance of a model can be stated only in terms of probability. With this in mind, the SCIPUFF tasks to be accomplished by the ATDD were:

1. Establish the model's general applicability and limitations.

   This task examined SCIPUFF's treatment of time and space scales relative to the input data requirements, and considered whether SCIPUFF can generate concentrations and dose predictions needed by the user community, given the available data. Sources of information were the technical documentation, refereed professional journal articles, published symposium presentations, and other documentation identified by DSWA.

2. Verify the scientific basis of the model.

   This task sought to determine the scientific validity and defensibility of the model. This required a detailed examination of all equations, parameterizations, and assumptions underlying the model, and verification of the necessary derivations in light of current understanding of atmospheric transport and diffusion. Particular attention was paid to the case of stable atmospheric conditions which can often result in very high concentrations for near-ground releases.

3. Verify the numerical code.

   This task examined the computer code in order to verify that the equations, parameterizations, and assumptions made by the model developers are accurately represented in the model. This required an examination of the numerical code, and the performance of a sensitivity study to verify that the model behaves as expected when input variables are carefully altered.

4. Test the model against data.

   After consulting with DSWA, the model was tested against available field data. Model performance was judged by statistical techniques.

5. Prepare a draft technical report.

   After the draft report is peer reviewed, a final report will be published. Significant findings will be summarized and presented at a technical briefing to DSWA at a time to be determined.

3. Overview of SCIPUFF

The following overview is taken directly from Sykes, *et al.* (1996a). SCIPUFF is a Lagrangian transport and diffusion model for atmospheric dispersion applications. It is based on (a) the Gaussian puff method (Bass, 1980) in which a collection of three-dimensional puffs is used to represent an arbitrary time-dependent concentration field, and (b) a turbulent diffusion parameterization based on the second-order turbulence closure theories of Donaldson (1973) and Lewellen (1977). This diffusion parameterization provides a direct connection between measurable velocity statistics and the predicted dispersion rates.

The Lagrangian puff methodology provides several advantages over the Eulerian method for predicting atmospheric dispersion from localized sources. The Lagrangian scheme avoids the artificial diffusion (numerical) problems inherent in any Eulerian advection scheme, and allows an accurate treatment over a wide range of length scales as a plume or cloud grows from a small source size and spreads to larger atmospheric scales. This range may extend from a few meters up to continental or global scales of thousands of kilometers. In addition, the puff method provides a robust prediction under coarse resolution conditions, giving a flexible model for rapid assessment when detailed results are not required. The puff methodology is highly efficient for multi-scale dispersion problems, since puffs can be merged as they grow, and resolution is therefore adapted to each stage of the diffusion process.

The efficiency of the puff transport calculations in SCIPUFF has been improved by the implementation of adaptive time stepping and output grids. Each puff uses a time step appropriate for resolving its local evolution rate, so that the multi-scale range can be accurately described in the time domain without using a small step for the entire calculation. The output spatial fields are also computed on an adaptive grid, avoiding the need for the user to specify grid information and providing a complete description of the concentration field within the computational constraints under most conditions.

The generality of the turbulence closure relations provides a dispersion representation for arbitrary conditions. Empirical models based on specific dispersion data are limited in their range of application, but the fundamental relationship between the turbulent diffusion and the velocity fluctuation statistics is applicable for a much wider range. Our understanding of daytime planetary boundary layer velocity fluctuations provides reasonably reliable input for the second-order closure description of dispersion for these conditions; however, the nighttime planetary boundary layer case is not so well understood. For scales larger than the boundary layer and upper boundary layer during stable conditions, the turbulence description is based on climatological information, but the closure framework is in place to accept improvement as understanding of these regimes improves. The closure model has been applied on local scales up to 50 km range

(Sykes et al., 1988) and also on continental scales up to 3000 km range (Sykes et al., 1993).

The second-order closure model also provides the probabilistic feature of SCIPUFF through prediction of the concentration fluctuation variance. In addition to giving a mean value for the concentration field, SCIPUFF predicts a quantitative value for the random variation in the concentration value due to the stochastic nature of the turbulent diffusion process. This uncertainty estimate is used to provide a probabilistic description of the dispersion result, and gives a quantitative characterization of the reliability of the prediction. For many dispersion calculations, the prediction is inherently uncertain due to a lack of detailed knowledge of the wind field, and a probabilistic description is the only meaningful approach.

4. Verification and Evaluation Methodology

The version of SCIPUFF code tested was v0.625.2R, as contained in HASCAL v2.1 which is in turn part of HPAC Ver.2.0. These are operational rather than scientific codes, and this complicated the code verification and model evaluation process. Operational codes have I/O requirements and formats which are fixed and not easily circumvented or changed. Scientific versions of SCIPUFF are available for examination, but to examine SCIPUFF out of context would not be meaningful to HPAC.

HASCAL/SCIPUFF is intended to operate over a wide range of space and time scales; however, for plume travel times greater than the Lagrangian integral time scale, diffusion will be controlled mainly by advection. The Lagrangian integral time scale is difficult to specify in practice, but it remains clear that when plume travel times are large, the mean transport winds will be more important than the dispersion parameterization. Thus our sensitivity tests and comparisons with tracer data were restricted to distances less than 20 km from the source. Evaluation of SCIPUFF on larger scales would require an evaluation of the wind field models used with SCIPUFF.

Tasks 1 to 4 of our study were performed somewhat independently by members of the Atmospheric Transport and Diffusion (ATD) branch of the ATDD. These teams included Nappo, Eckman, and Rao on Task 1; Eckman and Rao for Task 2; Herwehe, Gunter, and Nappo on Task 3, and Nappo and Gunter on Task 4. These scientists recorded not only their objective results, but also their opinions on the suitability of SCIPUFF for its intended use. These subjective results are based on many years of experience in model development and applications, and in verification and evaluation of other atmospheric dispersion models.

5. General Applicability and Limitations of SCIPUFF

5.1. General Comments

Our review of the SCIPUFF documentation indicates that the overall approach used by SCIPUFF to simulate turbulent diffusion is physically sound. The model uses a consistent approach based on second-order turbulence closure to estimate both the diffusion of individual puffs and the variance of the concentration fluctuations. The ability of SCIPUFF to estimate concentration fluctuation variance is a distinctive feature that is not currently available in most other dispersion models. SCIPUFF is a very complex model. This complexity is driven in part by the need to apply the model to a wide range of scenarios and meteorological inputs, and the need to quantify the uncertainty in the concentration predictions.

The complex second-order-closure approach used in SCIPUFF is likely to be of greatest benefit when extensive field measurements are available for the winds and turbulence, such as could be expected when simulating tracer releases during a field experiment. Under more operational conditions, when SCIPUFF must rely more heavily on the idealized wind and turbulence profiles given in Sections 7 and 8 of the TD, the accuracy of the second-order-closure approach may not be significantly better than simpler approaches.

For long range applications and upper atmospheric conditions, the turbulence input to SCIPUFF is based on climatological information. Predictions with such data will almost certainly be less reliable than with on-site measurements, and may not justify the use of a complex model such as SCIPUFF. It is therefore reasonable to conclude that the benefits of using SCIPUFF will be greatest for short-range atmospheric boundary-layer scale dispersion applications.

While it is relatively easy to generate output from SCIPUFF, especially using the many default options in the model, using meteorological input data files is not as straightforward. For example, when using the OBSERVATION boundary-layer mode, SCIPUFF calculates values for missing mixing layer heights; however, these values are computed using CALCULATED-mode values of surface heat flux instead of observed values. Though his may be necessary (because the heat flux must be integrated over time), it was not clearly explained in the TD, and it can lead to unexpected results. Using SCIPUFF as a research tool or for checking simulations requires access to the parameters and various values calculated in the code. Most of these values are contained in the internal PUFF files; however, these are in binary code and require a special FORTRAN program for reading. Our running of SCIPUFF was often frustrated by errors which were neither obvious nor understandable. We feel this was due to running SCIPUFF in modes for which it was not designed. However, some of these difficulties were also due to ignorance resulting from the lack of documentation for parts of the model. With these points in mind, we conclude that users of SCIPUFF must be well educated in running the model, and should also have a good understanding of atmospheric diffusion and boundary-layer meteorology.

Because SCIPUFF readily provides graphical output, it is easy to misapply the model. Errors in input values or misunderstanding of the many run options in SCIPUFF can lead to inaccurate results. Generally these input errors are not easily caught, and SCIPUFF does not flag physically inconsistent values. Hence, the user must be able to look at the output and determine if the result is physically realistic. Without this type of approach, SCIPUFF is at risk of being grossly misapplied. For this reason we recommend that the model be used by technically trained dispersion meteorologists, who can judge if the predictions are physically plausible.

5.2. Sources of Uncertainty in SCIPUFF

Uncertainty in atmospheric dispersion model predictions associated with a single event or occurrence (even when there are no coding errors) is associated with: (a) "data" uncertainty which results from errors or uncertainties in the parameters used to execute or evaluate the model; (b) "model" uncertainty which results from internal errors or incomplete knowledge of the modeling system itself; and (c) "stochastic" uncertainty which results from the turbulent nature of the atmosphere and the unpredictability of emissions due to human activities. Understanding of the various uncertainties and their causes is required to interpret monitoring data and modeling results correctly (Rao and Hosker, 1993). The objective of uncertainty analysis is to provide quantitative estimates of the overall uncertainty incorporated in model predictions, usually expressed in terms of a 90% or 95% confidence interval on the model predictions (Rao, 1997).

For a single event, the uncertainty associated with (a) and (b) in the above can be minimized through more accurate and representative measurements and improved model formulations. The stochastic or inherent uncertainty (c), arising from the natural variability of the atmosphere, can be expressed as $\sigma_c^2 = \langle [C - \langle C \rangle]^2 \rangle$, where σ_c is the standard deviation, $C(\mathbf{x}, t)$ is the concentration observed in one realization of the experiment at spatial location $\mathbf{x}$ at time t, and $\langle C \rangle$ denotes the ensemble-average concentration. σ_c is a function of averaging time, position, and the meteorology and source conditions defining the ensemble, and can usually be determined only from laboratory data or models because of the variability of the atmosphere.

For many atmospheric dispersion problems, the concentration fluctuations are large, *i.e.*, $\sigma_c \geq \langle C \rangle$. Nevertheless, air quality models presently used in regulation and safety assessment aim to predict only the ensemble-mean concentration, and generally ignore the concentration fluctuations because of the difficulty in making reliable estimates of σ_c for general atmospheric conditions and arbitrary sources. Lewellen and Sykes (1989) described a probabilistic framework for incorporating uncertainty in the model predictions. This method involves predicting the variance of concentration fluctuations from a second-order closure model, and estimating the probability distribution from the mean and the variance using a truncated Gaussian (also referred to as "clipped normal") function, which replaces any unphysical negative tail (*i.e.,* negative concentrations) in the Gaussian with a delta function at zero concentration. The expected cumulative distributions and associated confidence bounds can be estimated directly from repeated sampling of the predicted probability distribution function (pdf). Model evaluation then involves checking if the observed concentration samples are consistent with what could be expected from a single realization of the set of predicted pdf's. This is the approach used in the SCIPUFF model, one of the very few atmospheric dispersion models that accounts for the concentration fluctuations.

Though the clipped normal pdf (derived from the model-predicted ensemble mean and variance of concentration fluctuations) provides a reasonable description of the full probability distribution, a recent study by Yee and Chan (1997) shows that a clipped-gamma pdf (derived from the same two model-predicted parameters) fits the concentration data better and is more flexible in fitting the full range of observed pdf behavior in a dispersing plume.

It should be noted that SCIPUFF, in general, provides an estimate only of the stochastic uncertainty which arises due to natural variability of the atmosphere. But the model results will depend critically on the input data and internal parameter uncertainties, as well on errors due to our incomplete understanding and inadequate formulation of the modeling system itself (*e.g.,* behavior of chemical or biological agents in the atmosphere, the parameterization of turbulent diffusion, etc.). The ensemble is usually defined to include all wind and temperature fields that are consistent with the meteorological observations used to drive the model. While considering the errors in these meteorological measurements, one needs to deal with issues such as the relationships among different types of data (*e.g.,* tower, aircraft, rawinsonde, wind profiler, etc.), time-averaging, representativeness, and quantity and quality of data.

In general, the meteorological input (data) uncertainty increases rapidly as the complexity of the model (number of meteorological parameters) increases. Using a Monte Carlo method (*e.g.,* Rao, 1995), Lewellen and Sykes (1989) showed that the meteorological input errors account for more than 50% of the total uncertainty in predicting the observed 1-hr ground level concentrations (GLCs) with a second-order closure integrated plume (SCIMP) model. They found that the meteorological input error was dominated by the horizontal wind variance, *i.e.,* uncertainty in the transport direction (see Weil *et al.*, 1992). In general, the latter is a major contributor to the total model error even at short distances over flat terrain (Hanna, 1988). Simulation of the effective trajectory of mean transport of pollutants is even more difficult and uncertain in situations involving complex terrain (*e.g.*, Banta *et al.*, 1996) and long range transport (Kahl and Samson, 1986).

The above brings up the issue of the SWIFT model that provides the wind field input to the SCIPUFF model. As noted above, the present model verification effort did not include SWIFT. However, a cursory examination revealed that SWIFT is not unlike many other mass-consistent wind field models described in the literature (see Selvam and Rao, 1996, for references). Such diagnostic models are based on interpolation and objective analysis of available wind data, and satisfy the mass continuity equation by making adjustments such that the output wind field is divergence free. This approach is simple and fast, but it has several limitations. First, the method is data-intensive, and providing large amounts of representative data may be a problem in situations involving long range transport (over hundreds of km) and/or complex terrain. In the latter case, for example, the wind field interpolated from available data may not adequately represent the flow in some locations where there are no observations. Another limitation is due to the formulation of the mass-consistent model, where the imposed boundary condition changes either the tangential velocity or the normal velocity on the boundary while keeping the other one fixed. For better definition of the wind field, one may have to include additional physical constraints (*e.g.*, momentum and/or energy conservation) on the flow (Lamb and Hati, 1987; Eckman and Dobosy, 1989).

5.3. Scale Issues and Other Modeling Considerations

The SCIPUFF model is intended for use over a wide range of scales from short-range (30 km) boundary layer scales to long-range (3000 km) mesoscale dispersion applications. The concentration variance prediction permits estimation of the uncertainty in the predicted concentration field due to turbulent velocity fluctuations. However, the turbulent wind component depends on the detail of the available resolved wind field. The output quality of a diagnostic wind-field model such as SWIFT depends directly on both the quantity and quality of the input data.

For long-range applications, it is always difficult to obtain enough high quality wind observations. Even in research-grade long-range tracer experiments, the uncertainties due to spatial and temporal interpolation of the horizontal wind field are large, and lead to significant errors in the trajectory calculations (*e.g.*, Draxler, 1991; Stohl *et al.*, 1995). Utilizing the recent European Tracer Experiment (ETEX) data in a study involving the evaluation of 28 long-range dispersion models of varying formulations and complexity, Graziani *et al.* (1997) concluded that a factor of 5 characterizes the model uncertainty in unpaired concentration comparisons; even the best models have less than 50% of their predictions within that range. For larger scales and upper atmospheric conditions, the turbulence input to SCIPUFF is based on climatological information (according to the TD, p. 2). Predictions with such data will almost certainly be less reliable, and may not justify the use of a complex model such as SCIPUFF. As indicated above, it is therefore reasonable to conclude that the benefits of using SCIPUFF will be greatest for short-range atmospheric boundary-layer scale dispersion applications.

SCIPUFF incorporates a graphical user interface (GUI), which runs on the PC as a Windows application, to provide interactive I/O display. A SCIPUFF calculation can store the complete puff description and integrated surface deposition and dose fields at a specified time interval (Sykes *et al.*, 1996b). Though the GUI facilitates use of the model by relatively inexperienced personnel in the field, we have doubts about the ability of typical users to properly apply this model without adequate training and comprehension, given the complexity of SCIPUFF. If DSWA decides on proceeding with the full implementation and distribution of this model, then the documentation should be significantly improved (as discussed in this report) and considerable training must be provided to potential users.

6. Verify the Scientific Basis of SCIPUFF

6.1. General Comments

Dr. K.S. Rao of the ATDD was familiar with the early work by the Aeronautical Research Associates of Princeton (ARAP) that led to the development of the SCIPUFF model. This however did not make this verification task any easier because the TD is not complete and self-sufficient, in the sense that it relies heavily on the previous reports and papers for derivations of equations and other details of various topics. Much of the previous work by ARAP was scattered through a number of reports, journal publications, and conference papers. A complete and comprehensive "science" document, which explains the technical basis for the SCIPUFF model, and includes derivations of equations and other details missing in the TD, would have been very helpful. It would also have been very useful to have a List of Symbols, since much of the notation in the TD is non-standard.

Although the second-order turbulence closure scheme used in SCIPUFF is physically sound, the practical advantages of this approach over alternate approaches may be somewhat overstated in the SCIPUFF documentation. In Section 1 of the TD, it is stated that the second-order-closure approach is (a) more general than alternate approaches because it is less empirical, and (b) provides a fundamental relationship between turbulent diffusion and the velocity fluctuation statistics. However, a closer inspection reveals that SCIPUFF's approach also contains a significant degree of empiricism. Moreover, other approaches commonly used in puff models are also based on fundamental relationships between turbulent diffusion and the velocity fluctuation statistics.

In regard to advantage (a) above, we note that SCIPUFF's second order closure for the puff diffusion is based on the flux transport equation as provided by Eq. (2.12) in the TD. To make practical use of this equation, it is necessary to use empirical closure assumptions for the flux divergence and pressure-correlation terms. The closure assumptions developed by Lewellen (1977) are used in SCIPUFF to derive Eq. (2.13) in the TD. This equation contains two empirical constants A and ν_c, associated with the closure assumptions made for the flux divergence and pressure-correlation terms. An additional layer of empiricism is required in SCIPUFF to specify the length scale Λ and velocity scale q that appear in Eq. (2.13). The relations used by SCIPUFF for these scales are described in Sections 2.1.3.4 and 8 of the TD. From the derivation of Eq. (2.13), it is clear that the second-order-closure scheme used by SCIPUFF for the puff diffusion contains a significant level of empiricism. It is thus not obvious that SCIPUFF's treatment of puff diffusion is less empirical than the treatments used in many other puff models.

The other stated advantage (b) of the second-order-closure scheme used in SCIPUFF is that it provides a direct relationship between turbulent diffusion and the velocity fluctuation statistics. However, other modeling schemes also provide such a direct relationship, usually based on Taylor's (1921) diffusion equation (*e.g.*, , Irwin, 1983; Eckman, 1994). For diffusion in the y direction, Taylor's equation can be written as

$$\frac{1}{2}\frac{d\sigma_y^2}{dt} = \overline{v'^2}\int_0^T R(\xi)\,d\xi\,, \tag{1}$$

where σ_y^2 is the variance of the concentration distribution in the y direction, $\overline{v'^2}$ is the velocity variance in the y-direction, $R(\xi)$ is the Lagrangian autocorrelation for a time lag ξ, and T is the travel time. The rate of decrease of $R(\xi)$ with ξ is primarily determined by the Lagrangian time scale t_L. Hence, Eq. (1) can be considered to provide a direct relationship between the diffusion—represented by σ_y^2—and the velocity fluctuation statistics as represented by the variance $\overline{v'^2}$ and the time scale t_L used for $R(\xi)$. This is very similar to SCIPUFF's representation in Eq. (2.16) of the TD, where the diffusion is determined by $\overline{v'^2}$ and the time scale q_H/Λ_H. It is therefore not entirely clear whether one can make a general assertion that the second-order-closure approach used by SCIPUFF provides a superior representation of the diffusion as compared with other models based on Eq. (1). One argument in favor of the SCIPUFF approach is that Eq. (1) explicitly assumes that the turbulence is stationary, whereas the SCIPUFF approach does not.

The proceeding discussion is not intended to suggest that the second-order-closure approach in SCIPUFF is inferior to other approaches commonly used in dispersion models. Instead, the discussion is intended to show that some caution must be used in asserting that the SCIPUFF approach to dispersion is less empirical and has better theoretical underpinnings than other approaches. All diffusion parameterizations are based on some degree of empiricism and simplification. However, there is an important difference between an empirical estimate of turbulence statistics and an empirical estimate of dispersion rates. The former allows improvement of the model as our understanding of the turbulent dynamics improves provided there is a valid relation between the velocity statistics and dispersion. One feature of the second-order-closure approach that is difficult to replicate using other approaches is the estimation of the concentration fluctuation variance.

The pressure-gradient/scalar covariance of the second-order closure scheme appears to have been modeled only by Rotta's assumption, which leads to the destruction term $A\,(q/\Lambda)\,\overline{u_i'c'}$ in Eq. (2.13) of the TD. This represents only the turbulence-turbulence interactions. However, the buoyancy contribution is significant in the convective boundary layer (CBL), and this can be parameterized as one-half of the direct buoyant production rate (Moeng and Wyngaard, 1986). Similarly, it is well-known that the commonly used down-gradient diffusion for turbulent transport fares poorly in the convective boundary layer, due in large part to the direct influence of buoyancy (*e.g.,* Holtslag and Moeng, 1991). The characteristic length scales for the dissipation rates used in second-order closure models are typically a factor of 2–3 too small (Moeng and Wyngaard, 1989). It is not clear if SCIPUFF accounts for these recent revisions to the closure parameterizations that are derived from large eddy simulation (LES).

6.2. Specific Comments

There is an inconsistent use of overbars in the SCIPUFF equations. In Eq. (2.3) on p. 3, the overbar in $\overline{x}_i$ denotes a spatial average over a puff. Later in Eq. (2.6), an overbar is used in $\overline{u}_i$, $\overline{c}$, and $\overline{u_i'c'}$ to denote ensemble averaging. This leads to considerable confusion when the two kinds of averaging appear together, such as in Eqs. (2.9) and (2.10).

The procedures described on p. 5 of the TD for deriving Eqs. (2.9) and (2.11) are incorrect. According to the documentation, Eq. (2.9) is obtained by multiplying Eq. (2.6) by x_i and then spatially integrating over the puff. If Eq. (2.6) is multiplied by x_i, some of the resulting terms will have the index i repeated three times. This leads to confusion, since a basic rule in applying the tensor summation convention is that no index should appear more than twice. A similar problem with the index i occurs if Eq. (2.6) is multiplied by $x_i'x_j'$, as is stated on p. 5 for the derivation of Eq. (2.11). The correct tensor approach for deriving Eq. (2.9) is to multiply Eq. (2.6) by x_j and then integrate over the puff, whereas the correct approach for deriving Eq. (2.11) is to multiply Eq. (2.6) by $x_j'x_k'$ and then integrate over the puff. It should be pointed out here that Eq. (2.11) contains a typographical error in that the variables x_i and x_j should actually be x_i' and x_j'.

In Eq. (2.12), the pressure correlation term $\overline{c'\partial p'/\partial x_i}$ is missing a factor of $1/\rho$. This typographical error does not appear to lead to any problems in later derivations.

In deriving Eq. (2.21) in the TD from the flux transport relation given by Eq. (2.13), the first term on the left side of Eq. (2.13) provides a contribution of the form

$$\begin{aligned} \left\langle z'\frac{\partial}{\partial t}\overline{w'c'}\right\rangle &= \frac{\partial\langle z'\overline{w'c'}\rangle}{\partial t} - \left\langle \overline{w'c'}\frac{\partial z'}{\partial t}\right\rangle \\ &= \frac{\partial\langle z'\overline{w'c'}\rangle}{\partial t} + \langle\overline{w'c'}\rangle\frac{\partial\overline{z}}{\partial t}\,, \end{aligned} \tag{2}$$

where $\overline{z}$ is the vertical centroid location and $z' = z - \overline{z}$. This expansion produces a contribution of the form $\langle\overline{w'c'}\rangle\partial\overline{z}/\partial t$ that is not accounted for in Eq. (2.21). Some explanation is required as to why this term can be neglected or how it is possibly offset by other terms that are produced during the derivation. This term can probably be neglected for elevated releases but not for surface releases.

In Eq. (2.22) on p. 9 of the TD, the last term on the right side has the wrong sign; it should be subtracted instead of added. This may only be a typographical error, since the incorrect sign does not propagate through to Eq. (2.24).

On p. 10 of the TD, it is stated that Eq. (2.26) is required for consistency with Eq. (2.25). It would be helpful if either a reference were given here or alternatively a more detailed explanation was given on how these two equations are linked. There also appears to be a problem in interpreting the derivative $\partial K_z^{eq}/\partial z$. According to Eq. (2.23), K_z is obtained by performing a concentration-weighted spatial integration of the product $z'\overline{w'c'}$. The variable K_z^{eq} then represents the asymptotic limit of K_z for large travel times. Since the variable z was eliminated through integration in obtaining K_z, it is not clear how one should interpret spatial derivatives such as $\partial K_z/\partial z$ and $\partial K_z^{eq}/\partial z$. It appears that an alternate definition of K_z of the form

$$\overline{w'c'} = -K_z\frac{\partial\overline{c}}{\partial z} \tag{3}$$

may have been implicitly substituted for the original definition when deriving Eq. (2.26). This definition is not necessarily the same as Eq. (2.23) in the TD, because the former is representative of a fixed point, whereas the latter is representative of a material volume (*i.e.,* , the volume of the cloud).

On p. 15 of the TD, the scalar dissipation time scale τ_c is defined as

$$\frac{1}{\tau_c} = bs\left[\frac{1}{\tau_1} + \frac{1}{\tau_2} + \frac{1}{\tau_3}\right] , \tag{4}$$

where $\tau_1 = \Lambda_c/q_c$, $\tau_2 = \Lambda_{cH}/q_c$, $\tau_3 = \Lambda_{cV}/q_{cV}$, and b and s are turbulence model constants with values of 0.125 and 1.8 respectively. It not obvious why τ_1, τ_2, and τ_3 should be summed in this manner to obtain τ_c. A more straightforward approach would be to use either a weighted average as is done with the length scale Λ_H in Eq. (2.29) and the mean particle fall speed v_g in Eq. (2.78), or a series of max and min functions as in Eq. (2.70). The summation used in Eq. (4) above will tend to produce smaller values of τ_c than would be obtained using weighted averaging or max and min functions. If Eq. (4) is the proper approach for obtaining τ_c, some physical justification should be given in the TD.

Equations (2.46) and (2.47) describe modifications that are made to the length scales Λ_{cV} and Λ_{cH} to account for wind-shear effects. No explanation is given as to how these shear modifications were derived. It is also not entirely clear that these modifications, which are based only on a wind-speed shear, are applicable to situations with wind-direction shear. A directional shear affects the lateral variance σ_{22} and can thus change both of the horizontal length scales Λ_c and Λ_{cH} used in SCIPUFF. This is not accounted for in the derivation leading to Eq. (2.45) in the TD.

Another questionable feature of the shear representation in Section 2.2.3 is the contribution of the large-scale velocity fluctuations to the shear rate α in Eq. (2.48). Little is known about the values of $\partial\overline{u_L'^2}/\partial z$ and $\partial\overline{v_L'^2}/\partial z$, so it does not make much sense to include these vertical gradients in the computation of α. Moreover, u_L' and v_L' will at times tend to increase the overall vertical wind shear and at other times will decrease the shear. There is no reason to believe they always increase the shear as suggested in Eq. (2.48).

The multiple uses of the symbol α make it difficult to follow the discussion of puff interactions in Section 2.2.4. The symbol is first used to denote vertical wind shear in Section 2.2.3. In the following section, it is used both as a puff identifier [*e.g.,* , Eq. (2.51)] and as a tensor related to the puff spatial dimensions.

Section 2.2.5 describes a simple method for adjusting the velocity variances to account for changes in the sampling time T_{av}. The sampling time is converted to a length scale through Eq. (2.71). There are two possible problems with Eq. (2.71) that should be addressed further. First, it is not clear why a factor of 0.02 appears in this equation. Although some kind of empirical factor may be required here to make Λ_{av} consistent with the other length scales used by SCIPUFF, one would expect it to be closer to unity rather than 1/50. Second, the inclusion of the turbulent fluctuations in the definition of V needs to be explained further. Equation (2.71) is essentially an implementation of Taylor's frozen eddy hypothesis, and the turbulent velocity fluctuations are not usually included in the definition of the advection speed V. It could be argued that there is some "double counting" of certain atmospheric motions occurring in Eqs. (2.71)–(2.72), since the same eddies are contributing to both the mean flow and the turbulence. A similar problem is present with the definition of $\overline{V}$ in Eq. (4.7) and the definition of T_E in Eq. (5.23).

Equation (2.79) for the fall-speed variance σ_g^2 cannot be correct. The last term v_g^2 on the right side does not have the same units as the other terms. This term should be multiplied by the same weighting factor as σ_g^2.

The effect of the particle fall-speed variation σ_g on σ_{33} as given by Eq. (2.87) is incorrect. This equation should be

$$\frac{d\sigma_{33}}{dt} = \text{Terms from (2.11)} + 2\sigma_g\sqrt{\sigma_{33}}\,. \tag{5}$$

This provides consistent units on both sides of the equation.

The title "Rough Surface Model" given to Section 2.4.2.2 in the TD is rather misleading, given that it applies to all surfaces other than those covered by the canopy model in the foregoing section. The model described in this section is said to be a generalization of that developed by Lewellen and Sheng (1980) for smooth, flat surfaces. No indications are given, however, as to which parts of Eqs. (2.100)–(2.103) are from the original Lewellen and Sheng model and which parts are the generalizations specifically applied to SCIPUFF. It is stated that the model presented in this section compares favorably with Sehmel's (1973) data, but no references are given for this statement. Moreover, Sehmel's data are extrapolations of wind tunnel results, with which field data tend to disagree (see, for example, Wesely *et al.*, 1977, 1985).

On p. 35 of the TD, it is claimed that a two-dimensional split of a single Gaussian puff into smaller puffs provides better overlap and smaller errors than a one-dimensional split. Figure 3-1 shows the opposite result, with the error in the two-dimensional case increasing most rapidly with separation distance. Either the text on p. 35 is incorrect, or the curves in Figure 3-1 have been mislabeled.

The finite-difference approximation used by SCIPUFF for the movement of the puff centroid $\overline{x_i}$ is given by Eq. (3.11) in the TD. This equation is missing the turbulent-drift term $\langle\overline{u_i'c'}\rangle/Q$ that appears in the original differential equation for $\overline{x_i}$ as given by

Eq. (2.10). There is thus some question whether the turbulent drift is also included in the source code using an Adams-Bashforth scheme or even whether the drift is properly included in the finite-difference equation at all.

The right side of Eq. (3.13a) on p. 42 of the TD contains an error. The term $\Delta t\, \partial u/\partial y\, \hat{\sigma}_{22}^{(0)}$ should not be present.

In attempting to rederive Eq. (4.6) on p. 47 of the TD, a factor of $8\pi^{3/2}$ was obtained in the denominator instead of 4π. The reduction of the factor 8 to 4 can be explained if the spread σ_x along the downwind direction is taken to equal $0.5\overline{V}t$, but we cannot explain the factor of π in Eq. (4.6).

At first sight, the variable D_H used in Section 5.1 of the TD appears to be similar to the determinant D except that it is restricted to the x-y plane. A closer inspection reveals that this is not really the case; D is the determinant of σ_{ij} and has units of (length)^6, whereas D_H is the determinant of α_{ij} $(i, j = 1, 2)$ and has units of (length)$^{-4}$. These variables more closely resemble inverses of each other rather than three- and two-dimensional versions of the same physical quantity. The use of the notations D and D_H for these quantities is therefore rather confusing, especially when they are used together as in Eqs. (5.8) and (5.10).

Equation (5.21) on p. 53 of the TD is used to estimate the fluctuation intensity of a meandering plume. It would be helpful if a reference was given for this equation or some mention was made of how it was derived. Also, no explanation is given in the TD as to why a factor of 0.7 is required in Eq. (5.23) for the Eulerian scale T_E.

The description of radiation doses in Section 5.4 of the TD is not very informative. It is stated that the SCIPUFF treatment of radiation is based on that in the RASCAL code, but it is not clear what modifications (if any) may have been made to the original RASCAL approach. Some additional physical descriptions of the three terms in Eq. (5.29) would also be useful for users of the model.

According to Eq. (7.4) in the TD, the surface-layer reference wind speed U_{ref} used for computing the friction velocity includes contributions from the large-scale horizontal velocity variances (u'_L, v'_L). It is stated that these large-scale components are included because they represent fluctuations on time scales larger than the boundary-layer response time. However, these components can have either positive or negative signs, and thus can either increase or decrease the reference speed U_{ref}. Equation (7.4) assumes that these large-scale components can only increase U_{ref}. Further explanation is required here as to why one can assume that the large-scale components always increase the reference wind speed.

When SCIPUFF is run using the SIMPLE PBL mode, the surface heat flux H and boundary-layer depth z_i are respectively described by Eqs. (7.15) and (7.29) in the TD. These equations have the problem that the sun is always assumed to rise at 0600 local time and to set at 1800 local time. This will not be accurate in many parts of the world except near the vernal and autumnal equinoxes. Either the equations should be changed to account for variations in the length of day, or a caveat should be placed in the TD regarding the limitations of the SIMPLE mode. If the latter course is chosen, a warning about the limitations of this mode should appear in SCIPUFF's graphical interface when a user attempts to use this mode. Some members of the ATDD verification team have heard informally that the SIMPLE PBL mode is not intended to be used operationally. However, the latest versions of SCIPUFF available to ATDD still have this mode as a user option, and there is thus good reason to believe that it will be used operationally.

In CALCULATED mode, SCIPUFF uses the technique described by Holtslag and van Ulden (1983) to estimate the sensible H and latent LE heat fluxes. Holtslag and van Ulden used a simplified version of the Penman-Monteith equation to estimate the partitioning of the available energy into sensible and latent heat fluxes. Their model, represented by Eq. (7.16) in the TD, was based on data taken during the summer over well-watered grass in The Netherlands. Although there is some reason to believe that the model will also work at other locations with different surface characteristics, this has never to our knowledge been systematically tested. In particular, the assumption that $G = 0.1R_n$ in Eq. (7.16) is reasonable over land, but is an inappropriate assumption over water. If Eq. (7.16) is to be frequently used in SCIPUFF, its accuracy should be tested over a variety of surfaces using field data.

Another consideration in using Eq. (7.16) is whether it will in practice provide better turbulence estimates than would be obtained using simpler techniques such as Pasquill stability categories. An operational user of SCIPUFF would have to estimate cloud cover, albedo (based on Table 7-3 in the TD), and the Bowen ratio (also Table 7-3) to use the CALCULATED mode. Given the large uncertainties associated with these estimates and the assumptions that go into Eq. (7.16), it is not clear that the resulting values of H would be a significant improvement over simpler approaches. This is something that could be determined in a fairly straightforward manner using field measurements of H and LE.

The method SCIPUFF uses to estimate the incoming solar radiation R_0 is based on that described by Holtslag and van Ulden (1983), as stated on p. 73 of the TD. This method requires two empirical coefficients a_1 and a_2 that are respectively set to $990\,\mathrm{W\,m^2}$ and $-30\,\mathrm{W\,m^2}$ in SCIPUFF, based on a survey of northern mid-latitude sites. However, in going back to the original paper by Holtslag and van Ulden (1983), it is seen that the values of a_1 and a_2 used in SCIPUFF represent only a single set of measurements at Harrogate, U. K. which were reported by Collier and Lockwood (1974).

It is possible that the SCIPUFF developers performed their own survey of mid-latitude sites to estimate a_1 and a_2, but the resulting values do not appear to represent any kind of average of the data listed by Holtslag and van Ulden (1983).

The definition of the variable U_0^2 given just below Eq. (7.27) in the TD is incorrect. The factor U_{ref}^2 should not appear in the denominator, since U_{ref} already appears in the appropriate places in Eq. (7.27). We recommend that checking should be performed by the model developers to ensure that this error is limited to the documentation and does not appear in the SCIPUFF source code.

On p. 77 of the TD, a reference is made to a paper by Carson (1973). The listing in the References of the TD (and this report) for this paper is incorrect. In volume 99 of the *Quarterly Journal of the Royal Meteorological Society*, the paper starting on p. 171 is by Carson and Smith and is entitled "The Leipzig wind profile and the boundary layer wind-stress relationship". It is not clear what the correct reference should be for Carson (1973).

Equation (7.37b) on p. 78 of the TD allows the surface layer to occupy a progressively larger fraction of the total boundary layer as the stability increases. Further explanation is required for this assumption. The vertical extent of the surface layer is generally defined as the depth over which the vertical fluxes do not vary much from their surface values (*e.g.*, , Panofsky and Dutton, 1984, p. 113). In contrast, the total boundary-layer depth in stable conditions is often taken to be the depth of turbulent mixing (*e.g.*, , Nieuwstadt, 1984; Holtslag and Nieuwstadt, 1986), although other definitions are possible. Given these definitions, the surface-layer depth should generally be significantly smaller than the boundary-layer depth in stable conditions. The idealized boundary-layer structure given by Holtslag and Nieuwstadt (1986), for example, keeps the surface-layer depth at $0.1z_i$ under stable conditions, whereas the flux profiles given by Lenschow *et al.* (1988) also indicate that the surface layer occupies only a small fraction of the entire stable boundary layer. It is possible that the SCIPUFF parameterization is an attempt to differentiate between a region of intermittent turbulence in the upper part of the stable boundary layer and more continuous turbulence turbulence closer to the surface, but this needs to be explained further.

In Eq. (8.3b) for the function F_{22}, the empirical constant 2.5 is about 30% smaller than the more typical value of 3.7 often seen in the literature (*e.g.*, Panofsky and Dutton, 1984, p. 160). Some further explanation should be given as to why the smaller value was chosen. The constants used for F_{11} and F_{33} are closer to the values often seen in the literature.

7. Verify the Numerical Code.

7.1. Code Verification.

7.1.1. *General Comments*

This task was delayed as a result of inconsistencies in the version numbers for the SCIPUFF documentation, source code, and the runtime code. For example, the SCIPUFF documentation reviewed here is Ver. 0.2 (March 1996), the SCIPUFF runtime code in HASCAL Ver.1.0 is Ver. 0.338, and the source code is Ver. 0.441 (November 1996). We then received HPAC 2.0 (March 1997), with SCIPUFF runtime code Ver. 0.625.2R. Since changes in the runtime code may not be reflected in the older versions of source code and documentation, we are concerned that our verification work may not be up-to-date. We cannot tell how relevant our comments will be for the later runtime versions.

Our examination of the SCIPUFF Ver. 0.625.2R computer source code showed that there are 2260 subprograms in 534 source files, 76 include files, over 760,000 non-comment source lines, and over 85,000 non-empty comment lines mostly used to delimit subprograms and make "fossil" code inactive. Descriptive comments in the code are rare, and there is no documentation of the source code. Thus, it was not possible to do a comprehensive verification of the code in the time allotted. Instead it was decided to do a static analysis of the SCIPUFF FORTRAN code using a commercial code analyzer. The code analysis was conducted on the SCIPUFF v0.625.2R source code dated 11 March 1997. This version of the SCIPUFF source code matches the SCIPUFF runtime program included in the HPAC 2.0 distribution CD-ROM (which also contains HASCAL Ver. 2.1). NOAA/ATDD received the v0.625.2R source files at the end of July 1997. Due to lack of up-to-date technical documentation describing the scientific theory, equations and assumptions contained in this version of the SCIPUFF model, only a static code analysis of the SCIPUFF FORTRAN source code has been performed and is summarized here. No attempt was made to compare purported model equations with actual model source code statements.

The SCIPUFF v0.625.2R FORTRAN source code consists of 847 files occupying about 9.87 Mbytes of disk space. A search through the source files revealed that SCIPUFF v0.625.2R contains 650 functions and 1610 subroutines. A directory tree for SCIPUFF v0.625.2R, including brief descriptions, is shown in Figure 1.

Efforts to apply various FORTRAN code analyzers to the SCIPUFF source produced mixed results. Most of these analyzers expect relatively normal FORTRAN77 standard code with few extensions, but SCIPUFF contains numerous advanced

```
/scipuff/v0.625.2r/
├──pcscipuf ........... (empty)
│  └──Release.......... (only pcscipuf.mak, master makefile)
│     ├──help........... (SCIPUFF/GUI Interface Help RTF files for Ver. 0.625)
│     ├──lib............ (libs datums, opview, pcx, swift, wxview)
│     ├──make........... (22 different makefiles for compiling PCSCIPUF)
│     └──src............ (empty)
│        ├──absoft3 .... (absoft3.mak for making absoft3.lib, plus dummy *.f)
│        ├──arap........ (general *.f mathematical functions for ARAP lib)
│        ├──contri...... (*.f files for building the contri or plot lib)
│        │  └──inc ...... (4 *.inc files for contri)
│        ├──ncar........ (*.f files for building the NCARG lib)
│        │  └──inc ...... (*.inc file for the NCARG lib files)
│        ├──ntinc....... (*.f for building ARAP version of NTINC/Win lib)
│        ├──pcscipuf ... (PCSCIPUF.F main program, *.mak for libs under here)
│        │  ├──edit ..... (*.f files for GUI EDIT lib)
│        │  ├──inc ...... (*.inc and *.fd def files for these libs)
│        │  ├──plot ..... (*.f files for GUI PLOT lib)
│        │  ├──rc........ (resource files; *.bmp, *.ico, *.rc, *.h)
│        │  └──tool ..... (*.f files for GUI TOOL lib)
│        ├──scipuff .... (*.f science files for SCIPUFF lib)
│        │  └──inc ...... (*.inc files for above)
│        └──util ........ (empty)
│           └──sci2cats. (PCSCIPUF off-line CATS file generator src)
└──SWIFT................ (makefile for building SWIFT DLL)
   ├──data.............. (*.msg and *.rsc files)
   ├──make.............. (12 different *.mak files for SWIFT)
   └──src............... (empty)
      ├──absoft3 ....... (absoft3.mak for making absoft3.lib, plus dummy *.f)
      ├──dll............ (7 SCIPUFF/SWIFT interface *.f files)
      ├──inc............ (*.inc files for SWIFT)
      ├──library ....... (281 *.f files for ADSO SWIFT lib)
      └──ntinc.......... (*.f for building ARAP version of NTINC/Win lib)
```

Figure 1. Directory tree of "/scipuff/V0.625.2R" with descriptions.

extensions of the F77 standard. This is mostly due to specifying the Windows platform as its intended runtime target.

A commercial static FORTRAN code analyzer called FORCHECK was ultimately used to investigate the SCIPUFF model code. FORCHECK is F77/F90/F95 compatible and uses compiler-specific configuration files to properly analyze FORTRAN source code. For the SCIPUFF analysis, the Absoft compiler configuration was used, which correctly dealt with nearly all of SCIPUFF's F77 extensions. The basic FORCHECK analysis and cross-reference (without calling tree) of SCIPUFF produced a 165 Mbyte analysis output file. The analysis file was carefully examined for flagged errors that might corrupt SCIPUFF simulation results. The flagged errors gleaned from the analysis file are summarized in the section below, organized by SCIPUFF source file name.

The FORCHECK analysis of SCIPUFF v0.625.2R reported 2260 subprograms in 534 source files, 76 include files, over 760,000 non-comment source lines, and over 85,000 non-empty comment lines. By most standards, the SCIPUFF source code qualifies as one of the larger atmospheric dispersion model codes.

7.1.2. *General SCIPUFF Code Warnings from FORCHECK*

1. General trouble with named `RECORD`s being referenced before their `STRUCTURE` has been defined (the Absoft compiler apparently doesn't care about the order).

2. The Absoft compiler treats `LOGICAL` and `INTEGER` variables as interchangeable since there are many instances where `INTEGER`s are used in Boolean (*i.e.*, , `LOGICAL`) expressions. Plus, `INTEGER` values are assigned to `LOGICAL` variables in many cases.

3. Subroutine `julian_ymd` appears in both `ARAPUTIL.F` and `JULIAN.F`.

4. Subroutine `time_string` is defined as having one argument in SCIPUFF's `BUILDLST.F` and defined as having two arguments in SWIFT's `PROGRESS.F`.

5. Subroutine `time_cnv` is defined as having nine arguments in SWIFT's `PROGRESS.F` and defined as having 11 arguments in SCIPUFF's `TIME_CNV.F`.

6. Subroutine interp is defined as having 18 arguments in SWIFT's `INTERP.F` and defined as having six arguments in SCIPUFF's `INTERP.F`

7.1.3. *File/Subprogram Warnings from FORCHECK*

1. `ABORT.F`: No path to the 9999 statement.

2. `ANIMATE.F`: Functions that are `CALL`ed as if they were subroutines: `DeleteObject`, `ReleaseCapture`, `EnableWindow`, `UpdateWindow`, `TranslateMessage`, `DispatchMessage`.

3. `ARAPUTIL.F`: In subroutine `julian_ymd`, `IMPLICIT NONE` should appear before any other statements. In subroutine `c_format`, the line `ilog = float(ifix(alog10(1.0005*xx) + 5000.)-5000)` doesn't need the float reference and then the truncation back to integer `ilog`. In subroutine `year_month_day`, `COMMON` block array `nday` should be initialized in `BLOCKDATA`.

4. `BILMIN.F`: No path to the 990 statement.

5. `BITMAP.F`: Functions that are `CALL`ed as if they were subroutines: `EndPaint`, `ReleaseDC`.

6. `BUTTONS.F`: `CALL`s to subroutine `update_OpWx_climo` in subroutine `edit_button` pass two arguments, but definition of subroutine `update_OpWx_climo` in `METDEF.F` has three arguments.

7. `CONDRW.F`: In subroutine `fill3`, `COMMON` block variables `icolq`, `np`, and `itst` should be initialized in `BLOCKDATA`.

8. `CONLIM.F`: The `CALL` to subroutine `limget` in subroutine `limgetx` passes only two arguments, but the definition of subroutine `limget` in `SURFACE.F` has four arguments.

9. `CONLNS.F`: In subroutine `set_ATP_area`, `IMPLICIT NONE` should appear before any other statements.

10. `COPYFILE.F`: In subroutine `copy_file`, `IMPLICIT NONE` should appear before any other statements.

11. `DEFW32.INC`: The line `PARAMETER ( HWND_TOPMOST = ( -1 )` (line 175) needs an ending right parenthesis.

12. `DUMP.F`: In subroutine `year_month_day`, `COMMON` block array `nday` should be initialized in `BLOCKDATA`.

13. `EDITBOX.F`: The `CALL` to subroutine `update_material_buttons` contains no arguments, but the definition of subroutine `update_material_buttons` in `MATERIAL.F` has one argument.

14. `FILES.F`: In subroutines `AddPath`, `RemoveExtension`, `SplitName`, and `SubstituteName`, `IMPLICIT NONE` should appear before any other statements.

15. `GFA_GPL.F`: In subroutines `gellips` and `checkpoly`, `IMPLICIT NONE` should appear before any other statements; this can be fixed by moving the `include 'ncarplot.inc'` line to the top of the subroutine.

16. `GRIDAL.F`: In subroutine `gridal`, `IMPLICIT NONE` should appear before any other statements.

17. `HAS2SCI.F`: In subroutine `read_etac`, `COMMON` block array `jday_etac` should be initialized in `BLOCKDATA`.

18. `INCIDENT.F`: No path to the 9998 statement in subroutine `load_incidents`.

19. `INIT_MET.F`: In the statement `call calc_wt(zref,0.,r2,0.,zref,dum1,1, ---)` in subroutine `check_obs_grid`, the sixth argument (`dum1`) is a scalar, but subroutine `calc_wt` is expecting an array in that position.

20. `INP_PUFF.F`: No path to the 9998 statement in subroutine `skip_puff`.

21. `JOUVRL.F`: No path to the `IF(IFINAI.EQ.0) THEN` statement at line 172.

22. `JULIAN.F`: In subroutine `julian_ymd`, `IMPLICIT NONE` should appear before any other statements.

23. `MATERIAL.F`: In subroutines `load_current_material`, `delete_current_material`, `save_current_material`, and `find_material_list`, `IMPLICIT NONE` should appear before any other statements.

24. `MET_CLI1.F`: In subroutine `read_climo`, `COMMON` block array `jday_etac` should be initialized in `BLOCKDATA`.

25. `MET_MRF.F`: No path to the 9997 statement in subroutine `read_fields_mrf`.

26. `PCSCIPUF.F`: Function `MessageBox` is both `CALLed` (as if it were a subroutine) and treated as a normal function reference; this also happens to `TranslateMessage`, `DispatchMessage`, `ShowWindow`, `udateWindow`, `DestroyWindow`, `EnableWindow`,

GetClientRect, GetWindowRect, PostQuitMessage, DeleteObject, and ReleaseCapture. VAL(TOOLPROC) and VAL(DIALPROC) are the fourth args in the function reference CreateDialogParam, but both TOOLPROC and DIALPROC are functions themselves that require four arguments each, but none are provided. Likewise for VAL(INITPROC) in function reference DialogBoxParam. CALLs to subroutine fpcontrol pass two arguments, but the definition of dummy routine SUBROUTINE FPCONTROL in FPCONTROL.F has only one argument.

27. PENS.F: In subroutine setRGBcolor, IMPLICIT NONE should appear before any other statements by moving the include 'ncarplot.inc' line to the top of the subroutine, plus remove the IMPLICIT NONE that is already at the top of the subroutine.

28. PLCHHQX.F: In subroutine SetNCARFont, IMPLICIT NONE should appear before any other statements by moving the include 'ncarplot.inc' line to the top of the subroutine, plus remove the IMPLICIT NONE that is already at the top of the subroutine.

29. PLOTPROC.F: MouseCursor is illegally declared as LOGICAL in function PLOTWNDPROC when MouseCursor is actually a subroutine. The CALL to subroutine FlashBox in FUNCTION PLOTWNDPROC passes one argument, but the definition of subroutine Flashbox in MOUSE.F has no arguments.

30. PRINT.F: The CALL to subroutine HaltScipuff in logical unction cancel_print passes no arguments, but the definition of subroutine HaltScipuff in PROGPROC.F has one argument.

31. RELEASE.F: In subroutines load_current_release, delete_current_release, add_current_release, save_current_release, find_release_list, build_release_Munit, build_release_Tunit, build_release_Lunit, show_release_Lunit, release_spec_radio, compute_DMS, and compute_degrees, IMPLICIT NONE should appear before any other statements.

32. RESOURCE.INC: PARAMETER (SCI_ICON ='$InterfaceIcon ') should only have 20 characters, not 21, in the definition.

33. SAVEFILE.F: Remove the redundant second IMPLICIT NONE from subroutine SaveFileDlg.

34. SCIPUF_C.F: No path to the 9300 statement in subroutine create_restart.

35. `SET_MET.F`: In the statements `call age_wts(sumzi_ua,1,1,ua_fac)`, `call age_wts(sumpgt_ua,1,1,ua_fac)`, `call age_wts(sumhflx_ua,1,1,ua_fac)`, `call age_wts(sumzi_sfc,1,1,sfc_fac)`, `call age_wts(sumpgt_sfc,1,1,sfc_fac)`, `call age_wts(sumhflx_sfc,1,1,sfc_fac)`, in subroutine `set_met`, the first arguments are scalars, but subroutine `age_wts` is expecting an array in that position. In several of the `CALL`s to `COMB`, the fifth, sixth, eighth, and ninth arguments are scalars while subroutine `comb` is expecting arrays in those positions.

36. `SRF_EVAP.F`: The `CALL` to subroutine `lqd` in subroutine `srf_drop_evap` passes seven arguments, but the definition of subroutine `lqd` in `STEP_DROP.F` has six arguments.

37. `STEP_POOL.F`: The `CALL` to subroutine `lqd` in subroutine `step_pool` passes eight arguments, but the definition of subroutine `lqd` in `STEP_DROP.F` has six arguments.

38. `SUBGENSWI.F`: No path to the 9996, 9997, and 9998 statements.

39. `SUBSWIADS.F`: In subroutine `SWIADS`, `COMMON/PATDIA/NOMBCK` should be changed to `COMMON/PATBCK/NOMBCK` to be consistent with other declarations using `NOMBCK` in other subroutines.

40. `UNIDOS.F`: In line 269, `IERREU=20` appears at the end of the line beyond column 72 so that it is ignored, but instead it should be on a line of its own just before the `GOTO 9999` line.

41. `WINNT.F`: The `CALL`s to function `MAKELCID` in functions `LOCALE_SYSTEM_DEFAULT` and `LOCALE_USER_DEFAULT` pass only one argument, but the definition of function `MAKELCID` in `WINNT.F` has two arguments.

7.2. Sensitivity Tests.

Sensitivity tests relate changes in model output to changes in model input values. Sensitivity testing provides a means of assessing the integrity of the code; however, a sensitivity test is neither an accuracy nor a precision test. It is a test of the fidelity with which the model physics is being represented by the code. One way to obtain a clear picture of how model output is affected by changes in input, is to change one input variable at a time while holding the others fixed. For SCIPUFF, This was done by using meteorological input files as described in the TD. The key input variables tested were:

1. Wind speed
2. Mixing-layer depth

3. Surface heat flux
4. PGT (Pasquill-Gifford-Turner) stability class
5. Surface roughness
6. Release height
7. Averaging time
8. Boundary-layer parameterization

In these tests the following control values were used unless otherwise stated:

1. The wind is constant and from the west at 4 $\mathrm{m\,s^{-1}}$. Vertical wind shear is not considered.
2. The surface sensible heat flux is 200 $\mathrm{W\,m^{-2}}$ for the convective case and -10 $\mathrm{W\,m^{-2}}$ for the stable case.
3. The mixing depth is 1000 m for the convective case, and 50 m for the stable case.
4. The tracer is sulfur hexafluoride, SF_6; the release rate is 50 kg per hour, and the deposition velocity is set to 0.01 $\mathrm{cm\,s^{-1}}$.
5. The source height is 10 m, and the initial cloud size is $sy = 1\,\mathrm{m}$, and $sz = 1\,\mathrm{m}$.
6. The surface roughness is 0.01 cm.
7. The time averaging parameter was set to the default value, and the run length was 2 hours.

In our analyses, we use two different values for each input variable being tested, and examine the average relative change in ground surface concentration along a line of sampling points aligned with the plume axis, i.e., $C(x, 0, 0)$. This relative change is defined as $(C(\text{new input}) - C(\text{control}))/C(\text{control})$, and is expressed as a percentage change. We examined SCIPUFF sensitivity at the end of a two hour convective period, 1200 to 1400 LST, and at the end of a two hour stable period, 0200 to 0400 LST. We also plot these concentration values to get a better understanding of the model response. Because we are mainly concerned with the near-field response of SCIPUFF, the sensitivity analysis extended only to 10 km from the source. Table 1 lists the downwind-average (*i.e.,* out to 10 km from the source) changes in concentration for stable and unstable conditions. Figure 2 shows the downwind-average relative change in

Table 1. Relative change in the downwind-average concentration (averaged out to 10 km) resulting from changes in specific input variables.

	Convective		Stable	
Input Variable	Change in Input	Concentration Change (%)	Change in Input	Concentration Change (%)
Speed	+100%	44.5	+100%	38.4
Mixing height	-50%	122.3	+100%	-12.1
Heat flux	-50%	37.3	+100%	22.5
Roughness	+1000%	5.6	+1000%	15.4
Source height	0 to 250 m	-34.7	0 to 25 m	-19.3
Averaging time	0 to default	198.5	0 to default	316.3
PGT class	1 to 7	2362.0		

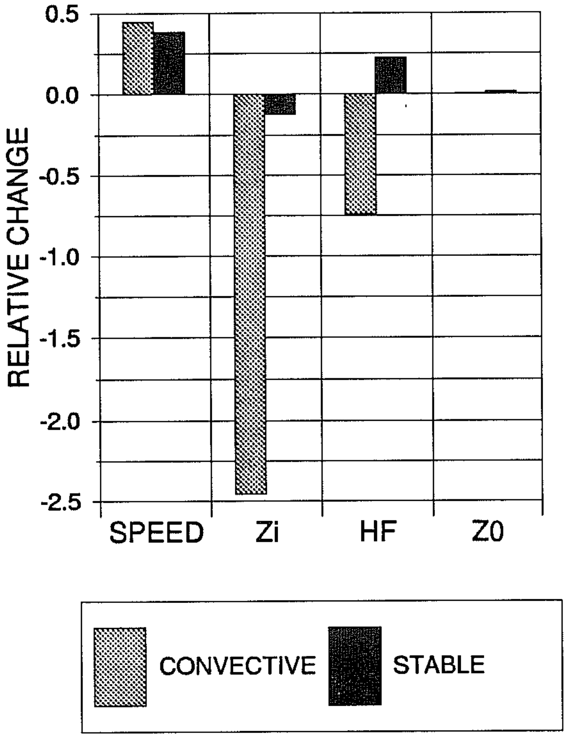

Figure 2. Downwind-average relative change in SCIPUFF concentration per unit relative change in wind speed (SPEED), mixing height (Zi), heat flux (HF), and roughness length (Z0).

concentration per unit relative change in input data for wind speed, PBL mixing height, surface heat flux, and surface roughness. We often observed large spikes in the fractional change curves; we cannot explain this behavior.

7.2.1. *Wind Speed*

Ground surface concentrations along the plume centerline, $C(x,0,0)$, as functions of downwind distance for wind speeds of 4 and 8 $\mathrm{m\,s^{-1}}$ are shown in Figure 3 for convective conditions and Figure 4 for stable conditions. Also shown in these plots is the downwind variation of the percent change in the ground level concentration due to the change in wind speed. Thus, the downwind-average percent change in concentration resulting from a 100% increase in wind speed,*i.e.,* from 4 to 8 $\mathrm{m\,s^{-1}}$, is about 44%.

In SCIPUFF, a continuous plume is modeled by a series of puffs. The dispersion of each puff is a function of the friction velocity u_*, which is a function of the boundary-layer reference velocities and the surface heat flux. Accordingly, for a constant heat flux, the vertical diffusion of puffs increases with increasing wind speed, but puff transport downwind from the source elevation also increases. For puffs released above the ground surface, it is possible that the effect of wind speed on the vertical diffusion is offset by the wind speed's effect on the horizontal transport, so that the downwind distribution of ground-level concentrations can be more or less independent of the wind speed. This kind of behavior is seen in Figure 4, *i.e.,* the concentrations are almost equal very near the source. The larger dispersion associated with the greater wind speed brings material downward to the ground surface at a rate greater than the horizontal transport. Thus ground-level concentrations increase with wind speed, but beyond about 8 km this trend begins to reverse, and eventually the concentrations become almost equal. For the stable case, Figure 4, the average change is about 38%; however, from the figure we see that this difference in concentration occurs mostly between about 1 and 7 km. Beyond that distance, the two concentrations are almost equal.

7.2.2. *Mixing Layer Depth*

Figure 5 shows the effects on $C(x,0,0)$ caused by lowering the convective mixing-layer depth, z_i, from 1000 m to 500 m. In this case the average relative change in concentration is about 122%. It is expected that once the plume material has dispersed through the depth of the mixing layer, concentrations will be inversely proportional to mixing depth. For a 50% decrease in mixing depth, one would expect the relative change to approach 50%, but this is not seen in Figure 5. Figure 6 shows the results of increasing z_i by 100%, *i.e.,* from 50 m to 100 m for the stable case. The average relative change is about -12%; the negative sign indicates a decrease in concentration

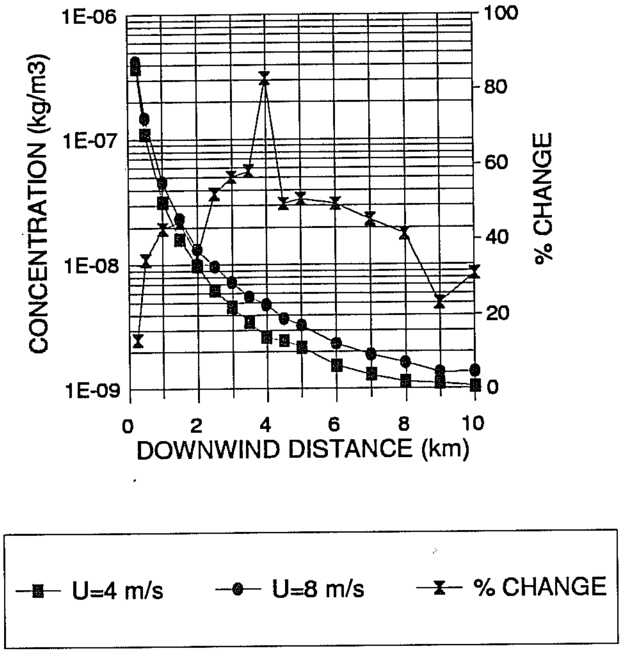

Figure 3. SCIPUFF sensitivity to wind speed: convective case.

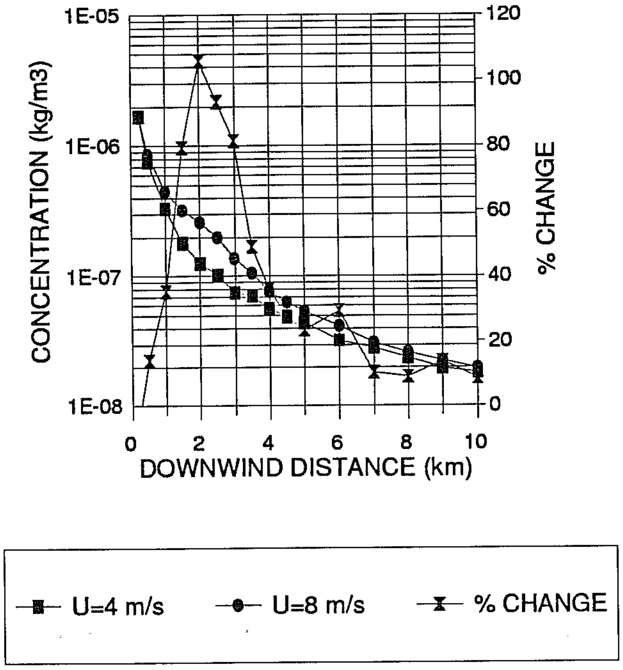

Figure 4. SCIPUFF sensitivity to wind speed: stable case.

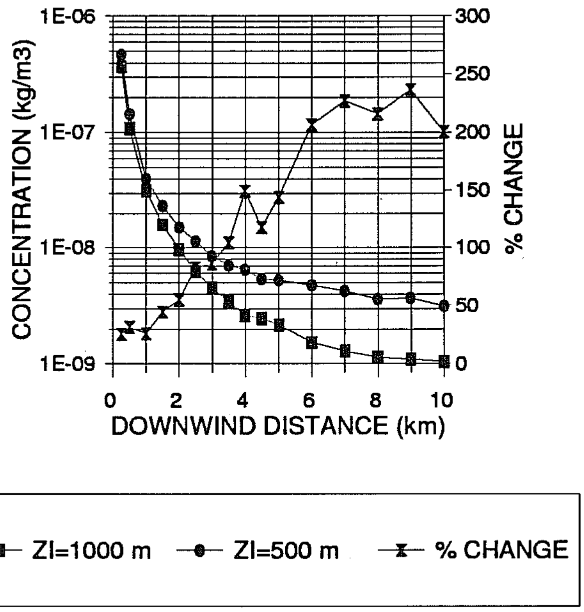

Figure 5. SCIPUFF sensitivity to mixing height: convective case.

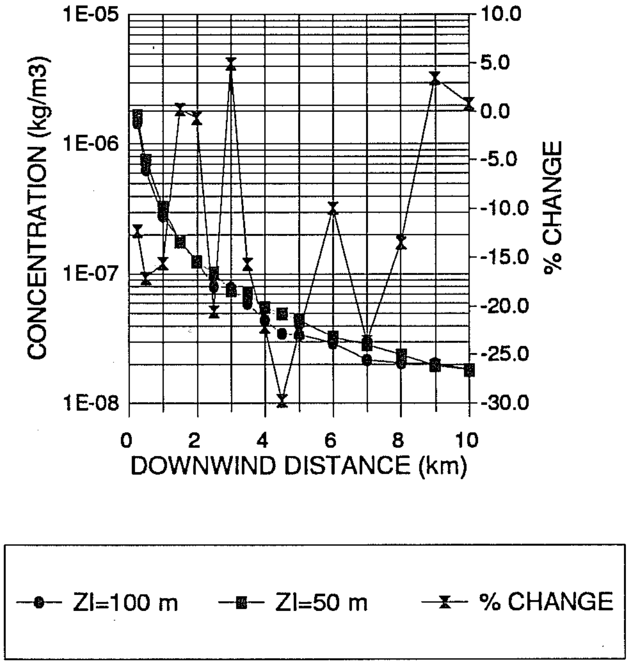

Figure 6. SCIPUFF sensitivity to mixing height: stable case.

which is expected when z_i is increased. However, the change in concentration is much less than the 100% expected for the case of uniform mixing. Under stable conditions turbulence decreases quickly with distance from the ground surface. Consequently, the depth of the mixing layer does not have the same influence on ground level concentrations as the convective mixing layer, *i.e.,* the plume in the stable mixing layer is not well mixed. Thus we expect the ground-level concentrations to be relatively insensitive to z_i, and this is observed in SCIPUFF.

7.2.3. *Surface Heat Flux*

Plots of $C(x, 0, 0)$ for convective and stable conditions are shown in Figure 7 and 8 respectively. Decreasing the daytime surface heat flux from 200 $\mathrm{W\,m^{-2}}$ to 100 $\mathrm{W\,m^{-2}}$ results in an average fractional increase in concentration of about 37%, and doubling the nighttime surface heat flux from -10 $\mathrm{W\,m^{-2}}$ to -20 $\mathrm{W\,m^{-2}}$ results in an average relative increase in concentration of about 22%. These results indicate that SCIPUFF is not very sensitive to surface heat flux; however, in the convective case it is perhaps unrealistic to hold z_i constant as heat flux varies.

7.2.4. *PGT Stability Class*

Figure 9 shows the changes in ground level concentration when the Pasquill-Gifford-Turner (PGT) values change from 1 (very unstable) to 7 (very stable). The average relative change is about 2360%. The differences between stable and convective conditions on concentrations is dramatic and consistent with diffusion theory.

7.2.5. *Surface Roughness*

Figures 10 and 11 show ground level concentrations for convective and stable conditions respectively when the surface roughness, z_0, is increased from 0.01 m to 0.10 m. The average relative change in concentration is about 5.6% for the convective case and 15.4% for the stable case. The higher value of z_0 leads to higher values of friction velocity, u_*, and consequently increased dispersion. During the stable period, the increased dispersion over the rougher surface mixes plume material downward to the ground surface faster than over the smoother surface resulting in higher concentrations. Overall, SCIPUFF shows little sensitivity to surface roughness.

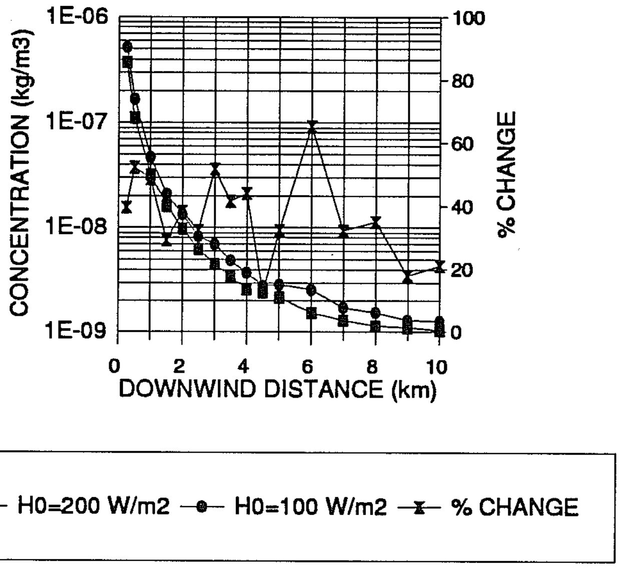

Figure 7. SCIPUFF sensitivity to surface heat flux: convective case.

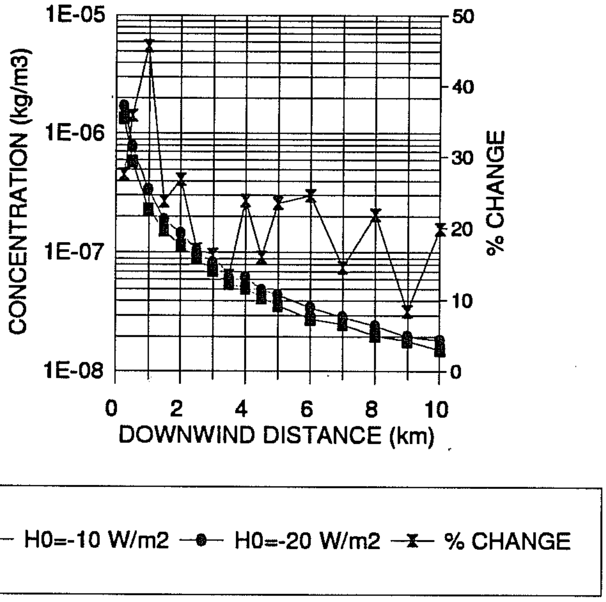

Figure 8. SCIPUFF sensitivity to surface heat flux: stable case.

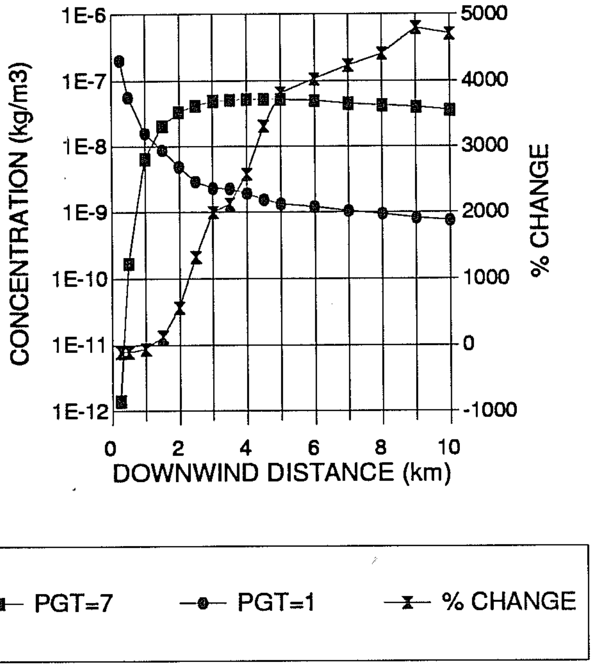

Figure 9. SCIPUFF sensitivity to PGT stability class.

7.2.6. *Release Height*

The sensitivity of SCIPUFF to changes in source elevation for convective and stable conditions is demonstrated in Figures 12 and 13 respectively. For the convective case, increasing the source elevation from the surface to 250 m resulted in an average decrease in concentration of about 35%. Initially there is about a 100% difference in these concentrations, but convection mixes plume material through the mixing layer so that by about 5 km downwind of the release point ground level concentrations are approximately equal. SCIPUFF treats the top of the convective mixing layer as an impenetrable surface. When a source elevation of 1100 m was used, plume material was not observed below z_i, even 100 km downwind. The downwind variations of ground-level concentrations seen in Figure 12 are in keeping with what is expected from diffusion theory. Figure 13 shows the case of a stable PBL. Changing the source elevation from the surface to 25 m results in about a 19% decrease in concentration. The greatest differences in concentration occur within the first 3 km from the source. Beyond that point, plume material is mixed through the stable layer, and surface concentrations become relatively insensitive to source height. These results are in agreement with diffusion theory.

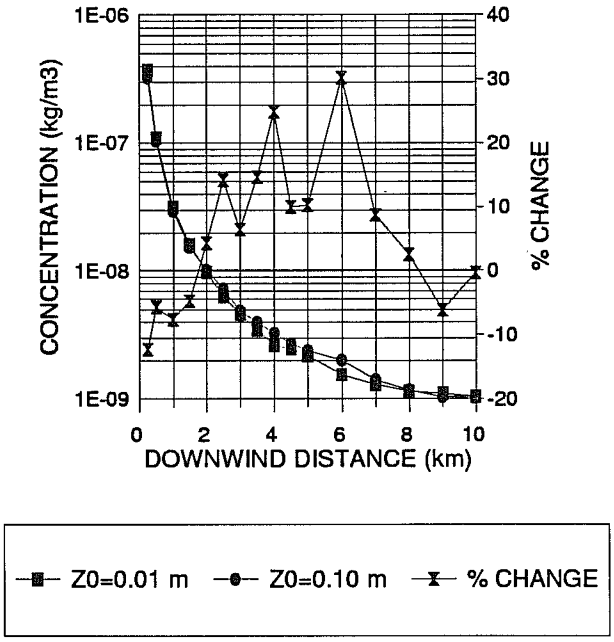

Figure 10. SCIPUFF sensitivity to surface roughness: convective case.

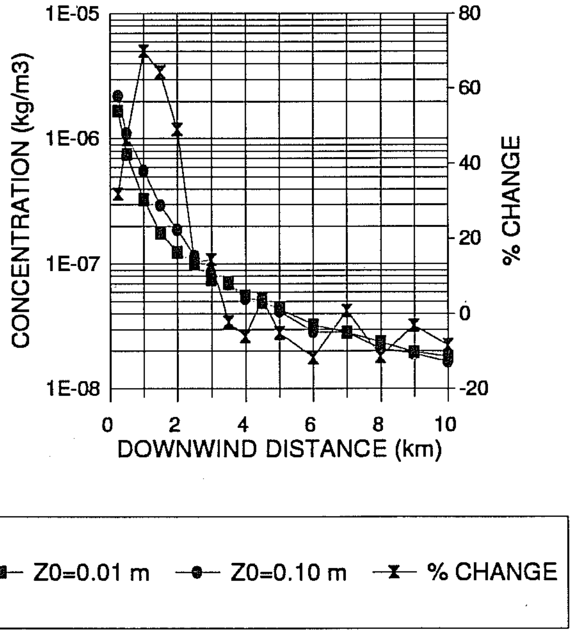

Figure 11. SCIPUFF sensitivity to surface roughness: stable case.

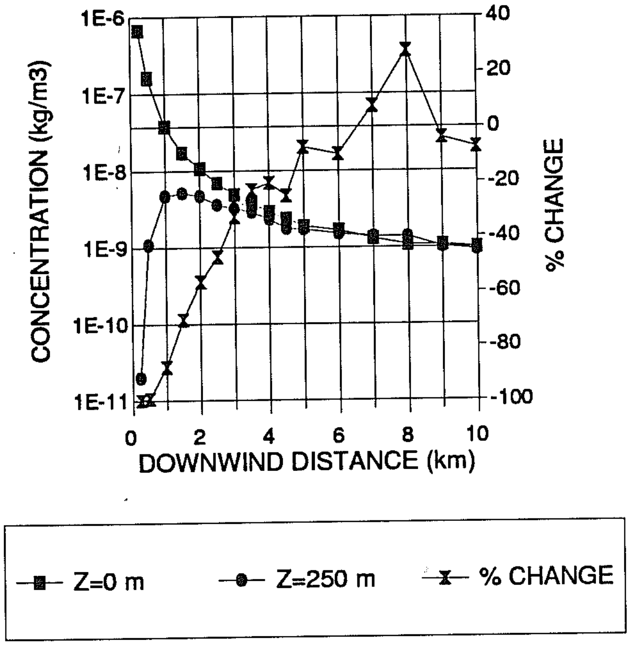

Figure 12. SCIPUFF sensitivity to source height: convective case.

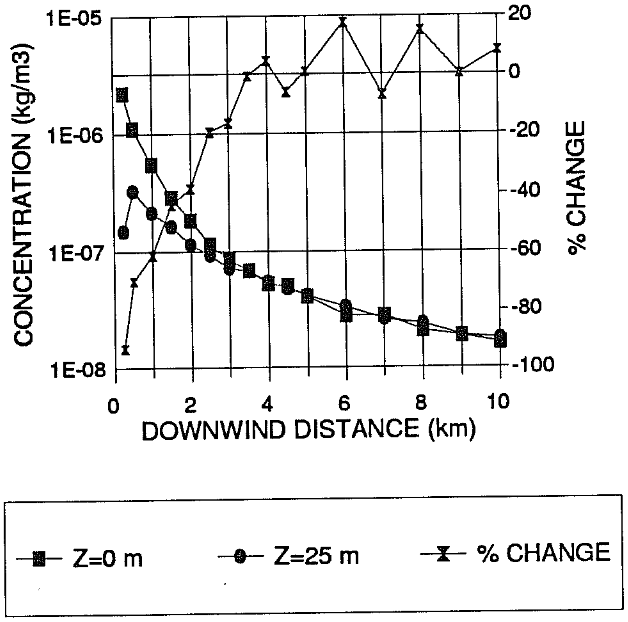

Figure 13. SCIPUFF sensitivity to source height: stable case.

7.2.7. *Averaging Time*

The averaging time parameter, T_{av}, along with the local wind speed defines an averaging length scale which is used to restrict the velocity variance to the diffusive range of turbulence scales. This averaging length scale is defined as the larger of the instantaneous length scale or $0.02\,V\,T_{av}$, where V is the velocity length scale. If the the averaging length scale is less than the length scale of the velocity fluctuations, a reduction factor is applied to the velocity variances. Turbulence theory predicts that velocity variances increase with increasing averaging time, and so we expect decreasing concentrations with increasing averaging time, and this is observed in Figures 14 and 15 for convective and stable conditions, respectively. For the stable case, changing the averaging time from the default value to zero resulted in an average fractional change in concentration of about 198%, and for the stable case this was about 316%. The default value of T_{av} is a large number so that no reduction of the variances occurs. When $T_{av} = 0$, variance reduction is determined by the cloud size. The greatest sensitivity to the averaging time is observed during stable conditions, but it is under stable conditions that the greatest uncertainty exists in the turbulence parameterizations.

7.2.8. *Boundary-layer Parameterization*

SCIPUFF is designed to run for a wide range of boundary-layer meteorological input data ranging from no data to observed values of surface heat flux and mixing depths. To examine the effects of increasing the quantity of boundary-layer data, the model was run with the SIMPLE PBL mode using the control values, and with the CALCULATED mode. The results of these runs are shown in Figure 16 for convective conditions and Figure 17 for stable conditions. For the convective case, the SIMPLE and the CALCULATED modes closely approximate the results from the control run (OBSERVED parameterization), but beyond about 3 km the CALCULATED-mode values become increasingly less than the control run and the SIMPLE values. In the stable case, the SIMPLE and the OBSERVED modes give identical results. This is because the surface heat flux is constant during the night in the SIMPLE mode. Since the control run and the SIMPLE mode use the same boundary conditions, it is expected that they will give the same results. The CALCULATED mode gives consistently lower concentration values at all downwind distances. These tests show that different boundary layer modes give different results, and the greatest differences, about a factor of 2, occur for the CALCULATED boundary-layer mode.

A possible source of user confusion was found in the vertical cross-section plots of the plume concentration contours produced by SCIPUFF. The mixing height is considered a reflecting surface, and so concentration contours are not expected above that height; however, the SCIPUFF plots show concentration contours above the mixing

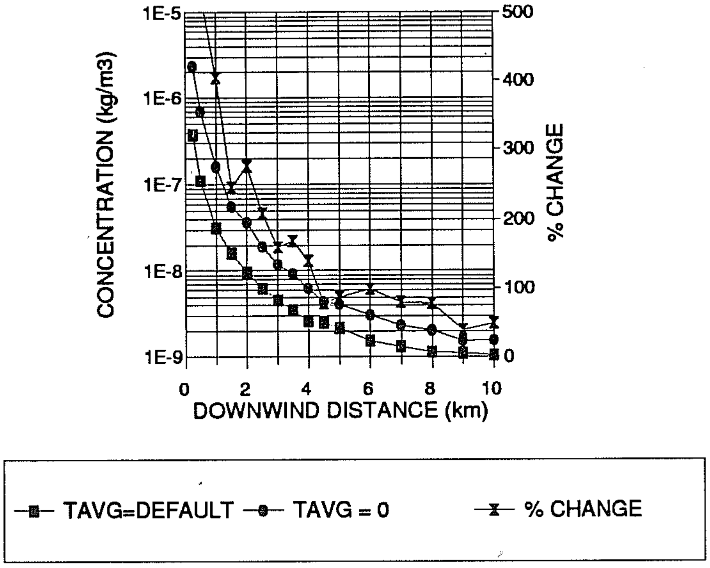

Figure 14. SCIPUFF sensitivity to averaging time: convective case. Note that zero averaging time corresponds to an instantaneous measurement of concentration.

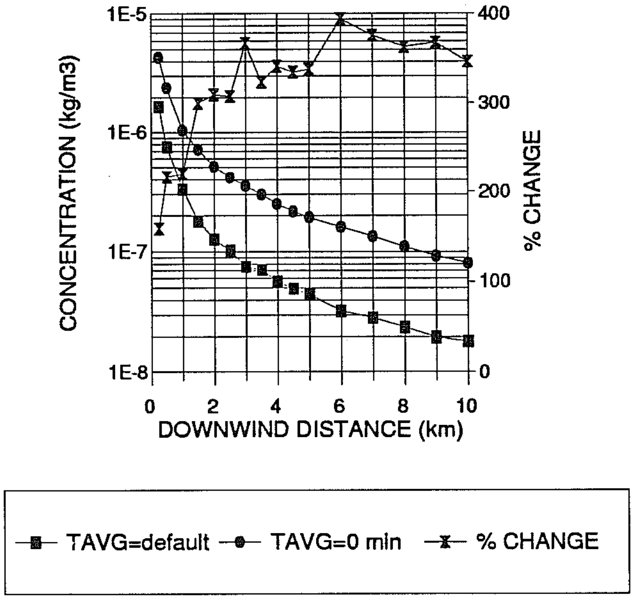

Figure 15. SCIPUFF sensitivity to averaging time: stable case. Note that zero averaging time corresponds to an instantaneous measurement of concentration.

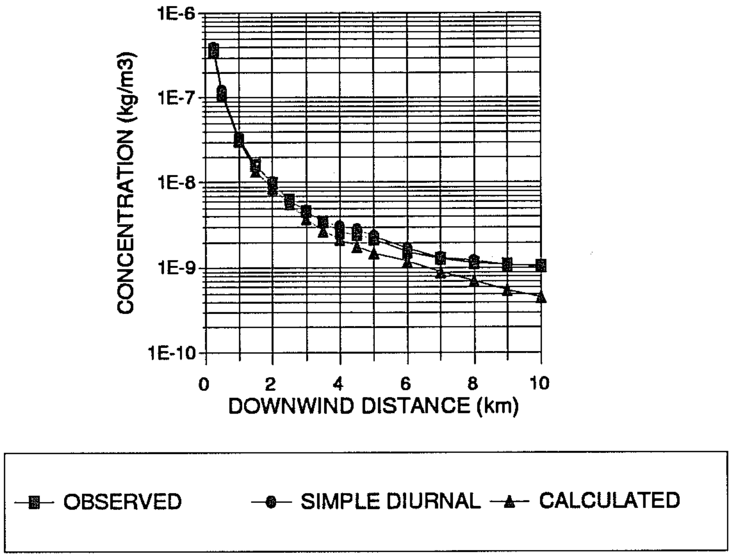

Figure 16. SCIPUFF sensitivity to boundary-layer parameterization: convective case.

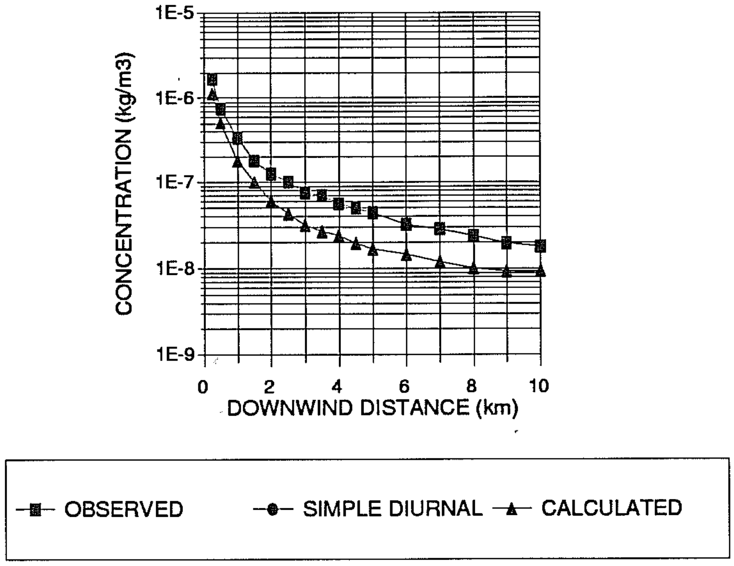

Figure 17. SCIPUFF sensitivity to boundary-layer parameterization: stable case.

height elevation. This problem was brought to the attention of the model developers, and their analysis revealed a coding error that essentially treated the atmosphere as having a uniform potential temperature when only a single temperature was specified on the surface observations file. It was reported to us that the problem has been fixed.

8. Test SCIPUFF Against Data

After discussions with DSWA staff, it was decided to compare SCIPUFF output with the SF_6 tracer test data taken as part of the U. S. Air Force Model Validation Program (MVP). These tests were performed at Cape Canaveral, Florida, and are described in Start and Hoover (1995), and Kamada *et al.* (1997). These tracer tests involved continuous (plume) and short-term (puff) releases near the ground surface and aloft using a blimp. Sampling was done with several vans traversing the plumes along roadways, and from an instrumented aircraft. Three tracer tests were selected from Session 2 of the MVP program:

> Test 208: 6 November, 1995. Plume release started at 1030 and ended at 1312 LST. Release height was 65 m (agl), and average release rate was $20.35\,\mathrm{kg\,hr^{-1}}$. We consider this to be a convective case.
>
> Test 209: 6 November, 1995. Plume release started at 1622 and ended at 1856 LST. Release height was 65 m, and average release rate is $20.57\,\mathrm{kg\,hr^{-1}}$. We consider this to be a transition case from convective to stable conditions.
>
> Test 215: 10 November, 1995. Plume release started at 0800 and ended at 1000 LST. Release height was about 2 m, and average release rate was $20.49\,\mathrm{kg\,hr^{-1}}$. We consider this to be a slightly stable case.

SCIPUFF calculates the concentration variance; however, the temporal resolution of the MVP concentration measurements is not fine enough to allow the formation of a statistically steady ensemble. For example, close to the release point where the plumes are generally less than a kilometer wide, concentration measurements (which require a complete pass through the plume to verify instrument baseline readings) can be made about every 5 minutes, but further away from the release point, 2 or 3 times more time is required. Because of the time required for the sampling vans to pass through the plumes, the resulting concentration values only approximate an "instantaneous" plume. On the other hand, SCIPUFF calculates the ensemble average of instantaneous plumes. It is not clear how these two quantities relate. Consequently, we chose to compare time-averaged, *i.e.*, Eulerian, MVP concentration values with time-averaged SCIPUFF values. To do this, a line of "virtual" samplers was established along straight sections of the various sampling paths. The concentrations measured by the moving sampling vans were then interpolated to these "fixed" sampler locations. By interpolating several sequential van passes in this way, we can construct the time-averaged MVP or observed plumes. These same virtual sampler locations are then used in SCIPUFF, and concentrations are calculated for these locations at every time step. These values are then averaged to form the time-averaged SCIPUFF plumes. We chose the averaging time to be 30 minutes.

Figure 18 is a schematic of the field setup for the three tests. The release points for Tests 208 and 209 were the same, and for Test 215 the release point was only a few hundred meters northeast of that point. The eastern-most meteorological towers generally follow the shoreline of Cape Canaveral. The origin of coordinates is arbitrary. The meteorological data have 5-minute resolution, and we used these observations in SCIPUFF. We ran SCIPUFF in the OBSERVATION PBL mode using only surface observations. The SCIPUFF time averaging parameter T_{av} was set to 5 minutes; this was also the time step size. Meteorological parameters included wind speed, wind direction, temperature, relative humidity, and surface heat flux. Mixing depth observations were not available. All SCIPUFF runs began at the time of SF_6 releases.

Figures 19, 20 and 21 show examples of observed and predicted concentrations for Tests 208, 209, and 215 respectively. Examination of these plume cross section graphs indicates a tendency for SCIPUFF to underpredict by more than a factor of two during convective conditions, to overpredict by about a factor of two during transition conditions from convective to stable conditions, and to be close to the observed values during stable conditions. However, we did not have observed mixing heights available for these calculations. As we have seen from the sensitivity tests, SCIPUFF is very sensitive to mixing heights during convective conditions. We feel that the use of observed mixing heights would greatly improve these comparison results.

In all, 24 half-hour averages were formed from the MVP data, and a scattergram comparing observed with predicted maximum values for each half-hour period is shown in Figure 22. Note that there are 23 points plotted in Figure 22; this is because for one case SCIPUFF predicted zero concentration, and the scattergram is on a log-log plot. From Figure 22, we see that about one-third of the points lie within a factor of 2 of agreement, and that almost all of the points are within a factor of 10 agreement. Hanna (1991) suggests several measures of model performance including the fractional bias (FB), the geometric mean bias (MG), the normalized mean square error ($NMSE$), the geometric mean variance (VG), and the correlation coefficient (R) which are defined as:

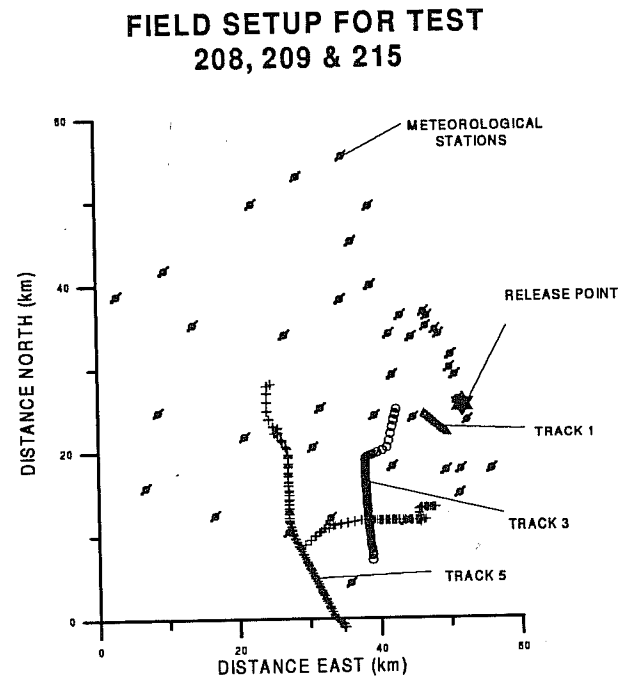

Figure 18. MVP experimental site at Cape Canaveral.

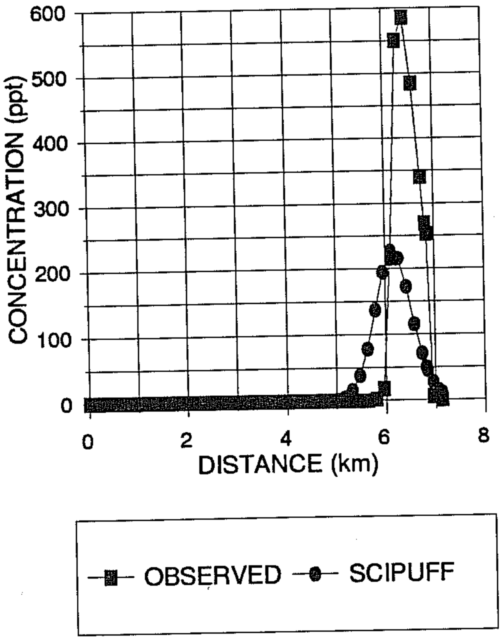

Figure 19. MVP and SCIPUFF average concentrations for Test 208 van 1: 1315 to 1335 LST.

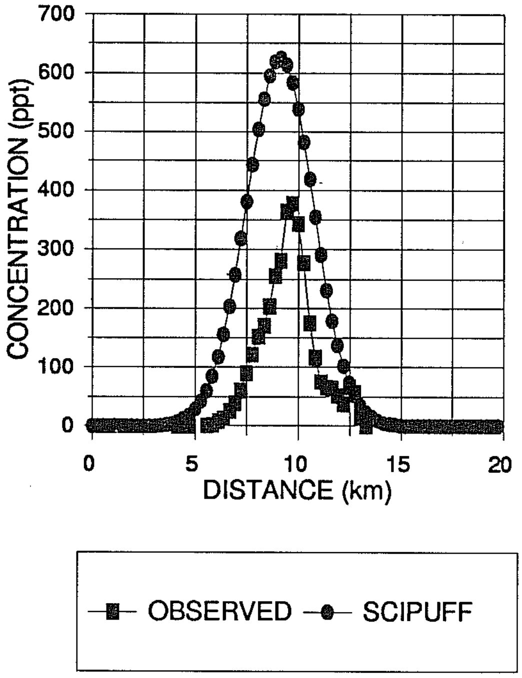

Figure 20. MVP and SCIPUFF average concentrations for Test 209 van 5: 2022 to 2057 LST.

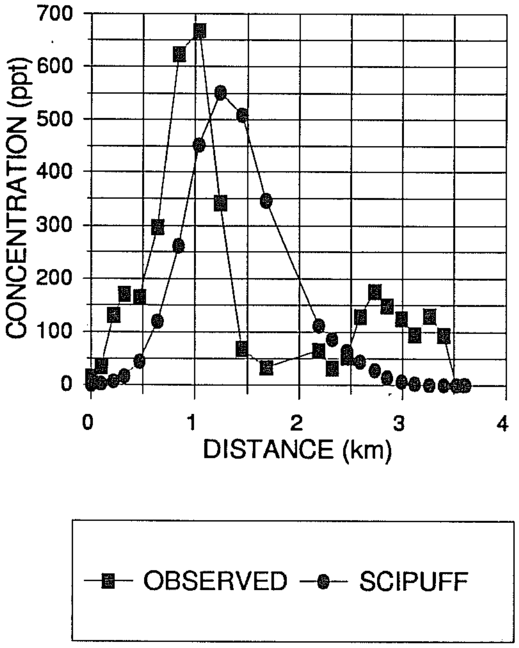

Figure 21. MVP and SCIPUFF average concentrations for Test 215 van 1: 0833 to 0929 LST.

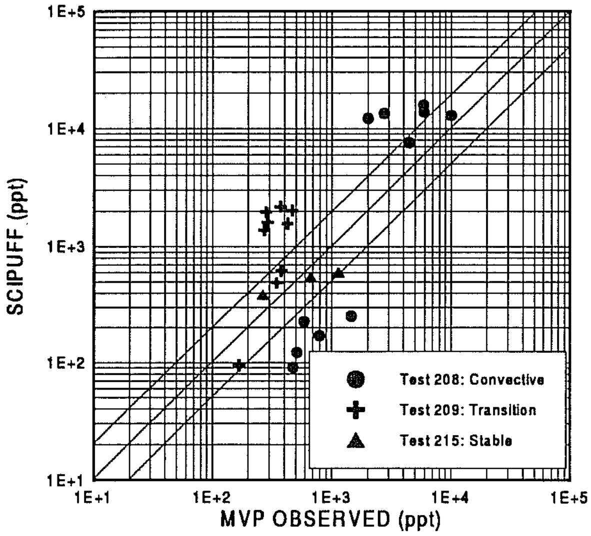

Figure 22. Scatter plot of SCIPUFF concentration estimates versus MVP observations.

$$FB = \frac{\overline{C_o} - \overline{C_p}}{0.5(\overline{C_o} + \overline{C_p})} \tag{6}$$

$$MG = \exp(\overline{\ln C_o} - \overline{\ln C_p}) \tag{7}$$

$$NMSE = \frac{\overline{(C_o - C_p)^2}}{\overline{C_o}\,\overline{C_p}} \tag{8}$$

$$VG = \exp\left[\overline{(\ln C_0 - \ln C_p)^2}\right] \tag{9}$$

$$R = \frac{\overline{(C_o - \overline{C_o})(C_p - \overline{C_P})}}{\sigma_{C_p}\sigma_{C_o}} \tag{10}$$

where C_o is the observed MVP concentration, C_p is the predicted SCIPUFF concentration, and σ is the standard deviation. Hanna (1991) cautions that if there is a wide range in the concentration values, then the statistics FB, $NMSE$, and R will be very strongly influenced by the large concentration values. In these cases, he suggests that MG and VG are more appropriate measures of model performance. Accordingly, we have calculated MG and VG using the half-hour average values plotted in Figure 22 with the result that $MG = 0.69$ and $VG = 4.89$. A perfect model would give values of 1 for both MG and VG. A geometric mean bias (MG) of 0.5 or 2.0 indicates an overprediction and an underprediction by a factor of two respectively, and a geometric variance VG of about 1.6 indicates a typical factor of two scatter between individual pairs of observed and predicted values. Thus, for these few specific tests, SCIPUFF can be said to overpredict (on average) by less than a factor of two, but there is a greater than a factor of two scatter between individual pairs of observed and predicted values.

9. Conclusions

Overall, the approach used by SCIPUFF to represent turbulent diffusion is physically sound. The second-order-closure approach used by the model allows estimates to be made of both the mean concentration and the concentration variance.

The complex second-order-closure approach used in SCIPUFF is likely to be of greatest benefit when extensive field measurements are available for the winds and turbulence, such as could be expected when simulating tracer releases during a field experiment. Under more operational conditions, when SCIPUFF must rely more heavily on the idealized wind and turbulence profiles given in Sections 7 and 8 of the TD, the benefits of the second-order-closure approach over simpler approaches may not be all that significant.

For long range applications and upper atmospheric conditions, the turbulence input to SCIPUFF is based on climatological information. Predictions with such data will almost certainly be less reliable than with on-site measurements, and do not justify the use of a complex model such as SCIPUFF. It is therefore reasonable to conclude that the SCIPUFF model is probably more suited for short-range, atmospheric boundary layer scale, dispersion applications rather than for long-range transport modeling.

The experiences of the study team indicate that there are deficiencies in the TD, and that running HASCAL is not straightforward. Several important diagnostic quantities are available in the PUFF files; however, these are binary files that are not easily accessible to the user. It would be useful to have a “research mode” switch in the code that would make such internal information readily available to the user. We anticipate that SCIPUFF users will require extensive training in the use of the model and in assessing the information provided in the results.

Although the second-order-turbulence closure scheme used in SCIPUFF is physically sound, the practical advantages of this approach over alternate approaches have been somewhat overstated in the SCIPUFF documentation. For example, it has been stated that the second-order-closure approach is more general than alternate approaches because it is less empirical and provides a fundamental relationship between turbulent diffusion and the velocity fluctuation statistics. However, a closer inspection reveals that SCIPUFF's approach also contains a significant degree of empiricism. Moreover, other approaches commonly used in puff models are also based on fundamental relationships between turbulent diffusion and the velocity fluctuation statistics. One feature of the second-order-closure approach that is different from other approaches is the estimation of the concentration fluctuation variance.

Our examination of the SCIPUFF Ver. 0.625.2R computer source code showed that there are 2260 subprograms in 534 source files, 76 include files, over 760,000 non-comment source lines, and over 85,000 non-empty comment lines mostly used to delimit subprograms and make "fossil" code inactive. Descriptive comments in the code are rare, and there is no up-to-date documentation of the source code. Thus, it was not possible to do a comprehensive verification of the code in the time allotted. Instead it was decided to do a static analysis of the SCIPUFF FORTRAN code using a commercial code analyzer. This analysis was conducted on the SCIPUFF v0.625.2R source code dated 11 March 1997. This version of the SCIPUFF source code matches the SCIPUFF runtime program included on the HPAC 2.0 distribution CD-ROM (which also contains HASCAL Ver. 2.1). No attempt was made to compare purported model equations with actual model source code statements. The FORTRAN code analyzer indicated 47 possible sources of coding conflicts or coding errors. These occurred mostly in the subroutine calling arguments, dimension statements, and type declarations. However, these inconsistencies can be resolved by the source code compiler, and so may not be a problem. Since we do not have access to the complier, we cannot verify that this is the case.

The sensitivity of SCIPUFF to changes in wind speed, mixing height, surface heat flux, PGT stability class, surface roughness, release height, conditional averaging time, and boundary-layer parameterization type showed that over a downwind distance of 10 km from the source, SCIPUFF behaved as expected from diffusion theory; *i.e.*, there were no unexplainable or extraneous results. However, in some cases the downwind plots of fractional changes in concentration due to changes in input values showed large spikes; we have no explanation for this behavior. For both daytime and nighttime conditions, the most sensitive parameter is the conditional averaging time, and the least sensitive parameter is the surface roughness. The next most sensitive parameters are mixing height for the daytime case and wind speed for the nighttime case. SCIPUFF is not very sensitive to changes in mixing height in the nighttime case. Heat flux and source height are about equally sensitive for both day and night conditions.

SCIPUFF output was compared with the SF_6 tracer test data acquired during the U. S. Air Force Model Validation Program (MVP). The tests used were performed at Cape Canaveral, Florida in November, 1995. The tracer tests selected for use in the present study involved continuous releases for about two hours, and ground level plume sampling was done with vans traversing the plumes along roadways. Three tracer tests were selected for comparison with SCIPUFF. These tests occurred during convective, transition, and stable conditions. SCIPUFF tends to underpredict by more than a factor of two during convective conditions, to overpredict by about a factor of two during transition from convective to stable conditions, and to be close to the observed values during stable conditions. However, we did not have observed mixing heights available for these calculations and, as we have seen from the sensitivity tests, SCIPUFF is very sensitive to mixing heights during convective conditions. We feel that the use of observed mixing heights would improve these comparison results.

The maxima of time-averaged observed and predicted plume concentrations were compared. The overall geometric mean bias MG is 0.69, and the geometric variance VG is 4.89. Thus, for these tests SCIPUFF can be said to overpredict on average by less than a factor of two, but there is greater than a factor of two scatter between individual pairs of observed and predicted values.

Acknowledgments

This work was performed under an interagency agreement between the Defense Special Weapons Agency (DSWA) and the NOAA Air Resources Laboratory (ARL).

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Appendix: Corrections to the Technical Document

Suggested by Dr. K. Shankar Rao

This section lists the specific comments consisting of corrections, revisions, and modifications to the Technical Document (Sykes *et al.*, 1996a) suggested by this reviewer. An interim partial list of these corrections was provided earlier to DSWA to guide the code verification effort.

Notation: A complete alphabetical listing of symbols used in the SCIPUFF guide, with brief definitions or explanations and units, should be provided at the beginning of the TD. Duplication or multiple use of symbols should be avoided in order to reduce confusion.

1. Puff Moment Equations

It is not clear why σ was used to denote the variance in Eq. (2.1) and elsewhere in this report, instead of σ^2 as is the standard practice. The latter would be preferable to avoid confusion.

p3, Eqs. (2.2): is true only for a non-reactive, non-depositing pollutant (such as an inert tracer), if Q is the emitted mass (Eq. 2.7 suggests this is the case). Otherwise, it is necessary to distinguish between the initial ($t = 0$) mass at release (say, Q_o) and the mass Q_t given by the volume-integrated concentration at time $t > 0$ in this equation. In any case, the assumptions leading to these equations should be clearly stated.

p4, para above Eq. (2.6): Change "Reynolds average technique" to "Reynolds averaging technique."

p5, Eqs. (2.9) and (2.11): The derivation of these equations should be provided in an Appendix. The x_i and x_j in the latter equation might be x'_i and x'_j. The physics and role of the "turbulent drift" term in Eq. (2.9) should be discussed here.

p6, Eq. (2.13): The turbulent transport term (third term on the RHS) should have a positive sign in front; see Donaldson (1973, p 362), for example.

p7, line above Eq. (2.14): Change x_i in $< x_i\overline{u'_j c'} >$ here to x'_i.

p7, Eqs. (2.15) and (2.16): should be derived in an Appendix.

p7, line below Eq. (2.16): What is a "horizontal value"? This sentence is awkward, and should be changed to "subscript H denotes values for the horizontal turbulent velocity and length scales..." or something similar.

p8, Eq. (2.19): is consistent with Taylor's (1921) exact analytical result for turbulent diffusion only for the assumption of homogeneous turbulence. This assumption should be emphasized.

p9, Eq. (2.22): The third term on RHS should have a minus sign instead of "+" sign in order to be able to derive Eq. (2.24), which appears to be correct.

p10, 1st para, last sentence: The mean concentration distribution tends to be uniform across a well-mixed layer, but only sufficiently far away from the source. What is meant by "non-uniform turbulence" here?

p10, 2nd para, last line: insert "turbulence" after "mesoscale/synoptic scale".

p10, 3rd para, last line: change "scale" to "scales."

p11, Eq. (2.30): Include the condition $\Lambda_{HB} > \Lambda_{VB}$ for the validity of this equation.

p11, sentence above Eq. (2.31): correct "simple" to "simply".

2. Concentration Fluctuation Variance

p12, 1st para, last sentence: delete "below".

p15, Eq. (2.41): How are the two values for α_{cH} given here determined? A reference would be useful.

p15, Eq. (2.42): With the given values b and s, one gets $bs = 0.23$, nearly the same as the constant in the first part of this equation. Why is the vertical scale growth given by the smaller of the two velocity scales in each part?

p16, Eq. (2.44): If these equations are nondimensional, then denote and redefine the LHS in these three equations as $\hat{\sigma}_{11} = \sigma_{11}/\sigma_o^2$, $\hat{\sigma}_{13} = \sigma_{13}/\sigma_o^2$, and $\hat{\sigma}_{33} = \sigma_{33}/\sigma_o^2$ to avoid confusion.

p16, Eq. (2.45): More steps and/or explanation (with a suitable reference, if available) between the two equations should be provided. In the paragraph above, rewrite the sentence as "the square of the mean is comparatively negligible".

p17, Figure 2-1 caption: Replace "Normalized" with "Nondimensionalized". The paragraph above this figure states that "smaller values of diffusivity give a lower minimum at later time". This is not what the figure shows! This should be written as "smaller values of diffusivity B give a larger minimum value of the timescale $\alpha\tau_c$".

p18, Eqs. (2.46) and (2.47): The derivation of these equations should be provided in the Appendix.

p18, Eq. (2.48): Why is the factor 1/4 needed in this equation? The last two terms and related assumptions need to be explained better. How is the linear distribution (with height) assumption for large-scale velocity connected to these terms? Is there any reference to support this assumption?

p20: The derivation of Eqs. (2.59) to (2.65) need to be provided in the Appendix.

p20, para. below Eq. (2.65), 2nd line: Insert "be" after "can".

p21, Eq. (2.66): should be derived in the Appendix. A clear statement is required of where and how this expression for f_R is used in the algorithms.

p21, last line: What is meant by "bounded below" here?

p22, 2nd para: Explain clearly what are the two variance calculations stored for multiple particle size bins, and how they are used.

p24, Eq. (2.71): How is the factor 0.02 obtained? A reference would be useful.

3. Particle Gravitational Settling

p24, Eq. (2.75): Insert "particle" before "Reynolds number".

p25, Eq. (2.78): The rationale for the inverse linear particle size weighting used here is not clear. Both Stokes' law as well as the widely-used velocity interpolation schemes suggest an inverse particle size-squared weighting in this equation. This same weighting scheme can also be applied in Eq. (2.79) for the fall-velocity variance.

p25, Eq. (2.79): The last term on RHS, given only as v_g^2, is dimensionally incorrect; I think it needs $\overline{r}$ in the denominator to be consistent with the other terms.

P26, Eq. (2.82): Define dA as the area element.

p26, Eq. (2.85): The RHS is wrong. It should be Q/F_s.

p27, Eq. (2.87): This equation is dimensionally inconsistent. The last term, given as $2\,\sigma_g/\sqrt{\sigma_{33}}$, has units of s^{-1}, while LHS and the first term on RHS have units of $\mathrm{m}^2\mathrm{s}^{-1}$ .. As the line below this equation notes, this is not an accurate representation of particle size variability.

4. Dry Deposition

p28, Eq. (2.89): This equation is valid only if F_c includes both turbulent flux and gravitational settling flux at the surface. This was not the case here however, since dry deposition was assumed to refer only to non-gravitational surface processes (p27, last para). This does not agree with the deposition boundary condition and related physics discussed by Monin (1959), Calder (1961), Smith (1962), and Rao (1981), among others. In their formulations, the deposition velocity v_d includes the gravitational fall speed v_g, and both need not be added as in the current version of SCIPUFF (p28, para 2).

p28, 4th para: Change "base" to "based".

p28, Eq. (2.91): applies only to small (submicron size) particles. This should be explicitly stated. Change "viscous boundary layer" in the next line to "viscous sublayer".

p29, 2nd para, line 1: Insert "in Eq. (2.90)" after "...shear-driven friction velocity".

p30, Eq. (2.96): Insert enough blank space and a "·" after f and $(1 - f)$ to avoid confusing these factors with the common notation for functions.

p31, Eq. (2.97): Though both Slinn (1982) and Davidson *et al.* (1982) use an equation similar to (2.91) for collection efficiency, their expressions for particle impaction efficiency (E_{IM}) and Stokes number (St) are different.

p31, 3rd para: The displacement height typically varies as 0.65 to 0.75 times the canopy height h_c; 0.5 being used now in SCIPUFF is too low.

5. Numerical Techniques

p33, 2nd para: How are ΔH and ΔV determined in practice? Rewrite the last sentence as "...displaced by a fraction r of the puff spread $\sqrt{\sigma_{11}}$ in the x-direction,..." Otherwise, r, σ_{11}, etc., are undefined in Eqs. (3.1) to (3.3).

p34, line above Eq. (3.2): Rewrite as "The diagonal moments for the two smaller puffs are obtained using the following relations." Similarly, the line above Eq. (3.3) is to be rewritten as "and the off-diagonal elements for the two smaller puffs are"

p35, 2nd para: states "...the multi-dimensional case provides better overlap between the new puffs and smaller differences for the same separation." I do not see the latter (*i.e.,* smaller ε_s for same δ_s) in Fig. 3.1. For a separation of 1.8, for example, the 2-D split gives a maximum dimensionless error of 0.2, while the 1-D split gives half of this error. Same para, 5th line from bottom: Insert "less than" before 1.8.

p36, Fig. (3-1) caption: Insert "concentration" between "maximum" and "value" in the third line.

p38, Eq. (3.6): How was the factor 4 in this equation obtained?

p38, 3rd para, 2nd sentence: "The puff requires 2 levels of grid refinement,.." needs to be restated clearly and explained.

p42, Eq. (3.13): It should be indicated here that these three equations are derived from Eq. (2.11) after neglecting turbulent diffusion terms. The second term within the brackets on RHS of Eq. (3.13a) could be wrong. It cannot be obtained from Eq. (2.11) and, I think, it should be zero.

p42, last para, 3rd line: "rapid time scales" does not make sense. This should be changed to "small time scales".

p43, 2nd para: The first line is confusing; rewrite this as "A large time step, Δt_L, is defined for the calculation. This time step must resolve the ...".

p43, 3rd line below Eq. (3.14): Correct "defines" as "defined".

p43, Eq. (3.15): Explain briefly with a reference, if available, why Δ_c was set to 1/2 of τ_c. The line above should be rewritten clearly as "The time step for dissipation of concentration fluctuation variance, Δt_c, is determined by the scalar dissipation timescale, τ_c defined in Eq. (2.40):"

p44, para below Eq. (3.18): w_T was not defined anywhere. The equation referred to here should be (2.86) instead of (2.82). It is better to rewrite this part of the paragraph as "... and w_T denotes the total vertical velocity defined in Eq. (2.86) as ..."

p44, last para: As noted above in the comment on Eq. (3.13a), I could not get this Δt^2 term.

6. Model Output

p51, line above Eq. (5.13): Q_s is not given by Eq. (2.79). Insert the correct equation number, or give the steps in the derivation of Eq. (5.13) here.

p53, line above Eq. (5.22): Eq. (5.21) should be Eq. (5.20).

P54, 1st line: Indicate here how $T_c = T_E \, \Lambda_C / \Lambda_y$ is obtained for $\Lambda_C > \Lambda_y$.

p54, Eq. (5.23): What are $\overline{u}$ and $\overline{v}$ here? If they are horizontal mean wind components, explain why they are included in the definition of the Eulerian scale of turbulence.

p54, sentence below Eq. (5.24): is rather cryptic and unclear. In fact, some parts of this section will benefit from clear rewriting.

p55-56, Eqs. (5.30-31): Define $\overline{R_j}$ and $\sqrt{\overline{R_j'^2}}$ as the mean and standard deviation of the dose, respectively.

p58, line above Eq. (5.37): Rewrite "... the number exposed ..." as "... the number of people exposed..."

p58, line below Eq. (5.38): Rewrite "... exposed to a level of X ..." as "... exposed to a concentration/dose level of X ..."

p61, 2nd para, last line: Insert "vertical" between "uniform" and "grid".

p62, Eq. (6.2b): set the RHS equal to $1/r_{ij}{}^2$, the inverse of squared distance.

p62, Eq. (6.2e): What is s here? This probably should be s_{ij}.

p64, Eq. (6.10c): The partial derivative on RHS, given as $\partial\phi/\partial\xi$, should be $\partial\phi/\partial\zeta$.

7. Planetary Boundary Layer

p66, 1st para, lines 7-8: Change "(See Wyngaard, 1985, 1988 or Lewellen, 1981)" as "(See Wyngaard, 1985; Venkatram and Wyngaard, 1988; and Lewellen, 1981)"
Change "... ideal condition both ..." to "... ideal conditions, both ..."

p66, list of parameters: "3) the Monin-Obukhov length, L," is a calculated parameter, not a measured one. It would be better to replace it with the surface heat flux, $H/(\rho_a \, c_p)$, so that the parameters in this list would permit calculation of L.

p66, last para: z_{ref} cannot be set arbitrarily. It is important to point out that z_{ref} has to be within the surface layer so that Eqs. (7.1) and (7.3) apply.
Change "more fundamental parameters..." to "important PBL parameters..."

p67, 1st para, last line: Replace "L is singular" with "$L \to \infty$".

p67, last line: Insert "z_{ref}" to read as "height z_{ref} used in Eq. (7.3)..."

p68, Eq. (7.7): Ψ_1 on the LHS should be Ψ_m.

p68, Eq. (7.9): The definition and sign are incorrect. This should be defined as $\theta_* = -H/(\rho_a\, c_p\, u_*)$. Rewrite the line above this equation as "The temperature scale for stable conditions is defined as". The line below this equation seems to suggest that u_* appears in the temperature profile equation. Change this line to "and it appears in the temperature profile equation given by".

p69, 2nd para, last line: Rewrite "an estimate of H is found from a ..." as "H is estimated from a ...".

p70, Table 7-1 caption: Include "(Saucier, 1987)" at the end of the caption.

p73, para under Eq. (7.20): Correct "theses" to "these".

p73, Eq. (7.24): needs a reference. What is r here? Where is it used?

p74, 2nd para: Section number should be (7.2.4) instead of (7.2.3.3).

p75: This Table number should be 7-4 since the previous Table number is 7-3.

p74-75, Tables 7-3 and 7-4: Include relevant references in the captions and text.

p75, Eq. (7.27): needs a reference and more explanation leading to its derivation.

p76, 2nd para: Change "used in the setting mean velocity profile ..." to "used in setting the mean velocity profile ...".

p77, 2nd para: Change "solves an model evolution equation for ..." to "solves an evolution equation for ...".

p77, line above Eq. (7.33): Rewrite "Then" as "Then, from Eqs. (7.30) to (7.32),".

p80, Eq. (7.40): is confusing. $u_*^2 T/(k^2 g L)$ should be replaced with θ_*/k, since θ_* is already defined in Eq. (7.9).

p81, last line: Change "... Schumann, 1989), and a ..." to "... Schumann, 1989). A ..."

p83, 1st para: In line 2, change "turbulence conditions for the stable atmosphere remote from the ground ..." to "in the stable atmosphere, the conditions above the boundary layer ...".

p83, line 5: the units should be corrected as "m^2s^{-2}". Same correction applies in 2nd line from bottom of this para. Rewrite the latter line as "...suggest that horizontal velocity variances, ..., be taken as ...". Why is the typical vertical length scale, Λ_{VB}, taken as 10m? Is there any reference?

p84, 3rd line: Change "data presently exits ..." to "data presently exist ...".

p84, line below Eq. (8.11): The Λ_r should be Λ_T.

p84 Eq. (8.12): Why is the filter scale Λ_G defined as $\sqrt{2}$ times the diagonal spacing of the wind field grid?

8. File Formats

p88, namelist group: The correspondence between these input parameters and the mathematical symbols used in the text and equations, if any, should be indicated, to help model users. It is necessary to indicate where some of the parameters (*e.g.*, t_{avg}, *mgrid*) are used or discussed in the text.

p90, *lon*0 and *lat*0: The definitions are not clear. How can CARTESIAN coordinates be specified in degrees? "CARTESIAN" should be replaced with "LATLON" (see *xmin* definition on p89).

p91, *epstrop*: The default value given here is $4.0\text{x}10^{-3}$, while on p84 it is given as $4.0\text{x}10^{-4}$.

p91, *nzbl*: Insert "vertical" between "boundary layer" and "grid".

p93, *cmass*: Specify units here for total mass of material or mass flux.

p94, *rel_param*(5): Change "particle material" to "particulate material".

p94, Fig. 9-3: Why are canopy height (*H_CNP*) and surface roughness (*ZRUF*) given the same value? What does this mean physically?

p95, *bl_type*: Include "SBL stands for 'standard boundary layer' parameters" in the definition.

p95, *sl_ensm*: The default value here is $1.0\text{x}10^5$ m, while the recommended value is 1000 m (p83).

p95, *zimax*: Change "...with 'standard' boundary layers." to "...with 'SBL' boundary layers."

p96, below *cloud_cover*: Include *LOCAL_MET* (see Fig. 9-3) definition also in this list.

p101, 2nd para: Change "...data is ..." to "... data are ...".

p104, 1st para: The temperature input is given here is deg. C, while in the MEDOC format (p101) it is assumed to be potential temperature in deg. K.

p 104, last line: Correct "Figure 9-3" as "Figure 9-7".

9. References

p115: Correct the Wyngaard and Venkatram (1988) reference as "Venkatram and Wyngaard (1988)" (listed below).