Appendix A

Verification and Validation of the Air Module

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A.1 Overview of air module

The purpose of the atmospheric modeling for the Multimedia, Mulipathway and Multireceptor Risk Assessment (3MRA) is to provide an annual average estimate of air concentration of dispersed constituents and annual deposition rate estimates for vapors and particles at various receptor points in the area of interest, which is defined by a 2-km radius measured from the edge of the largest area source at the site. The chemical constituents are assumed to be in the form of volatilized gases or fugitive dust emitted from area sources. The atmospheric module simulates the transport and diffusion of the constituent. The simulated air concentrations are used to estimate bio-uptake from plants and human exposures due to direct inhalation. The predicted deposition rates are used to determine chemical loadings to watershed soils, farm crop areas, and surface waters.

The atmospheric concentration and deposition of constituents can be determined in several ways. The initial design of the air module was strongly influenced by the needs and constraints of the proposed HWIR application of 3MRA. The requirements for the air model included: 1) able to produce estimates of concentration, wet deposition, and dry deposition for particles and gases at distances within 10 km of the source for a variety of time scales; 2) able to model rectangular area sources to be consistent with other media models being considered for inclusion; 3) able to use readily available meteorological data for sites across the nation; and 4) short runtime. After consideration of several models, we selected the Industrial Source Complex-Short Term (ISCST3) model, a steady-state Gaussian plume model. ISCST3 fit most of the design criteria with two notable exceptions: 1) the gas deposition algorithms were not appropriate for most of the chemicals to be modeled and 2) the runtime for modeling area source was longer than specified, particularly when including the effects of plume depletion due to dry deposition. We opted to use bio-transfer factors to account for the exchange of gases between the air and other media. To address the runtime issue, we embarked on a series of investigations into ways to develop options for reducing the runtime. These are described in more detail in Section 2.0.

ISCST3 is used as "legacy code" in the 3MRA framework. That is, the model is left intact and the necessary interfacing to the framework is handled using pre- and postprocessors. Together, the EPA air quality model (ISCST3) and the pre- and postprocessing code that integrates ISCST3 into the 3MRA environment are referred to as the Air Module. The pre- and postprocessing code also provides additional functionality to support other 3MRA framework requirements. For example, the preprocessor determines whether to execute ISCST3 to model the site-specific x-y coordinates requested by the 3MRA framework or, alternatively, to model to a fixed set of polar coordinates and then use a two-dimensional cubic spline method to interpolate from this polar set to the x-y coordinates of interest.

A.2 Verification History of ISCST3

The ISCST model has had a long history of use, dating back to 1979 (Bowers et al, 1979), by the EPA for modeling sources of nonreactive pollutants. Over the years, ISCST has undergone a number of updates as needed to address particular applications. A history of the development is detailed in Irwin (2002). This section details much of the verification efforts that have occurred during the continued model development to show that the FORTRAN program accurately solves the intended equations. A significant overhaul of the program occurred in 1992 when the code was modified to produce the ISCST2 model. During this effort, a substantial amount of recoding was done to make the code more modular. A detailed test plan was followed to assure that the re-coded model produced results equivalent to the original model (U.S. EPA, 1992a).

There have been several components of the ISCST2 model that have been revised since 1992. In response to concerns related to emission sources at Superfund sites, a study was undertaken to compare area source algorithms used by various dispersion models (U.S. EPA, 1989). The results of the study showed that the finite line source approach used in ISC to model area sources predicted unrealistic concentrations for receptors located within and near the area source. A new area source algorithm which uses an integrated line source algorithm was implemented in ISCST2 and tested in 1992 (U.S. EPA, 1992b; U.S. EPA 1992c) and released to the public in draft form as AREA-ST. The need for better estimates of the intermedia transfer of pollutants from the atmosphere to land, water and vegetation to support environmental impact analyses prompted a study to compare existing algorithms for calculating the dry deposition velocity of particles (U.S. EPA, 1994). The algorithm in the original ISCST2 model was not designed for small particles. An additional component of this study was to compare plume depletion algorithms and propose a revised algorithm. A new deposition velocity algorithm and plume depletion algorithm were proposed and implemented into ISCST2 and released to the public in draft form as DEPST. In 1993, the EPA Administrator announced that risk assessments, including indirect exposure, would be required for permitting hazardous waste incinerators and industrial furnaces. Since there were no regulatory models capable of quantifying wet and dry deposition in all terrain, EPA Region 5 sponsored further development of the ISCST2 model to address their immediate need for performing an assessment as well as the more general need of the Agency. In this effort, the AREA-ST and DEPST versions of the ISCST2 model were combined into a single version referred to as ISC-COMPDEP. Testing was performed to demonstrate equivalence between ISC-COMPDEP and AREA-ST and DEPST. The methodology used in the COMPLEX I model for modeling point sources in complex terrain was added to ISC-COMPDEP with equivalence tests begin performed against the original COMPLEX I model. Finally, wet deposition and depletion algorithms were selected and implemented in ISC-COMPDEP. The development and testing of the ISC-COMPDEP model including the equivalency test is documented in Strimaitis et al (1993). ISC-COMPDEP was provided to EPA's Office of Air Quality Planning and Standards, renamed ISCSTDFT, and proposed as part of Supplement C to the Guideline on Air Quality Modeling. As part of the rulemaking process, the model and associated documentation was subject to public review and comment. Supplement C was promulgated on 8/9/95 (60 FR 40465) and model was renamed to ISCST3 and released to the public for use in regulatory applications.

To meet some of the needs and constraints of the proposed HWIR application, ISCST3 was further modified. One of the major areas of concern for the HWIR application was the runtime of ISCST3. There were two modifications made to ISCST3 to address this issue. The first change was the addition of an option to sample from the meteorological data at regular intervals rather than run each consecutive hour. This option is used to calculate annual values for concentration and deposition. This use of this option, referred to as the Sampled Chronological Input Methodology was tested over a range of sources, climate regimes, and sampling rates (U.S. EPA, 1998). The testing resulted in a recommended sampling interval for the HWIR application, however the use of the sampling option and the selection of the sampling interval are not mandated by the 3MRA software system. A second modification to ISCST3 involved an analysis of the plume depletion algorithm since this is a numerically intensive calculation for area sources. A comparison of available depletion schemes was completed and a new algorithm was proposed, tested, and implemented (Venkatram, 1998) to replace the existing scheme (Horst, 1983).

In addition to the testing of the individual model components described above, the model, preprocessors, and postprocessors have undergone internal and independent testing as part of the software development process supporting the HWIR application(ref). The testing plan addressed the following specific requirements:

1. The air module should correctly develop the input file needed to run ISCST3, run the model, archive results for use in subsequent runs, output results in the correct format for use by other models, write an error messages to the 3MRA system log file.

2. The air module should be successfully implement the spline option and produce a reasonable spline surface and output values in the format appropriate for use by subsequent models.

3. The air module should correctly implement the plume depletion option. Concentration and deposition values should be higher when depletion is not considered.

4. The SCIM option should be correctly implemented by the air module. Values determined when every hour is sampled should approximate those calculated when the option is not used.

A.3 Validation of the ISCST3

The ISCST3 model provides point estimates of concentration, dry deposition, and wet deposition. While there have been a number of studies that have compared concentrations predicted by ISCST3 (or its predecessors) with observational databases, the deposition estimates are harder to validate since field studies of dry and/or wet deposition flux from point or area sources are seldom found in the literature. The subsections that follow discuss validation studies that have been performed on the various components of the ISCST3 model with the intent to show that the modeling approach adequately represents the physical processes in the atmosphere.

A.3.1 Concentration estimates

The ISCST model (Bowers et al, 1979) evolved from earlier plume models such as CRSTER (U.S. EPA, 1977), inheriting the same dispersion algorithms and adding building downwash algorithms. So, evaluation studies done for CRSTER (and its derivatives) are also applicable to ISCST and subsequent revisions to it. Concentration estimates from CRSTER were extensively evaluated for a number of point sources using databases for coal fired power plants. These studies are listed in Table A-1.

Table A-1. Coal-Fired Power Plants used for ISCST3 Evaluation

Database	Location	Stack height(s)	Terrain type	Reference
Clifty Creek	Indiana	3 stacks; all 208 m	low ridges and rolling hills	Londergan et al (1982)
Muskingum	Ohio	2 stacks; all 252 m	low ridges and rolling hills	Cox et al (1985)
Paradise	Kentucky	3 stacks; 183 m, 183 m, 244 m	flat terrain surrounded by rolling hills	Cox et al (1987)
Kincaid	Illinois	1 stack; 187 m	flat terrain	Cox et al (1986)

Separate studies were performed to evaluate the concentrations predicted for area sources. Field studies of area sources, particularly ones measuring impacts near and within the source are scarce. Alternative methods for evaluating the algorithm were used by EPA to prepare for recommending the algorithm for regulatory modeling applications. As described above, a comparison of area source algorithms used by various dispersion models (U.S. EPA, 1989) was conducted to select an algorithm for inclusion in ISCST2. In this study, a set of prediction scenarios was developed for testing and intercomparing the algorithms. A follow-on study examined the sensitivity of the selected area source algorithm across a range of source characteristics and compares the results to those from the original ISCST model algorithm. Finally, the algorithm selected for ISCST2 was compared to data from a wind tunnel study (U.S. EPA, 1992d).

A.3.2 Dry deposition estimates

Particle dry deposition flux is calculated in the model by multiplying the concentration by the deposition velocity. Studies of particle deposition flux attributable to individual sources are difficult to find. In the absence of flux studies to be used for validation, the emphasis has been placed on validating the algorithm for estimating the particle deposition velocity and relying on the previously noted validations of the concentration algorithms. To select the dry deposition algorithm to be added to ISCST3, EPA evaluated and intercompared a number of deposition velocity algorithms and implemented the “most appropriate approach” (U.S. EPA, 1994). The algorithms were evaluated on their ability to parameterize important physical processes while requiring only readily available meteorological, chemical and physical input data. Additionally sensitivity tests were done by Schwede and Paumier (1997) which exercised the algorithms and demonstrated the ability of the model to produce estimates within expected ranges. Another aspect of the deposition calculation is the accounting for the material lost from the source due to deposition. This is referred to as depletion. For use in the HWIR application, the depletion algorithm in ISCST3 was changed to use one that was shown to be faster and more robust (Venkatram, 1998). The algorithm was validated against a full numerical solution to the eddy diffusivity equation (Venkatram, personal communication).

A.3.3 Wet deposition estimates

ISCST3 is used to calculate the wet deposition of both particles and gases for the HWIR assessment. Wet deposition is dependent on the concentration, the scavenging coefficient (dimensionless), and the precipitation rate. For particle deposition, the scavenging coefficient is specified for ISCST3 by particle size category. For wet deposition, the scavenging coefficient is chemical specific. To reduce the number of model runs frequired for the HWIR application, the air module was configured to use a single value was used for all gases which causes gases to be scavenged as if they were small particles. The general approach for calculating the wet deposition flux and resulting depletion was proposed by Maul (1980) based on an analysis of ambient data.

A.4 Peer Reviews

The ISCST3 model has had a long history of use by the EPA for modeling sources of nonreactive pollutants and is designated as a "preferred model" in the Guideline on Air Quality Modeling. As such, the model has undergone substantial public review and comment over a number of years as the model was originally promulgated and subsequently revised. Copies of the comments received by the EPA during these reviews and the Agency's response to them have been placed in Docket No. A-92-65. The docket is available for public inspection and copying.

For use in the HWIR application, ISCST3 was modified to reduce the computational burden and to provide additional outputs needed by other modules. The first modification involves no change to the actual dispersion algorithms within the model, but simply allows the user to select an option that causes the model to sample from an extended record of meteorology at a user specified interval rather than use each hour in the data. The second modification involves the calculation of plume depletion resulting from dry deposition. The Horst (1983) method which had been previously used in ISCST3 was replaced by a method developed by Venkatram (1998) that provided consistent results with faster runtimes. To further reduce runtimes, ISCST3 was run for the HWIR application using a unit emission rate. Annual varying estimates of concentration and deposition were obtained by multiplying the ISCST3 annual average estimates by an emission rate defined by the source module for a particular year. Additional runtime savings were obtained by using a single scavenging coefficient for all vapor phase wet deposition calculations rather than running ISCST3 for each chemical individually.

The revised ISCST3 model and its implementation for the HWIR application was peer reviewed. The runtime considerations and requirements for the HWIR application were not adequately represented to the peer reviewers which was reflected in their comments. While computer processor speeds have greatly increased over the last few years, the ISCST3 model continues to require a great deal of runtime, particularly considering the number of sources and chemicals in the HWIR application. However, the framework is flexible and allows the modeler to reuse stored ISCST3 results (provided with the software system), rather than running the ISCST3 model each time, to decrease overall system runtimes. When running the ISCST3 model, the modeler may select the sampling interval, if any, to use depending on available computing power, the number of sources to be modeled, etc. The ISCST3 model does allow the use of time varying emission rates and chemical specific scavenging coefficients, but the framework does not allow the use of these features at this time. As far as the technical merits of the modifications, the reviewers felt that the new depletion algorithm was appropriate for HWIR-type sources and that the algorithm was based on current scientific knowledge. However, the reviewers felt that the documentation for the new depletion algorithm was not complete enough to allow them to fully evaluate the new algorithm. The reviewers agreed that sampling the meteorology at regular intervals should produce reasonable results, particularly with the inclusion of a separate sampling rate for wet hours. The reviewers suggested that studies be undertaken to further examine the issues related to developing annually varying concentration and deposition estimates as well as those related to chemical specific scavenging coefficients.

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