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MMS 98-0050

A Critical Review of Four Types of Air Quality Models Pertinent to MMS Regulatory and Environmental Assessment Missions

MMS U.S. Department of the Interior
Minerals Management Service
Gulf of Mexico OCS Region

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Authors

Joseph C. Chang
Mark E. Fernau
Joseph S. Scire
David G. Strimaitis

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1 INTRODUCTION

1.1 BACKGROUND

The Minerals Management Service (MMS) is responsible for leasing federal offshore lands for oil and gas exploration and development, and for regulating the activities of offshore operators. These responsibilities require the MMS to use different types of air dispersion models to perform tasks such as environmental assessments and regulatory analyses. The MMS would like to expand the current suite of air quality models used for the above tasks, which must be performed based on scientifically credible approaches and tools. As a result, there is a need to conduct a critical review of different air quality models to ensure MMS' model selections can withstand the peer-review process within the scientific community, and legal challenges in the regulatory arena.

The potential model scenarios to be considered by the MMS cover a wide range, including:

- a routine release (with a long time scale) of combustion products such as SO_2 versus an accidental release (with a short time scale) of highly toxic chemicals,
- an offshore source that is only a few kilometers versus a few hundred kilometers from the shoreline,
- elevated pollutant concentrations caused by local sources versus by long-range transport,
- a buoyant versus denser-than-air release, and
- an inert versus reactive pollutant.

It is evident that there is no single model that could address all of the above issues. One model that is appropriate for one scenario may not be suitable for another scenario. Thus, the MMS identified the following four general types of air quality models for its mission work:

Regional-Scale Dispersion Models
For regional-scale (i.e., up to 1000 km) environmental assessment, where phenomena such as advection, deposition, and potential chemical transformation of pollutants are important. The number of sources is usually large due to the size of the model domain. The MMS suggests that an Eulerian grid model might be best for the purpose.

Lagrangian Trajectory Models
For instantaneous and short-duration emissions, or for releases when spatially-varying meteorological fields are important. The MMS suggests that a Lagrangian puff model might be best for the purpose.

Toxic Release Models
For analysis of consequences of accidental releases of hazardous pollutants from both above-water and under-water sites. These releases might be highly buoyant (e.g., due to temperature), high momentum (e.g., due to pressure), highly reactive, water soluble, multi-component or denser than air.

Steady-State Gaussian Models

For general review of offshore operator's plan. These models are generally applicable to source-receptor distances less than 50 km. The Offshore and Coastal Dispersion (OCD) model has been used by the MMS for this purpose.

The above four types of dispersion models consider a wide range of spatial (from a few kilometers to hundreds of kilometers) and temporal (from less than an hour to multiple years) scales. As a result, their respective data and computational requirements, degree of sophistication, and physical processes simulated are also quite different. We used the following evaluation criteria and methodology in order to conduct a credible, objective review.

1.2 EVALUATION CRITERIA

During the 24 October 1997 project kickoff meeting between the MMS and Earth Tech, the following six major model evaluation categories were identified:

A. Science and Credibility
B. Ease of Use (from User's Perspective)
C. Computational Requirements
D. Cost
E. Availability / Restrictions / Terms
F. Language for Model and GUI (Graphical User Interface)

Categories A, B, and C each has a number of subcategories or attributes. Definitions of each category and attribute are given below. The results for Categories A, B, and C will be used to rank the models. Categories D, E, and F are for reference only; their results will not be used in model ranking.

A. Science and Credibility

Describes how the model simulates processes in pollution meteorology (dispersion, chemistry, transport, numerical methods, etc.), and whether the model has direct relevance to the MMS Gulf of Mexico OCS (Outer Continental Shelf) region. The category is further divided into six attributes.

A1. Technical and general descriptions

Lists and briefly describes the processes, and types of emissions simulated. Lists citations for further reference. Describes model assumptions and limitations. Determines whether model outputs are suitable to MMS needs (e.g., annual averages for environmental impact study).

A2. Grid options for Eulerian and trajectory models

Rates whether the model allows variable grid size, grid telescoping (ability to zero in onto individual locations) and nested grids in all dimensions. Determines types of coordinate systems allowed.

A3. Quality of physical processes simulated

Rates whether the physical processes simulated are state-of-the-art (i.e. agrees with current understanding) and of high quality.

A4. Sparse data treatment

Rates whether the model requires input data not commonly available from an offshore environment.

A5. Overwater dispersion

Rates whether the model includes algorithms to parameterize the marine boundary layer and the land-sea interface.

A6. Model evaluation history

Describes any previous evaluation studies for the model performance against observations.

B. Ease of Use (from User's Perspective)

Describes how easily the user can use the model with or without prior knowledge and existing input files. This category is further divided into seven attributes.

B1. User's guide

Lists available user's guides (hard-copy and on-line) and determines how beneficial documents are to new or experienced users.

B2. Model options

Lists the options for input data, processes simulated, and output data. Also rates how easily the options can be applied.

B3. Data preparation time

Rates the time (e.g., in man-hours) and effort to prepare a new model run with and without existing files.

B4. Ease of data acquisition

Lists sources for data, such as emissions, meteorological, and geophysical, required to run the model; tells potential costs; and describes the steps to extract and prepare data from various sources (data archives).

B5. Model interfaces to preprocessors / GUI

Lists and evaluates preprocessor applications (emissions, meteorology, etc.) and the graphical user interface (GUI) program assisting the user to run the model.

B6. Run-time diagnostics

Lists whether debugging routines exist for models and data inputs, and whether debugging routines include visualization methods.

B7. Post-run diagnostics

Describes outputs from the model and analysis programs (postprocessors), and any methods for visualizing the results.

C. Computational Requirements

Describes whether the model and any supporting programs have system requirements that are difficult to meet. The category is further divided into four attributes.

C1. Multiple sources

Rates whether the model can easily determine effects from a large number (e.g., > 1000) or different types of sources of concern to the MMS.

C2. UNIX / PC portability

Rates whether the model can be used on both operating systems without extensive modifications. Describes how specific model codes, control files, and binary data files are to computer platforms.

C3. Run time

Rates the CPU time required to run the model and supporting programs for MMS applications.

C4. Code flexibility and readability

Tells how easily can code changes, such as array dimensions, subroutines, and input/output formats, be implemented to meet MMS needs.

D. Cost

Describes the financial costs for acquiring the model, GUI, technical support, necessary hardware, and annual user's license.

E. Availability / Restrictions / Terms

Describes the legal restrictions on procuring the model, code changes by MMS allowed, and acquisition methods (from the vendor or download from the Internet).

F. Language for Model and GUI

Lists the programming languages and their dialects used by the model and the GUI program.

1.3 EVALUATION METHODOLOGY

We used the following composite scoring scheme to establish a ranking or rating of the models reviewed. The 17 model attributes (under Categories A, B, and C) mentioned above can have a score between 1 to 3, where 3 = good, very flexible, or state-of-the-art; 2 = fair, less flexible, or somewhat out of date; and 1 = poor or not flexible. Intermediate scores such as 1.5 and 2.5 are allowed. Each attribute will be assigned a different weight, *reflecting varying degree of importance*. During the 24 October 1997 project kickoff meeting between the MMS and Earth Tech, it was decided that the attributes for Categories A and B shall have a weight of 2, and the attributes for Category C shall have a weight of 1. This means that the "Science and Credibility" and "Ease of Use" categories are more important than the "Computational Requirements" category for the MMS. A composite score, S_C, will then be calculated with the following formula:

$$S_C = \Sigma s_i w_i$$

where s_i is the score for Attribute i, and w_i is the weight (2 or 1) for Attribute i. Note that the summation is based on *applicable attributes only*. For example, if the source code for a proprietary model is not available for review, then Attribute C4 ("code flexibility and readability") will not be included in the calculation of S_C. The highest possible value of S_C for a model is $90 = 13\times3\times2 + 4\times3\times1$, where 13 is the number of attributes in Categories A and B with a weight of 2, 4 is the number of attributes in Category C with a weight of 1, and 3 is the highest possible score for each attribute.

S_C for each model is further normalized by the highest possible score to obtain a normalized score (0-100%), S_N, to produce the final model ranking:

$$S_N = (S_C / \Sigma 3 w_i) \times 100\%$$

where 3 is highest possible score for Attribute i. Again, the summation is based on *applicable attributes only*. This is to prevent a model from being overly penalized for some attributes that are not simply applicable to the model. Therefore, two models might have identical S_N but different S_C.

Because of budget constraints, the review is not intended to be comprehensive. Instead, we reviewed four to seven "representative" models in each type of air quality models, except for the steady-state Gaussian models described below. The omission of a model in this study does not mean that the model is inferior or less desirable in any way.

For the traditional, steady-state Gaussian models, since (1) the MMS has been using the Offshore and Coastal Dispersion (OCD) model for general review of offshore operator's plan, (2) the MMS has just recently funded a project to develop a graphical user interface (GUI) program for OCD (Chang and Hahn, 1997), and (3) OCD is one of the official EPA "guideline" models (USEPA, 1986a), the review is limited to only the technical components of the OCD model.

The evaluation exercise mainly consisted of reviews of user's guides, technical reports, peer-reviewed journal articles, conference proceedings, World Wide Web (WWW) pages, and the source code for each model. We also interviewed model developers and users when additional information is necessary. In most cases, we have prior experience of directly applying the models reviewed in this study. We did not conduct any "performance evaluation," in which case the model results are compared against

observations. However, Attribute A6 (" model evaluation history") briefly summarizes previous model evaluation studies for the models.

Eulerian regional-scale dispersion models are the most computationally-intensive among the four model types reviewed in this study. They are usually run on more powerful UNIX workstations or even supercomputers. Consequently, for this type of models, we conducted an additional benchmark comparison, where we ran many models on the same computer with data sets that are as similar as possible and compared the CPU times.

Critical reviews of Eulerian regional-scale dispersion models, Lagrangian trajectory models, toxic release models, and the Offshore and Coastal Dispersion (OCD) model are presented in Sections 2, 3, 4, and 5, respectively. Section 6 contains the summary.

2 EULERIAN REGIONAL-SCALE DISPERSION MODELS

2.1 INTRODUCTION

Eulerian regional-scale dispersion models are used in environmental analyses, with spatial scales up to 1000 km or so, to study the transport, dispersion, deposition, and possibly chemical transformation of pollutants emitted from spatially gridded emission sources. In this section, we reviewed the following five popular Eulerian models:

- CALGRID
- CAMx
- SAQM
- UAM-IV
- UAM-V

All models have a three-dimensional grid, and are mainly designed to study the photochemical production of ozone in urban areas. They have extensive data requirements and are very computationally intensive due to chemistry routines. Although most models have the option of "turning off" the chemistry, it is not a good practice to use these models to simulate the fate of primary pollutants such as SO_2. This is because the models' grid structure causes pollutants from large point sources to be immediately spread within a grid cell, thus creating unrealistic diffusion. The effects of the initial diffusion on transported pollutants may be felt for tens to hundreds of kilometers downwind. In addition to affecting mass distribution in primary pollutants, the artificial dilution also affects chemical reactions through its effect on pollutant ratios in the plume and the subsequent impact on reaction product amounts. Some newer models, such as CAMx, SAQM, and UAM-V, have a plume-in-grid (PiG) algorithm that attempts to solve the problem. However, it is still much more efficient and accurate to apply Lagrangian regional-scale models, such as CALPUFF reviewed in Section 3, if the chemical transformation of pollutants is not of primary concern. Lagrangian model applications do not have to be limited to those treating only a limited number of point sources. Earth Tech applied CALPUFF successfully to domains in Wyoming, Washington, and elsewhere that were several hundred kilometers on a side and contained several hundred point sources. Another source of error in Eulerian models as a plume travels tens to hundreds of kilometers downwind is numerical diffusion caused by the computational methods used. Tests have shown that centerline concentrations can degrade by 25% to more than 50% after a few time steps, depending on what numerical scheme is employed.

The following discussion contains references to grid options such as nested grids, high vertical resolution, and plume-in-grid. A nested grid (see Figure 2-1) is one that has higher resolution (smaller volume in each cell) and is contained fully within a larger and less highly resolved grid. They are generally placed in areas with dense and interesting receptor and/or source characteristics. The inner nests receive mass and boundary conditions from the coarser grid and then repeat the physical and chemical steps on a finer scale. The results from the inner nest sometimes feed back into the coarse domain (two-way nesting) and sometimes do not (one-way nesting). Two-way nests must run simultaneously with the coarse grid. One-way nests can run simultaneously or sequentially. Vertical resolution (see Figure 2-2) refers to both the number of vertical layers in a model and the vertical spacing (thickness) of those layers. Both of these factors vary by model. Usually layers are thinner near the ground, with the magnitude of the spacing dependent on how many layers the model employs. Plume-in-grid (see Figure 2-3) refers to methods that segregate large point source emissions from the mass of the surrounding grid cell(s) until the physical

dimensions or the pollutant concentrations of the plume approach those of the cell, at which time the plume mass is introduced into the surrounding cell. Within the plume, physical and chemical transport and transformation are maintained separately from what is occurring outside the plume. The chemistry within the plume is usually simplified compared to that of the full chemical mechanism.

In Sections 2.2 through 2.6, each model is critically reviewed. Note that although the five models are alphabetically listed, we recommend that the user read Sections 2.5 (for UAM-IV) and 2.6 (UAM-V) first, since the two models are frequently mentioned in other sections.

Refer to Section 1 for a description of the evaluation methodology. Section 2.7 provides a benchmark comparison of computational requirements for all models except CAMx. A summary and our recommendations are given in Section 2.8.

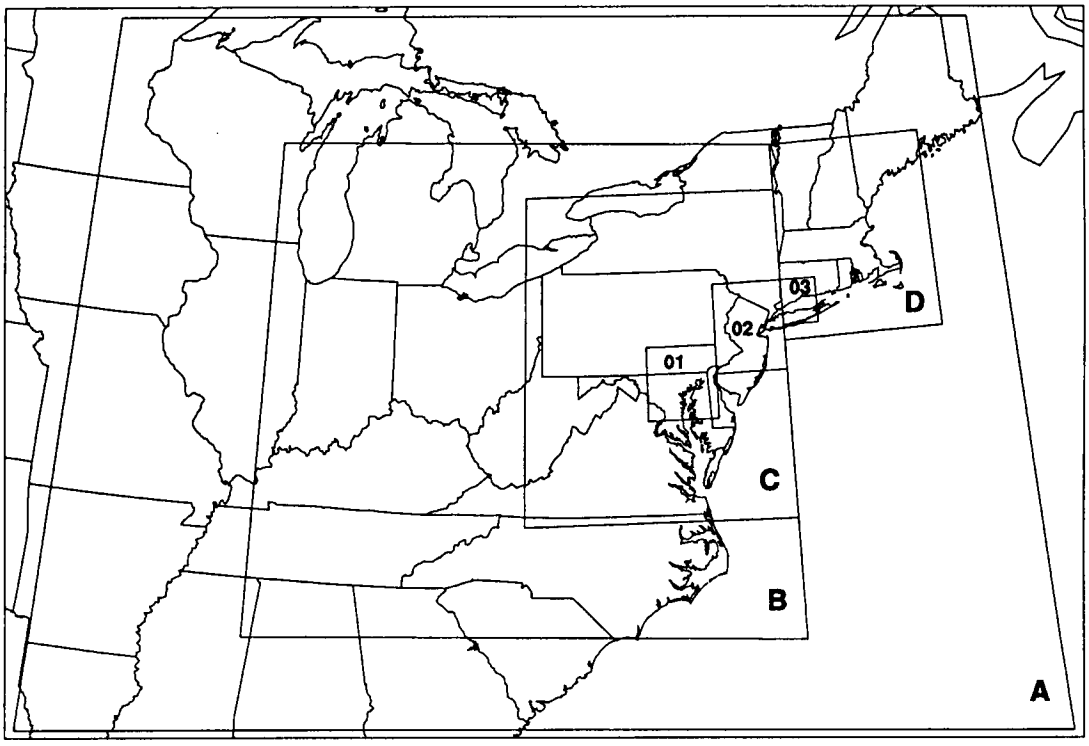

Figure 2-1 An example of a nested UAM-V modeling domain for the eastern United States. Domain A has about 40 km resolution, domain B has 20 km resolution, domains C and D have 10 km resolution, and domains 01, 02, and 03 have 5 km resolution. Mass is allowed to move between the domains (two-way resolution). This domain set was used in the Modeling Ozone Cooperative (MOCA) experiment. After Douglas et al. (1995).

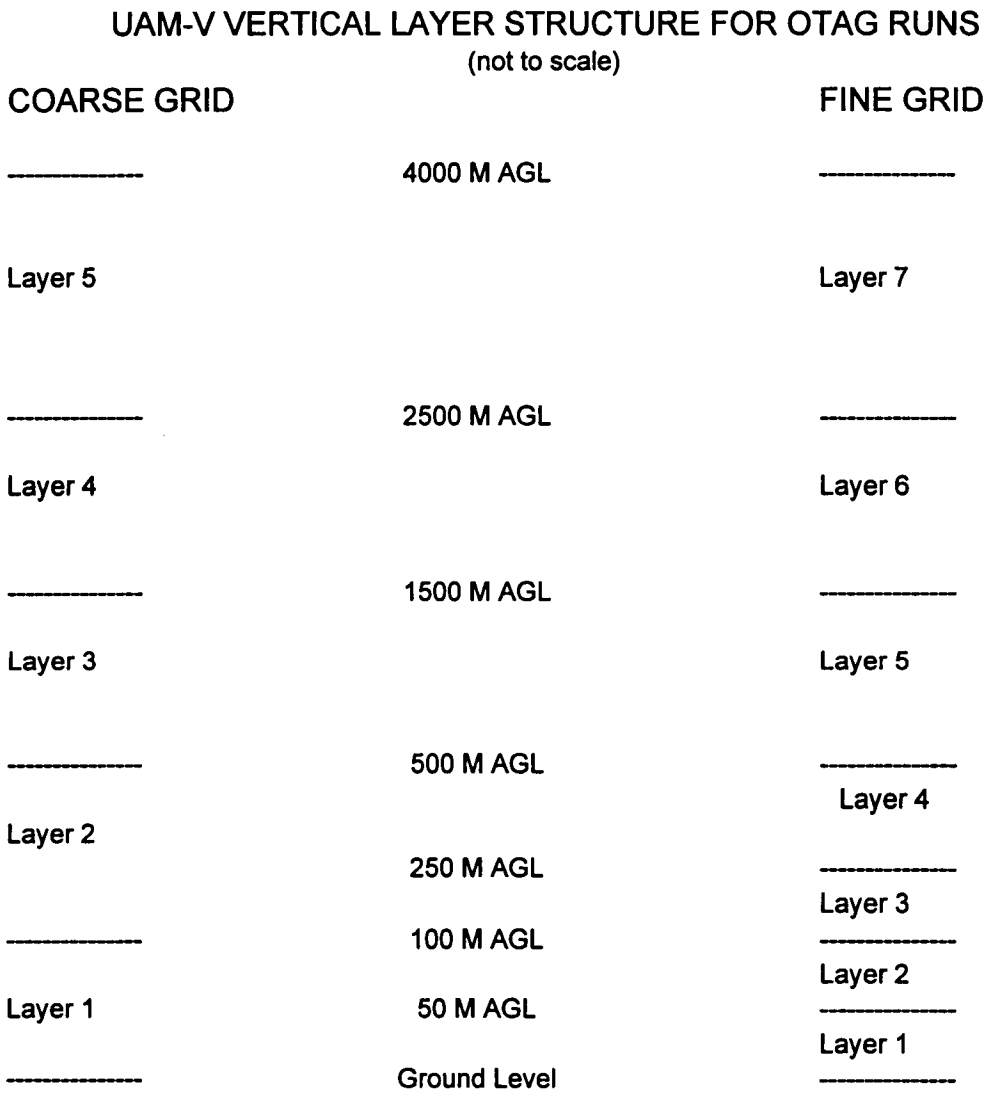

Figure 2-2 This figure depicts differences in vertical resolution between the horizontal coarse (36 km) and fine (12 km) domains used by UAM-V in the Ozone Transport Assessment Group (OTAG) modeling experiment. The fine domain has two additional thinner layers near the ground. After Hao (1996).

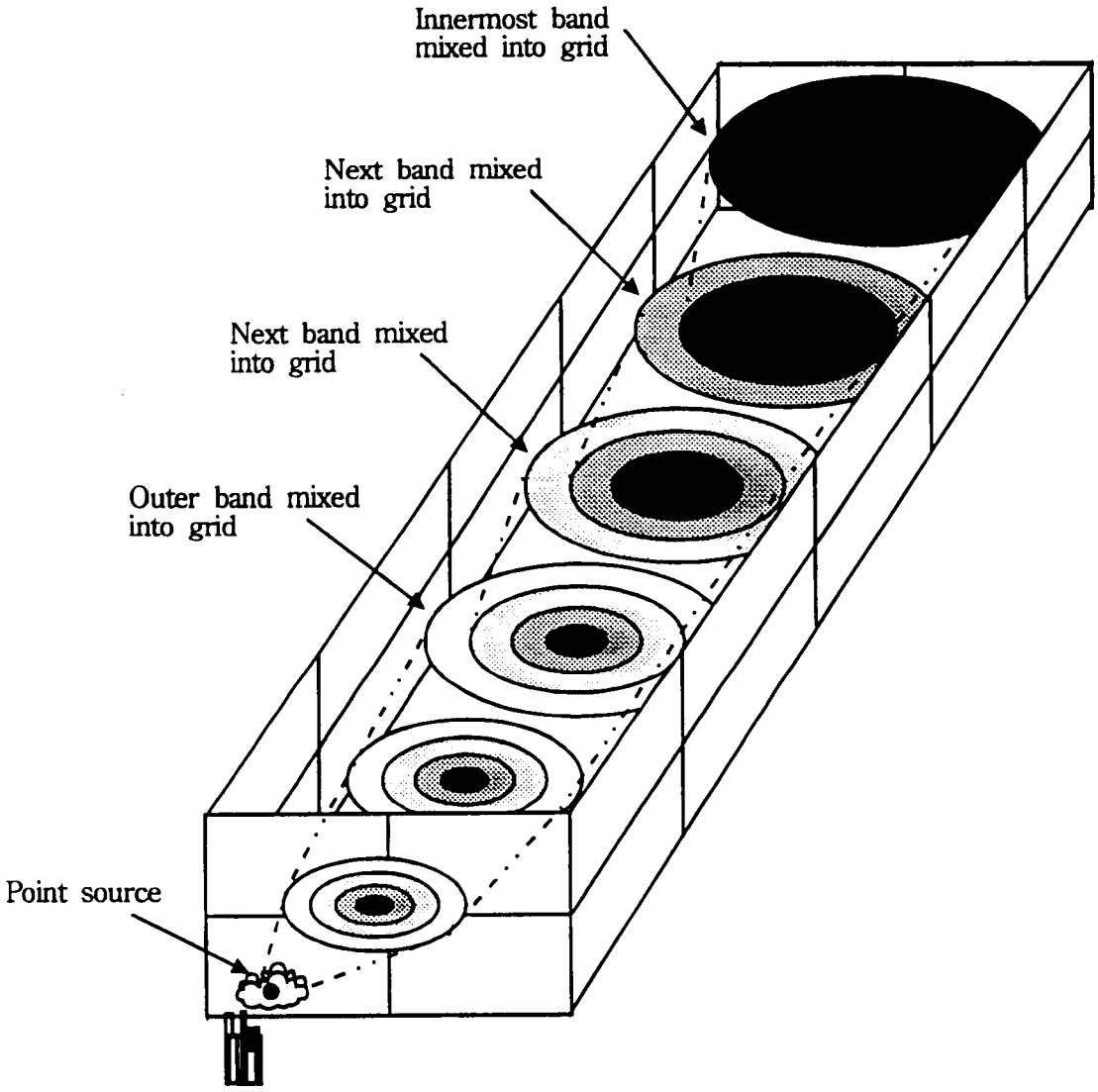

Figure 2-3 A schematic depiction of the UAM-V plume-in-grid algorithm. Emissions from major point sources experience separate chemistry and diffusion until their size, age, or chemical make-up dictates that they mix with the surrounding air. After SAI (1996a).

2.2 CALGRID

Note that, like other sections in the report, the five Eulerian regional-scale dispersion models are also alphabetically listed in this section. It is recommended that Sections 2.5 (for UAM-IV) and 2.6 (for UAM-V) be read first since the two models are frequently mentioned in other sections.

Model Name: CALGRID	
Person of Contact:	
	Joseph Scire Earth Tech, Inc. 196 Baker Avenue Concord, MA 01742 Tel (978) 371-4270 Fax (978) 371-2468 E-mail jss@src.com
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	***Score: 1.5***
	CALGRID is a three-dimensional, comprehensive, Eulerian photochemical model incorporating formulations for transport and dispersion, transformation of precursor gases to secondary species and particles, and dry deposition of gases and particles. Its technical formulation has been described in the peer reviewed literature (Yamartino et al., 1992) and in the user's guide (Scire et al., 1989). The model is primarily used to study short-term episodes of poor air quality. It is not yet practical to calculate annual averages with the model. CALGRID was originally developed for California Resources Board (CARB) as a replacement to UAM-IV (see Section 2.5). Its main strengths are: It is designed to use the same CALMET meteorological inputs as its sister Lagrangian puff model, CALPUFF, so that the models can be used in a complementary way to examine in more detail the behavior of point sources. • It has very low numerical diffusion compared to other models. • It correctly conserves mass. • It has high resolution near the surface. • It has a state-of-the-art dry deposition algorithm. CALGRID uses the Carbon Bond 4 (CB-IV) lumped chemical mechanism (Gery et al., 1989), in which hydrocarbon species are classified, partitioned and aggregated by the number and type of carbon bonds that they contain. The sulfur/sulfate chemistry is very simple, and generally is not used. It ignores wet deposition and aqueous processes. The model has been used on regional and urban domains for studying the photochemical production of ozone. It also has

	an option to use the SAPRC (State Air Pollution Research Center) lumped chemical mechanism (Carter, 1990). The model uses point and area source emissions as inputs. Area sources can be from natural sources, mobile sources, low-level point sources with minimal plume rise, or miscellaneous area sources. The emissions species generally consist of lumped hydrocarbons, nitrogen oxides, and carbon monoxide. Boundary and initial chemical concentrations must be specified. The model requires three-dimensional meteorological fields to advect the materials and to calculate chemical reaction rates. CALGRID is limited in that it does not contain plume-in-grid treatment, two-way nesting, or a detailed aerosol component incorporating aqueous processes and organic species, although one is under development. Inert tracer experiments can be done by simply setting reaction rates to zero.	
A2. Grid Options for Eulerian and Trajectory Models		***Score: 2***
	CALGRID does not have a two-way nested grid option. It does contain an option to output model-generated boundary conditions for a one-way nested run on a sub-domain. The horizontal coordinate system can be either Mercator (UTM) or Lambert conformal. The model allows three types of vertical coordinates: fixed, UAM-IV emulation (but with a 20 m first layer), and dynamically varying.	
A3. Quality of Physical Processes Simulated		***Score: 3***
	The fixed layers (with a 20-m thick first layer) vertical coordinate system is the preferred option. The model contains the most recent version of the CB-IV chemical mechanism, which includes the latest understanding of isoprene chemistry. The photolysis rates used by CALGRID are based on the latest literature. Cloud processes, which affect photolysis rates, are included. The numerical advection scheme is peer-reviewed (Yamartino, 1993) and state-of-the-art, and gives minimal numerical diffusion. The dry deposition algorithm is current.	
A4. Sparse Data Treatment		***Score: 2.5***
	CALGRID is driven by the CALMET meteorological model, which has been shown to produce realistic (terrain-influenced) wind, temperature, and mixing height fields, given a sparse input data set. Additionally, CALMET can take as supplemental inputs the outputs from prognostic models such as MM5 (Penn State/NCAR Mesoscale Model, Version 5) or CSUMM (Colorado State University Mesoscale Model) that use the equations of continuity and motion to yield realistic fields in areas of sparse data. The approach of using prognostic model outputs is technically sound, and our experience so far has shown that realistic wind fields are produced. However, the lack of observed data has so far made a comprehensive assessment difficult of CALMET's performance over areas of sparse data. Furthermore, the lack of observed data may result in diminished model performance because of difficulties in assigning boundary and initial conditions and providing data for nudging for prognostic models.	

A5. Overwater Dispersion		*Score: 2.5*
	The overwater boundary layer methods in CALMET are the same as those used in the OCD model. Effects such as plume fumigation and the thermal internal boundary layer (TIBL) are treated in the model. For the Lake Michigan and New England areas, CALGRID produced realistic ozone concentrations over water and near the land/water interface with meteorological fields prepared by CALMET. This good performance is likely due to its high vertical resolution near the ground and CALMET's good handling of overwater meteorological conditions. CALMET uses a different set of equations to calculate mixing height and surface layer micrometeorological parameters over water as opposed to over land. The user's manual has omitted some of these equations and some appear to be different in the code from what appears in the manual. The mixing height equation in the manual is based on neutral barotropic scaling, which is adequate for mid-latitude open ocean purposes as suggested by Garratt (1995). CALMET has a mixing height advection algorithm that can transport mixing heights from coastal areas into the near-shore area. Prognostic model outputs can be introduced into the model as "pseudo buoy data" if necessary.	
A6. Model Evaluation History		*Score: 3*
	An early version of CALGRID has been compared to observations in a peer-reviewed article (Kumar et al., 1994). Another recent peer-reviewed article found that CALGRID, using SAPRC chemistry and driven by a prognostic meteorological model, performed comparably to UAM-V, driven by SAIMM and using CB-4 (Jiang et al., 1998). The model has been used by Earth Tech for several different domains with differing characteristics. The model compared favorably to observations and other models in the Midwest, California, New England, and the OTAG domains. The model has a tendency to overpredict ozone concentrations at night compared to both observations and other models. This overprediction possibly is caused by underpredicting dry deposition. The model has been widely used and evaluated against observations by several research groups in Europe.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		*Score: 2*
	The documentation consists of user's guides for both CALGRID (Scire et al., 1989) and CALMET (Scire et al., 1995). The CALGRID document is in-depth and easy to read, although it does not include descriptions of the most recent changes to CALGRID (e.g., cloud module, arbitrary time-steps, etc.). Data file formats are clearly defined. The CALMET manual also is useful. Some aspects of the model and preprocessors have been changed since the last manual update. Some of the more intricate aspects of using CALMET are not discussed as well as the basics.	
B2. Model Options		*Score: 3*
	The self-documenting CALGRID control file allows access to many option	

	switches. It is easy to modify the file for a particular model simulation. Within the input file, the user can specify the domain, the run time/date and duration, file names, file formats, chemical specifications, deposition parameters, output and print options, and diffusivity settings. CALGRID allows the area source emissions to be spread over multiple vertical layers. A global parameter statement sets the maximum array sizes. A very few parameters are hardwired in the code. These include the number of species that are emitted and advected in the CB-4 chemistry scheme. CALGRID produces hourly average concentrations for user-selected species and levels. It also has a continually updated restart file containing the last two hours of instantaneous concentrations for all species.	
B3. Data Preparation Time		***Score: 2***
	To prepare a CALGRID run from scratch with no existing data is very labor-intensive, could take on the order of weeks to months, depending on available labor resources, and requires some prior knowledge of the various physical and chemical issues involved. Inputs from three different areas must be prepared: meteorological, emissions, and chemical boundary concentrations. The user must acquire raw input data, run CALMET, and develop emissions and chemical concentration files. Except for meteorological inputs that are prepared by CALMET, CALGRID does not contain separate processors to prepare other data. The user either needs to write custom software, or use the UAM-IV processor suite (see Section 2.5 for more details). CALGRID does have a conversion program to reformat UAM-IV input fields to the CALGRID format. To modify an existing run is generally straightforward and requires much less time. However, the user may still need to develop custom software to achieve the desired input file modifications.	
B4. Ease of Data Acquisition		***Score: 1***
	The CALMET meteorological processor for CALGRID requires land use, terrain, surface and upper air observations, and optional prognostic model (e.g., MM4 and MM5) output. Land use and terrain data: 200-m resolution USGS (U.S. Geological Survey) land use data are available for free from the Web (http://edcftp.cr.usgs.gov). Terrain data are available from the same source or can be purchased on CD-ROMs for several hundred dollars. For simple domains or applications, one can use a low-resolution data set (e.g., just land vs. water rather than detailed descriptions of different land use types). Meteorological data: Surface and upper air data are available from a variety of sources. Data since the early 1990s can be acquired for free via ftp from the OASIS (On Line Access and Service Information System) database (http://hurricane.ncdc.noaa.gov/codiac/oasis-www.html) at NCDC (National Climatic Data Center). However, these on-line data sometimes have quality control problems. NCDC will also send data for a charge of several hundred	

	dollars depending on the amount of data requested (http://www.ncdc.noaa.gov/op/). Data can also be purchased from NCAR (National Center for Atmospheric Research) for a cost of about $50 to $100 per tape (http:/www.scd.ncar.edu/dss/). Alternatively, the user could purchase data on CD-ROMs from private companies for a cost of about $100 per CD-ROM (covering different parts of the country and many years). Some meteorological data are available through the U.S. EPA AIRS data base (free of charge) or from state regulatory agencies. Outputs from prognostic models usually have to be produced in-house or obtained from outside sources. A gridded MM4 database for 1990 exists and is available for free. The above data are then processed by CALMET to create a CALMET.DAT file for use in CALGRID. Emissions data: See discussions under UAM-IV (Section 2.5) and UAM-V (Section 2.6). For selected episodes and areas, the user can run the EPA GMISS/ROM-UAM interface program to acquire and reformat Regional Oxidant Model (ROM) inputs and outputs. The GMISS program can create meteorological data, emissions data (biogenic only), and boundary and initial conditions for use in UAM-IV. These data can be further reformatted for use in CALGRID. This process is less time-consuming overall, but involves interacting with the EPA mainframe, downloading large files, and running several processors. Cooperation with regional EPA and state regulatory agencies may facilitate data acquisition, because they access AIRS and GMISS on a routine basis, or may already have data in-house.	
B5. Model Interface to Preprocessors / GUI		***Score: 2***
	The CALMET meteorological processor consists of a diagnostic wind field module and micrometeorological modules for overwater and overland boundary layers. It accounts for slope/valley flows, kinematic terrain effects, terrain blocking effects, and divergence minimization; and generates a mass-consistent wind field. CALMET can use outputs from prognostic models to supplement input data. This is extremely useful for large data-sparse areas where it is not practical to run prognostic models at a high spatial resolution. CALMET has a good Graphical User Interface (GUI) program for the PC platform. The GUI guides the user to set model options in order to produce the model control file and runs the code. It has extensive help functions and uses Visual Basic to allow menus and point-and-click usage. It is available for free from Earth Tech or the EPA. The GUI program does not work on the UNIX platform. The CALGRID model does not have a GUI program. The GUI does not set up or run the CALMET preprocessors that are described below. CALMET requires land use, terrain, surface, upper air, and, optionally, prognostic model output data to run. There are various processors to prepare most of the data files from raw data. The TERREL preprocessor produces gridded terrain data. The CTGCOMP, CTGPROC, MAKEGEO and LUPLOT programs process and display the USGS land use data. (Note that the	

	MAKEGEO processor is not the same as the MAKEGEO processor for the OCD model discussed in Section 5.) The METSCAN and SMERGE preprocessors produce the surface meteorological data file from National Weather Service (NWS) or other observations. The PXTRACT and PMERGE programs produce site-specific hourly precipitation files from the NWS TD3240 data. The READ62 program produces individual upper air meteorological files from NWS data. These processors are available from Earth Tech or EPA. CALGRID requires a chemical information file, boundary conditions, point and area source emissions, and the CALMET output meteorological file (CALMET.DAT). CALGRID lacks a suite of formal preprocessors to create the chemical and emissions files. Since a large number of similar data files (for different geographical areas and episodes) already exist for UAM-IV, and sometimes UAM-V, one can take these existing files and reformat them for use in CALGRID if they exist for the desired episode and domain.	
B6. Run-Time Diagnostics		***Score: 2***
	The FORTRAN code contains a number of run-time error messages and diagnostic messages. The code carefully compares user input settings vs. declared array sizes, and flags suspect or wrong values. Optional debugging switches are available in CALMET to output intermediate data fields and variable values for review.	
B7. Post-Run Diagnostics		***Score: 2***
	CALMET and CALGRID can use the PRINTMET and CALPOST programs to produce listing of selected model outputs. In addition, Earth Tech has written interactive software to extract user-specified concentration fields for subsequent analysis or plotting. CALMET can interact with the commercial plotting package SURFER to produce colored vector and contour plots of model outputs. CALGRID does not have a graphics program. The user must write interface software and use his favorite plotting package. See the UAM-IV table (Section 2.5) for other available generic options for plotting and analyzing output fields.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 2***
	CAGRID handles multiple point and area sources easily. However, it is difficult to detect the effects of any one or several sources on the final predicted pollutant concentrations. CALPUFF could be used in conjunction with CALGRID to examine further any sites or areas that seem to be of significance.	
C2. UNIX / PC Portability		***Score: 3***
	CALGRID is easily ported between the UNIX and PC platforms. Minor changes are necessary in the job scripts and certain machine-specific	

	FORTRAN utility functions and routines (e.g., the date and time routines). However, the necessary code is already provided with CALGRID.	
C3. Run Time		***Score: 2***
	CALGRID's run time is comparable to that of UAM-IV. On a 34x60x10 (in x, y, and z directions, respectively) grid, CALGRID takes about 4 hr of CPU time to complete a 48-hr simulation on an HP 735 workstation (~ 200 times faster than a VAX 11/780 workstation, and ~ 2 times slower than a SUN Ultra 2 with a 200 MHz CPU). See Section 2.7 for more details.	
C4. Code Flexibility and Readability		***Score: 3***
	The code is well commented and modular, so that alternate subroutines can be added, as long as they properly interact with existing model algorithms.	
D. Cost (Non-Ranking)		
	CALMET, CALGRID, the associated pre- and post-processors, and documentation are available from Earth Tech at no charge.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	There are no restrictions on CALMET/CALGRID availability or use, except that research versions under development at Earth Tech will not be made available until satisfactory quality assurance exercises have been completed.	
F. Language for Model and GUI (Non-Ranking)		
	CALMET and CALGRID are written in FORTRAN 77. The CALMET GUI is written in Visual Basic.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**17**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**74.4**

2.3 CAMx

Note that, like other sections in the report, the five Eulerian regional-scale dispersion models are also alphabetically listed in this section. It is recommended that Sections 2.5 (for UAM-IV) and 2.6 (for UAM-V) be read first since the two models are frequently mentioned in other sections.

Model Name: Comprehensive Air Quality Model with Extensions (CAMx)	
Person of Contact:	
	Ralph E. Morris Environ International Corporation 101 Rowland Way, Suite 220 Novato, CA 94945 Tel (415) 899-0700 Fax (415) 899-0707 E-mail rmorris@environ.org
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	***Score: 2***
	CAMx is an Eulerian model that expresses transport, diffusion, emissions, deposition, and chemical processes in mathematical forms to simulate ozone, ozone precursor, carbon monoxide, and (optionally) sulfur and sulfate pollutant concentrations on a three-dimensional grid. The reader is referred to the user's guide (Environ, 1997) for the model's technical formulation. It is not well-suited for calculating annual averages, but rather is used for episodic investigations in which maximum hourly and eight-hourly averages are examined. Sulfur and aerosol chemistry is present but simple. The manual does not clearly explain whether nonreactive tracer studies can be easily done. CAMx uses the CB-IV lumped chemical mechanism (Gery et al., 1989), in which hydrocarbon species are classified, partitioned and aggregated by the number and type of carbon bonds that they contain. Gas-phase sulfur reactions are present but not used in ozone studies. It has an aqueous-phase aerosol chemistry routine and an optional wet deposition algorithm. The model has been applied to several domains but does not yet have regulatory or pseudo-regulatory status, since the model is relatively new. The standard version of CAMx contains two-way horizontal nesting, a plume-in-grid algorithm, and a source attribution algorithm. Emissions data include contributions from point and area sources. The emissions species generally consist of lumped hydrocarbons, nitrogen oxides, and carbon monoxide. Boundary and initial chemical concentrations must be specified. Three-dimensional meteorological inputs are needed for calculating plume rise, advecting the materials, and calculating chemical reaction rates.	

	CAMx is designed to replace UAM-IV and be competitive with UAM-V. Although CAMx is in the public domain, as explained later it relies heavily on proprietary UAM-V pre- and post-processors. Thus, unless all necessary CAMx input files are already available, the open nature of the model is somewhat diluted.	
A2. Grid Options for Eulerian and Trajectory Models		***Score: 3***
	CAMx has a two-way nested grid option (Figure 2-1) and a plume-in-grid (Figure 2-3) option. The coordinate system can be either Mercator (UTM) coordinates or latitude/longitude coordinates. Winds can be represented at either the cell face or the cell center.	
A3. Quality of Physical Processes Simulated		***Score: 3***
	The technical aspects of CAMx have not yet been peer-reviewed in the refereed literature. Kumar and Lurmann (1997a) found that the model's technical aspects are modern and comparable to those of UAM-V. Its computational aspects compare favorably to UAM-V. It contains the most up-to-date CB-IV chemistry with the new isoprene reactions, and has up-to-date photolytic reaction rates. The model conserves mass by advecting species in mass concentrations rather than in volume concentrations. It has high vertical resolution near the surface and uses fixed layers. It uses three-dimensional temperature, pressure, and humidity fields, which is an improvement over UAM-IV. The plume-rise algorithm is current. The horizontal advection scheme no longer is state-of-the-art. The source apportionment algorithm received good technical reviews, but has not been extensively tested in actual use. The aerosol component is a simplified representation of the current knowledge.	
A4. Sparse Data Treatment		***Score: 2.5***
	CAMx requires meteorological inputs generated by either the SAIMM or RAMS prognostic meteorological models, which perform well over water and in coastal thermal internal boundary layer (TIBL) situations. The effects of lack of data over water are minimized because the meteorological models rely on physical equations, rather than data interpolation, to produce three-dimensional fields. In addition, sophisticated initialization methods also minimize reliance on observed data. Observed data over water, if available, can be used to "nudge" the model back towards a realistic solution based on four-dimensional data assimilation (FDDA). However, even with use of prognostic models, the lack of observed data may result in diminished model performance because of difficulties in assigning boundary and initial conditions and providing data for nudging.	
A5. Overwater Dispersion		***Score: 2.5***
	As mentioned above, the sophisticated treatment of the marine boundary layer and the land/water interface in the SAIMM and RAMS prognostic models assure relatively good performance over water, even in data-sparse situations. The lack of data, however, can lead to a degradation of performance over water because of the difficulty of calculating micrometeorological parameters and	

	dispersion coefficients. The RAMS model offers a variety of turbulence closure and lower boundary treatment options. These are summarized at http://rams.atmos.colostate.edu/detailed.html, and include Smagorinsky-type eddy viscosity, closure methods with eddy viscosity as a function of turbulent kinetic energy, constant fluxes, constant fluxes with similarity, and surface energy flux methods that depend on ground temperature. SAIMM uses first-order closure to parameterize turbulent exchange. Similarity theory is used to parameterize fluxes near the lower boundary. Flux-profile relationships are used to calculate the surface fluxes in the surface layer. Two methods can be used to calculate vertical exchange coefficients and PBL heights: one involves diagnostic relationships that depend on the sign of the heat flux and the other depends on turbulent kinetic energy. The details are contained in SAI (1995c). This reference does not explain clearly how the model handles air-sea interaction among temperatures, etc. or how some of the fluxes are calculated.	
A6. Model Evaluation History		***Score: 2***
	CAMx performance has not yet been reported in peer-reviewed journal articles, and it does not have as long an application history as do the other major photochemical models. Kumar and Lurmann (1997b) found that its performance against observations on the OTAG domain was essentially the same as that of UAM-V. Its developers have applied the model to several domains and compared the results with observations. It is difficult to evaluate the performance of the source apportionment algorithm against measured data, since such studies have not been done.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 1.5***
	The user's guide (Environ, 1997) is clear and easy to understand. The documentation is available for download at the CAMx Web site (http://www.camx.com) as PDF files. There is another guide (Yarwood et al., 1997) to the source apportionment tool. Since CAMx does not have its own pre- and post-processing software, no guides exist for these. The source apportionment manual actually describes the implementation of the procedure for the UAM-IV model. However, the implementation for CAMx should be similar. A sample control file is given in the user's guide. Whether individual input lines in the control file are optional or mandatory is much more clearly depicted in the CAMx documentation than it is in the UAM-V documentation. Unfortunately, the CAMx user's guide does not include formats or examples of other input and output files. The user needs to refer to UAM-V's manuals for more details. The user's guide does not include discussions of the aerosol algorithm and its application.	

	The user guides for the UAM-V preprocessors are described in UAM-V Section B1 and include a useful manual for using SAIMM (SAI, 1995a). They can be downloaded from EPA's SCRAM bulletin board, as described in Section E. The RAMS user guide does not appear to be available via the Web but there is a homepage that describes the model at http://rams.atmos.colostate.edu/. The literature description of the model is contained in Pielke et al. (1992).	
B2. Model Options		***Score: 3***
	The main model options in CAMx are whether to include the source apportionment methodology, the nested grids, and the plume-in-grid treatments. These options and their associated parameters and definitions can be set in the control file. Selections of these options usually lead to the need for additional input files. File names, output species, run information (date, time, duration, message, etc.), domain information, time step, deposition information, diffusivity information, chemical integration information, and other logical switches and default values are also set in the control file. CAMx outputs include the two most recent hours of instantaneous concentrations for all layers for restart purposes, hourly average concentrations, restart files for PiG, three diagnostic output files to monitor run performance and track mass flux, and an optional source attribution output file. If source attribution is used, the hourly average files will contain only Layer One information.	
B3. Data Preparation Time		***Score: 2***
	Like all other photochemical models, to prepare a CAMx run from scratch with no existing data is very time consuming. The process could take from a few weeks to a few months, and requires some scientific and modeling expertise. Since CAMx directly runs off UAM-V input files, the reader is referred to the corresponding section for UAM-V for more details.	
B4. Ease of Data Acquisition		***Score: 1***
	CAMx uses the same input data as are required by UAM-V (see Section 2.6).	
B5. Model Interface to Preprocessors / GUI		***Score: 1***
	CAMx does not have a graphical user interface program. It does not contain its own set of formal preprocessors. The user must use the UAM-IV/UAM-V preprocessors and EPS-2 or EMS-95 emissions preprocessors (see UAM-IV and UAM-V descriptions and Section 2.8). Similar to CALGRID, an option would be to take existing UAM-IV or UAM-V files if available and reformat them for use in CAMx.	
B6. Run-Time Diagnostics		***Score: 2***

	CAMx does not contain the formal run-time debugging switches that are present in UAM-V. The code contains many run-time variable value checks and error messages.	
B7. Post-Run Diagnostics		***Score: 2***
	CAMx does not have its own postprocessor code, except for an Excel "browser" designed to analyze the source-apportionment output. The user could use UAM-V post-processors or other programs to analyze the results. The UAM-V postprocessing routines may not be available to private users without a license.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 3***
	CAMx is an Eulerian model that can easily handle multiple point and area sources. However, it is difficult to detect the effects of any one or several sources on the final predicted pollutant concentrations. CAMx has an innovative source attribution algorithm that gives some information as to the influence of various subregions on predicted concentrations.	
C2. UNIX / PC Portability		***Score: 3***
	CAMx is easily ported between the UNIX and PC platforms. For a specific UNIX platform, minor changes are necessary in the job scripts and certain machine-specific FORTRAN utility functions and routines. For the PC, the job script logic should also be changed slightly. We did not try to compile CAMx on a PC but did not detect any obvious obstacles to doing so. CAMx has built-in subroutines to perform certain data conversions that are necessary to use a DEC ALPHA machine and swap binary files across platforms.	
C3. Run Time		***Score: 3***
	We did not run CAMx to assess its run time. However, the documentation claims that a fast chemical solver leads to overall run times three to four times faster than those for a standard model, so CAMx's run time likely is on a par with that of UAM-V. The number of PiG sources will influence run time to some degree. It is likely that the source apportionment option will slow down the model and greatly add to memory requirements, since the procedure is performed during run time. The user manual does not provide estimates of performance for the source apportionment option.	
C4. Code Flexibility and Readability		***Score: 3***
	CAMx is composed of many modular subroutines. With a few exceptions, the code is extensively commented as to the purpose of each algorithm and subroutine. Compared to UAM-V, the coding is more efficient in the number of subroutines used and in the improved consistency among routines. The code contains parameter files to set the maximum array sizes. The I/O subroutines	

	are easy to locate and change, if necessary.	
D. Cost (Non-Ranking)		
	CAMx and its documentation are available to the public free of charge. The UAM-V preprocessors, postprocessors, and manuals are also freely available from EPA's SCRAM bulletin board (http://www.epa.gov/scram001/), although special licenses (see below) are sometimes required before the programs could be used.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	CAMx and its documentation can be freely downloaded via the Web with no restrictions, except that any projects or derived products based on the model must have proper acknowledgment. CAMx is designed to use the UAM-V pre- and post-processing software to prepare model inputs and examine outputs. The UAM-V software can be used by government agencies for "bona fide government purposes" without restrictions. However, permissions from the model developers, SAI, are required for any code modifications. A licensing agreement with SAI is necessary before a private user can use the UAM-V software. SAIMM and its user manual are available for download from EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/) under the UAM-V section, with the restrictions mentioned above. The RAMS code does not appear to be available via the Web but there is a home page describing the model that is located at http://rams.atmos.colostate.edu. CAMx inputs and outputs for the OTAG test case are available via ftp from ftp.environ.org (user name "camx", password "pass4camx").	
F. Language for Model and GUI (Non-Ranking)		
	CAMx is written in FORTRAN 77.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**17**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**74.4**

2.4 SAQM

Note that, like other sections in the report, the five Eulerian regional-scale dispersion models are also alphabetically listed in this section. It is recommended that Sections 2.5 (for UAM-IV) and 2.6 (for UAM-V) be read first since the two models are frequently mentioned in other sections.

Model Name: SARMAP Air Quality Model (SAQM)	
Person of Contact:	
	Dr. Saffet Tanrikulu Modeling Support Section California Air Resources Board 2020 L Street Sacramento, CA 95814 Tel (916) 322-7298 Fax (916) 327-8524 E-mail saffet@cupid.arb.ca.gov
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	***Score: 1.5***
	SAQM is an Eulerian grid model that simulates concentrations and deposition using a resistance dry deposition model, a cloud sub-model for simulation of aqueous chemical conversions and precipitation scavenging, and a chemical mechanism involving the photochemistry of organic and inorganic species. It is derived from the Regional Acid Deposition Model (RADM; Chang et al., 1987). SAQM's technical formulation is described in Chang et al. (1997). It is mainly used to study short-term episodes. Its computational requirements currently prohibit the model from performing long-term runs in a realistic time frame, as with all similar models. SAQM uses the CB-IV lumped chemical mechanism (Gery et al., 1989), in which hydrocarbon species are classified, partitioned and aggregated by the number and type of carbon bonds that they contain. It also can use the SAPRC lumped chemical mechanism. The CB-IV mechanism has simple sulfur/sulfate chemistry. Because of its roots as an acid deposition model, SAQM has very good wet deposition and aqueous process capabilities. These processes are disabled in summer-time ozone applications. The model is suitable for use on a regional or urban scale. The model has similar input data (meteorological, emissions, and chemistry) requirements as other photochemical models. SAQM is designed to accept inputs generated by the MM5 prognostic meteorological model. SAQM exists in several different versions. In addition to the two chemical mechanisms, there is a plume-in-grid (PiG) version, a two-way nested version,	

	a one-way nested version, a telescoping version, and a surface layer submodel (SLS) version. A process analysis version and a sophisticated aerosol version have been developed and are being tested by the California Air Resources Board (CARB). Note that all these versions of SAQM are actually separate codes, and not merely different options in an all-encompassing system.	
A2. Grid Options for Eulerian and Trajectory Models		***Score: 2***
	Operational versions of SAQM with one- and two-way horizontal nesting (Figure 2-1) exist. A plume-in-grid version (Figure 2-3) recently has been developed. A telescoping version exists but has not been fully tested. The coordinate system is limited to Lambert conformal. The SLS version allows increased resolution near the ground, but is no longer supported by the CARB because of disappointing performance.	
A3. Quality of Physical Processes Simulated		***Score: 2***
	The operational version of SAQM uses 16 fixed vertical layers. The recently installed PiG module is almost identical to that in UAM-V. The model contains an outdated version of the CB-IV chemical mechanism that does not include the current understanding of isoprene chemistry, although the updated mechanism currently is being installed. One weakness of the operational version is that the lowest layer is about 60 m thick, which is not adequate to represent surface layer processes. The surface layer submodel (SLS), which attempted to resolve this problem, has not given satisfactory performance versus observations. Work is under way to better match the vertical layer structure and the boundary layer physics of SAQM with that of its meteorological model (MM5), so that vertical resolution can be improved without harming performance. A second concern with SAQM is that the meteorological processor that converts MM5 output to SAQM input may not preserve the divergence and vertical velocities that are present in the original wind fields.	
A4. Sparse Data Treatment		***Score: 2.5***
	SAQM is driven by meteorological inputs provided by the MM5 prognostic meteorological model. MM5 performs well over water and in coastal thermal internal boundary layer (TIBL) situations. Since MM5 uses physical equations rather than data interpolation to produce three-dimensional fields, the effects of lack of data over water are minimized. Four-dimensional data assimilation (FDDA) nudges the model predictions towards observations at areas where observed data are available. As with SAIMM and RAMS, the lack of observed data may result in diminished model performance because of difficulties in assigning boundary and initial conditions and providing data for nudging.	
A5. Overwater Dispersion		***Score: 2.5***
	The sophisticated treatments of the marine boundary layer and the land/water interface in MM5 assure relatively good performance over water, even in data-sparse situations. The lack of data, however, can lead to a degradation of performance over water because of the difficulty of calculating micrometeorological parameters and dispersion coefficients. MM5 does not	

	treat water differently from land, except that the underlying land use, terrain and ground (water) temperature information is different. It offers several planetary boundary layer (PBL) options: a bulk-aerodynamic method, the Blackadar method which uses similarity theory to calculate heat and moisture fluxes that are dependent on stability, and the Gayno-Seaman method in which the eddy viscosities are based on turbulent kinetic energy (TKE) and the PBL is defined as the height where the TKE falls below a threshold value. The reader is referred to the MM5 web site and Grell et al. (1995) for details on the PBL methods and the interaction between the surface and the atmosphere. The current 60 m thick first layer in SAQM may be too coarse to retain the information contained in the original MM5 fields.	
A6. Model Evaluation History		***Score: 3***
	SAQM's ancestor RADM is one of the most heavily-evaluated and peer-reviewed models in history because of its central role in the National Acid Precipitation Assessment Program (NAPAP). SAQM has been applied and/or evaluated against observations by both the CARB and outside consultants and users on several California domains, in the Lake Michigan area, and for the Ozone Transport Assessment Group (OTAG) domain. As mentioned above, some questions remain about its treatment of meteorological inputs. The CARB has used the model in regulatory applications within California.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 2***
	The user documentation for SAQM consists of five volumes: 1. an overview that gives the technical description of the model (Chang et al., 1997), 2. a user's guide that describes model implementation (Chang et al., 1996), 3. a user's guide for the meteorological processor (Chang and Li, 1996), 4. a description of the emissions preprocessor system (CARB, 1996), and 5. a user's guide for the plume-in-grid (PiG) version (Myers et al., 1996). The overview document (report 1) is not completely satisfactory. It is lacking in detail and parts of it read like a draft. The user's guide (report 2) describes the necessary steps to prepare input files and to perform a model simulation. It is relatively complete and fairly useful. The report also contains a detailed description of all the subroutines and their variables, although such information is probably of interest to only advanced modelers. The user's guide for the meteorological processor (report 3) is also useful and informative. It gives suggestions for porting the processor to other machine platforms and using it with newer versions of SAQM. The PiG documentation (report 5) is very comprehensive, clear, and useful. An overview and details of the MM5 model can be found at the web site http://www.mmm.ucar.edu/mm5/. The documentation also is available there	

	for viewing, downloading, and ordering in hard copy. There is a technical description of the model (Grell et al., 1995), a document that describes the source code, variable list, input options, and model overview (Haagenson et al., 1994), and several other preprocessor manuals and tutorials. These appear to be comprehensive and useful for implementing the work station version of MM5.	
B2. Model Options		***Score: 2***
	The SAQM family has many version options (PiG, chemical mechanism, boundary layer treatment or SLS, etc.) but they tend to be implemented as separate codes rather than one all-encompassing system. Rather than specifying an option switch value in an input file, one must obtain the desired code version, modify it for the desired computer platform if necessary, and compile the code. This procedure must be repeated for each desired option. The PiG algorithm has been implemented in both the one- and two-way nested versions. These would be the most desirable versions to obtain. The PiG version has not yet been extensively used or tested. The SLS version does not include the PiG algorithm. The user sets various other model options in the control file, including whether plume-in-grid treatment is used (if available), run duration information, print and file-write interval information, and various chemical integration information. The domain and grid information is contained in parameter files. These files must be edited for a new domain or grid resolution. However, even when this is done, the user still needs to consider many subtle code features, mainly because values for some other related parameters are "hardwired" in the code for the California applications. SAQM produces hourly average output for layer one and instantaneous concentration output for all layers. It also has a restart file to allow a prematurely terminated run to resume.	
B3. Data Preparation Time		***Score: 1***
	The level of effort required to create SAQM inputs depends on: • whether the user could obtain MM5 outputs from an external source or has to run the MM5 model himself, • whether emissions data sets already exist or have to be created from scratch, and • whether the user uses the pre-existing 4 km and 12 km preprocessors and SAQM code or tries to implement a different grid resolution or nesting ratio. The SAQM code and processors are hardwired to a large extent for the California applications. All aspects of the code must be carefully examined to assure that the code will perform properly for a different domain or grid resolution. As a new user, trying to run the MM5 prognostic meteorological model is a	

	major undertaking by itself. It requires significant resources and expertise, and could take several months to complete. Developing emissions inventories from scratch also is a major task. The user normally would use one of the existing systems (EPS-2 or EMS-95) to complete this task. We did not review the SAQM emissions systems. One should use the initialization methods recommended in the SAQM user's guide to prepare boundary and initial chemical conditions. The procedure is relatively simple. However, observations still must be obtained first in order to develop realistic initial profiles and boundary conditions. At Earth Tech, in order to set up SAQM, we obtained an existing MM5 data set, and we wrote a filter to convert UAM-formatted emissions files into the SAQM "merge" format so that they could go directly into the SAQM processor. This greatly minimized the data acquisition needs and the file preparation work. However, we still invested significant effort in modifying the SAQM meteorological processor to handle the new MM5 Version 1 format and the new 8-km grid resolution. (SAQM was originally designed to handle only 4- and 12-km resolutions.)	
B4. Ease of Data Acquisition		***Score: 1***
	Like all other photochemical models, SAQM requires meteorological, emissions, and air quality data to run. Meteorological Data: Meteorological inputs for SAQM consist of MM5 prognostic model output files, which can be obtained in two ways if they do not already exist. The first way would be to enter into contracts or agreements with existing users of MM5 (Penn State University, the CARB, etc.) to make model runs for the areas and time periods of interest, and then to receive the outputs via the Internet or in some storage medium. The cost would have to be negotiated with the supplier and would depend on the amount of work requested. The alternative is to run MM5 in-house, which is really not recommended since it is a major undertaking as mentioned above. In this case, the user normally would have to gain access to the Cray supercomputers at NCAR (National Center for Atmospheric Research). There is no need to order raw data from sources such as the National Climatic Data Center or the U.S. Geological Survey, since enormous meteorological and geophysical data archives already reside at NCAR. These data archives are intimately connected to MM5's preprocessing system installed at NCAR's supercomputers. Although the data are available to the user free of charge, it will still take months for a new user to learn how to use the complete MM5 system at NCAR. After the MM5 inputs are prepared, the user can then run MM5 on supercomputers or typical UNIX workstations. Air Quality Data: One could in theory run SAQM without obtaining any actual air quality data by using climatological values in a "spin-up" run. However, it is better to base input files on observed data. Some air quality data sets are available for download on the Web from state agencies. However, in general, the user has to formally request the data with state regulatory agencies or to	

	obtain the data from EPA's AIRS database. These data should be free to government agencies such as the MMS. Emissions Data: Emissions data are very complicated to acquire or generate. Gridded data are available from the Office of Air Quality Planning and Standards (OAQPS) of the EPA for some episodes, years, and areas. The data must be reformatted for use in the SAQM emissions preprocessor. One can also obtain the "raw" emission data from the AIRS database.	
B5. Model Interface to Preprocessors / GUI		***Score: 1***
	The SAQM preprocessors are available for free from the California Air Resources Board (CARB). These processors, described below, are all designed to run on Cray supercomputers or UNIX workstations. Emissions preprocessor: We did not review the SAQM emissions system. We did review the final program that converts a SAQM "merge" emissions file into a SAQM input file, applying any desired controls at the same time. This preprocessor has an interactive UNIX script that acts as a crude user interface, but it and the underlying FORTRAN programs are hardwired to the California case and need to be edited to work for other domains. Meteorological preprocessor: SAQM has a preprocessor that converts the MM5 outputs to SAQM inputs. The preprocessing for MM5 is normally done on NCAR's supercomputers; afterwards the user can run MM5 on either supercomputers or UNIX workstations. Air quality preprocessor: SAQM uses simple FORTRAN programs to create an initial air quality field based on observations or climatological data. This field is then used for the "spin-up" run which provides air quality inputs for the model on coarse and nested grids. SAQM does not have any GUIs except as previously described for the emissions preprocessor.	
B6. Run-Time Diagnostics		***Score: 2***
	The FORTRAN code contains some run-time error messages.	
B7. Post-Run Diagnostics		***Score: 2***
	The SAQM RAP postprocessor, Macintosh-based, is very poorly documented. The user usually needs to write custom software to analyze the SAQM outputs, or reformat the outputs in order to use the postprocessors of other photochemical models.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 2***

	SAQM can easily handle multiple point and area sources. However, it is very difficult to detect the effects of any one or several sources on the final predicted pollutant concentrations. This is a common problem among all Eulerian grid models. SAQM contains a tracer option to determine the transport direction and extent of materials originating from an urban area, but the option is not documented well.	
C2. UNIX / PC Portability		***Score: 1***
	SAQM was originally designed for a Cray supercomputer. There are some difficulties in porting the code to UNIX workstations, although it has already been done. To date, SAQM has not been executed on a PC, to the best of our knowledge.	
C3. Run Time		***Score: 1***
	Run time is one of SAQM's great weaknesses. It is very slow compared to the other leading photochemical models, especially when SLS or many vertical layers near the ground are used. On a 26x56x18 (in x, y, and z-directions, respectively) grid, SAQM takes about 15 hr of CPU time to complete a 48-hr simulation on an HP 735 workstation (~ 200 times faster than a VAX 11/780 workstation, and ~ 2 times slower than a SUN Ultra 2 with a 200 MHz CPU). This is much slower than other models (see Section 2.7). Myers et al. (1996) also show roughly 16 to 17 hr of CPU time per 24 hr simulated hour for a California application on an IBM RS6000 workstation (comparable to an HP 735).	
C4. Code Flexibility and Readability		***Score: 1***
	The parts of SAQM that date to RADM are well documented internally and in the user's guide. Many of the changes made in the conversion from RADM to SAQM are poorly documented, making it difficult to understand or change the code. In addition, much of the model and preprocessor codes are hardwired for the California applications, for which the model was first developed. This hardwiring often is not documented, making it difficult and time consuming to convert to another domain or configuration.	
D. Cost (Non-Ranking)		
	SAQM, its processors, and the user documentation are available for free from the California Air Resources Board (CARB).	
E. Availability / Restrictions / Terms (Non-Ranking)		
	SAQM, together with its processors, test data sets, and the user documentation are available for free from the CARB by contacting S. Tanrikulu. The code is in the public domain and can be customized if necessary. Not all the versions described in Section A1 are available at this time. The workstation version of	

	MM5 and its documentation are available via the Web at http://www.mmm.ucar.edu/mm5/.	
F. Language for Model and GUI (Non-Ranking)		
	SAQM and its processors are written in FORTRAN 77. The emissions processor uses UNIX shell scripts.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**17**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**60.0**

2.5 UAM-IV

Model Name: Urban Airshed Model, Version 4 (UAM-IV)	
Person of Contact:	
	Ellen Baldridge U.S. Environmental Protection Agency OAQPS/TSD/SRAB MD-14 Research Triangle Park, NC 27711 Tel (919) 541-5684 Fax (919) 541-2357 E-mail kwb@ladybug.rtpnc.epa.gov
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	*Score: 1*
	The Urban Airshed Model, Version 4 (UAM-IV) is a three-dimensional Eulerian model that expresses transport, diffusion, emissions, deposition, and chemical transformation in mathematical forms to simulate ozone, ozone precursor, carbon monoxide, and (optionally) sulfur and sulfate pollutant concentrations. Its technical formulation can be found in Scheffe and Morris (1993) and in Volume I of the user's guide (Morris and Myers, 1990). The model was mainly designed for urban-scale applications, and for investigating episodes (on the order of a week) of poor air quality. It is not practical to apply the model to calculate annual averages due to its computational requirements. Like all other photochemical models reviewed here, UAM-IV also uses the CB-IV lumped chemical mechanism (Gery et al., 1989). The mechanism consists of over 80 reactions and over 30 chemical species. CB-IV uses a quasi-steady-state assumption for the low-mass fast-reacting species, and the more computationally efficient Crank-Nicholson algorithm for the remainder of the species. It ignores wet deposition and aqueous processes. The model accounts for point and area sources (biogenic and anthropogenic). The emissions species generally consist of lumped hydrocarbons, nitrogen oxides, and carbon monoxide. Boundary and initial chemical concentrations must be specified. Three-dimensional meteorological fields are needed for use in calculating layer heights, advecting materials, and calculating chemical reaction rates. Several versions of UAM-IV with an aerosol module have been developed for the South Coast Air Quality Management District in California. One example is UAM-AERO, which is very sophisticated and resource-intensive. The other example is UAM-LC, which is a simplified version designed to do annual average particulate studies. Both of these models and their documentation are	

	publicly available upon request but were not reviewed in this study. UAM-IV is the most widely-used and the only official EPA "guideline" photochemical model; its roots date back more than 25 years. However, as described below, the science and physics for the model (at least the official version) are somewhat outmoded. There are many next-generation photochemical models, such as UAM-V, CAMx, and CALGRID also reviewed in this study, gradually rising up to replace UAM-IV.	
A2. Grid Options for Eulerian and Trajectory Models		***Score: 1***
	UAM-IV does not have a nested grid option. However, the model boundary can be "jagged" or "stair-stepped," i.e., the definition of the boundary is not constrained to be a rectangle with constant sides but rather can vary by grid cell as one moves around the model domain perimeter, leading to an irregularly shaped domain (see Figure 2-4). UAM-IV uses only the Mercator (UTM) coordinates.	
A3. Quality of Physical Processes Simulated		***Score: 1***
	One major shortcoming for UAM-IV is its variable-thickness layer structure that depends on the spatially-varying mixing height field. The state-of-the-art is to use fixed layers with high resolution near the ground. The EPA version of UAM-IV contains an outdated version of the CB-IV chemical mechanism that does not include the current understanding of the isoprene chemistry. (The new reactions are described in Carter (1996)). The new mechanism predicts incremental ozone reactivities of isoprene in urban atmospheres that are half those predicted by CB-4 in smog chamber experiments. Our experience with actual photochemical modeling is that the mechanism can change peak ozone predictions by several tens of ppb at times. Over the Gulf of Mexico, isoprene emissions are minimal but local and regional pollutant mixes transported from shore may affect concentrations over the Gulf, depending on the scale of the model domain and how much land it encompasses. The photolysis rates used in the model are not based on the latest literature. Cloud processes, which affect photolysis rates, are not included. Moreover, the model does not use three-dimensional temperature, moisture, and pressure fields. All of the above deficiencies plus the lack of nesting capability make UAM-IV unsuitable for regional applications, and place the model behind the state-of-the-art. Another problem with UAM-IV is that it does not strictly conserve mass compared to newer models. This is because the model transports chemical species in volume concentrations rather than in mass concentrations. Furthermore, UAM-IV is prone to a larger degree of numerical diffusion than newer models. Its lack of plume-in-grid treatment may lead to unrealistic diffusion of large point sources.	
A4. Sparse Data Treatment		***Score: 1.5***
	Most model input fields are based on interpolated observations. The model requires meteorological and air-quality data over water to avoid spurious interpolation of land-based values. Buoys and other overwater data sources are often widely scattered or even outside the modeling domain. The typical way	

	of dealing with this problem is by introducing "pseudo observation sites" where data values from adjacent sites are specified to produce a smoother and more realistic interpolation field. The quality of the input fields over water often is determined by the cleverness of the model user in applying limited data. Difficulties in interpolation and uncertainties in assigning boundary and initial conditions can affect model performance in areas of sparse observational data.	
A5. Overwater Dispersion		***Score: 1***
	The model always assumes neutral conditions over the water. In the vicinity of the land/water interface, the variable-thickness layer structure employed in UAM-IV and its lack of vertical resolution often lead to rapidly shrinking or expanding cell height and loss of wind shear and temperature gradient information. There often is unrealistically large transport between land and water along the sloping cell interfaces. The model performance suffers as a result. The minimum layer thickness in the first layer (about 50 to 100 m) is sometimes not adequate for modeling the thin polluted layers that occur over water. The domain-wide temperature gradients used in UAM-IV also cause problems in a domain that has large bodies of water, because they usually are representative of overland conditions.	
A6. Model Evaluation History		***Score: 3***
	UAM-IV has been in existence for over 25 years, and has been applied in many regulatory and exploratory studies on many domains. Its strengths, weaknesses, uncertainties, and average level of performance are well-known to the user community. For example, Scheffe and Morris (1993) documented the evaluation history of UAM-IV.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 3***
	The user's guide for UAM-IV consists of eight volumes, the most comprehensive among the models reviewed, that cover various aspects of the model. The Information is complete and instructions are helpful. The volumes available include: overall user's manuals (Morris and Myers, 1990; Morris et al., 1990), a guide to the diagnostic wind model (Douglas et al., 1990), a guide to the EPS-2 emissions preprocessor system (USEPA, 1992a), a guide to the UAM-ROM interface program (Tang et al., 1990), a guide to the postprocessing system (USEPA, 1992b), a guide to the performance evaluation system (USEPA, 1992c), and a guide to the quality assurance system (USEPA, 1993a) The user's guides must be purchased from the National Technical Information Service (NTIS). Electronic versions of the reports are not available via the Web, unlike other newer models.	

B2. Model Options		*Score: 2*
	There are some model options that can be set in the control file and the chemical parameter file. In the chemical parameter file, the user can change upper and lower bound concentrations (also used as defaults for missing species) and whether to perform an inert tracer run. In the control file, one can indicate whether the run is a restart, the time/date information for the episode, whether surface removal takes place, whether point sources are used, whether a temperature file is included, whether land use is used, the maximum time step, various chemistry integration controls, the file output interval, and several optional debugging print options. The model can output average concentration fields, instantaneous concentration fields (also used for restarting a failed model run), and deposition fields. Some parameters are hardwired in the code and are not documented, such as the maximum number of species.	
B3. Data Preparation Time		*Score: 2*
	To prepare a UAM-IV run without any existing data files is very time-consuming due to model's extensive data requirements. (This is common among all the photochemical models reviewed.) The process could take up to a few months and requires some modeling and programming expertise. The user needs to prepare input data in three areas: meteorological, emissions, and chemical boundary concentrations. The normal procedure is to obtain raw input data; quality assure the data; run many preprocessing programs, including the Diagnostic Wind Model (DWM) and the Mobile model for vehicle emissions, process the data; and validate the processed data. Sometimes, parts of the procedure may have to be repeated because some problems with the data, either raw or processed, are not so obvious initially. To modify an existing run, on the other hand, is in general straightforward and requires much less time. However, the user almost always has to develop custom software to achieve the desired input file modifications.	
B4. Ease of Data Acquisition		*Score: 1*
	Acquisition of various input data for UAM-IV is described below. Land Use: Gridded land use data are required. If one wants to have a level of data accuracy beyond what is available from visually inspecting a map or aerial photo, then the USGS land use data must be acquired. The data are available from the Web free of charge (see Section 2.2). However, UAM-IV does not contain processors to handle the USGS data, so the user must write custom software to process the data. Air Quality Data: UAM-IV requires hourly ozone and ozone precursor concentrations or background values for inputs and to assess model performance. Some air quality data sets are available from state agencies via the Web. But the data generally are acquired through a formal request to state regulatory agencies or to the AIRS data base manager. The data should be free. Meteorological Data: The UAM-IV processors require wind, temperature,	

	moisture, and pressure data from surface and upper air sites. Data for recent years (since the early 1990s) are available via the Web for free from the National Climatic Data Center (NCDC). Historical data would have to be ordered from NCDC. The cost is typically within a thousand dollars. The National Center for Atmospheric Research (NCAR) also provides data with comparable pricing. See Section 2.2 for some specific Web addresses. There are commercial companies who put historical meteorological data on CD-ROMs at about $100 per disk. Each disk contains data for many states and many years. Specialized observations may be available from industry or from the AIRS data base. Emissions Data: Emissions data are probably the most complicated to acquire and process, and the most uncertain. Gridded data are available from the Office of Air Quality Planning and Standards (OAQPS) of the EPA for some episodes and geographical areas. If one has access to the AIRS emissions data base through state agencies, one can obtain "raw" AFS (point source) and AMS (area and mobile source) data. Alternatively, one can develop domain and time-specific "raw" emissions data based on surveys and measurements. Data obtained from all these sources often must be reformatted for use in preprocessors. Link data also are necessary to map mobile source emissions. For selected episodes and areas, the user can run the EPA GMISS/ROM-UAM interface program to acquire and reformat the Regional Oxidant Model (ROM) inputs and outputs for use in UAM-IV. This process, although less time-consuming overall, still involves accessing the EPA mainframe, downloading large files, and running several processor files. Only biogenic emissions are available from this system.	
B5. Model Interface to Preprocessors / GUI		***Score: 1***
	Currently, there is no formal graphical user interface to the UAM-IV model or its preprocessors. At one time, a system called UAM-Guides was available from the MCNC, but the system no longer appears on MCNC's Web site (http://www.iceis.msnc.org). UAM-IV has a collection of preprocessors, as described in various user's guides listed in Section B1. The UAM-IV preprocessors, freely available from EPA's SCRAM bulletin board, can be run on many computer platforms. Some of the emissions preprocessors require meteorological input files to already exist. Therefore, the execution sequence for preprocessors is important. Since certain photochemical models, such as UAM-V and CAMx, also use some of UAM-IV's preprocessors or processed data, the standard UAM-IV preprocessing system is described in detail below: The description also gives the reader some idea concerning the level of effort required to prepare necessary input data for a photochemical model. Control data preprocessors and files: SPREP produces the simulation control file (SIMCONTROL), in which the user specifies various simulation characteristics and options. CPREP produces	

	the chemical parameters file (CHEMPARAM), in which reaction rates and other information are given. Meteorological preprocessors and files: MIXHT, RAMMET-X and DFNSBK produce the DIFFBREAK hourly gridded mixing height file from meteorological input data. REGNTP produces the REGIONTOP gridded model top height file based on user inputs. SUNFUNC and METSCL produce the METSCALARS file which contains hourly NO_2 photolysis rates, water vapor concentrations, pressure, stability, and vertical temperature gradient information based on user inputs and meteorological observations. TMPRTR produces the TEMPERATUR gridded hourly surface temperature field from interpolated observations. PRESFC, PREUPR, DWM and UAMWND produce the three-dimensional hourly wind vector file (WIND) using reformatted surface and upper air weather observations. DWM has many switches and options that can affect the appearance of the final wind field. Initial and boundary conditions preprocessors and files: CRETER produces the TERRAIN input file of roughness lengths and vegetation factors from gridded land use data. AIRQUL produces the AIRQUALITY initial chemical concentration file by interpolating observed and background hourly pollutant observations. BNDARY produces the BOUNDARY file which contains the model boundary concentrations. TPCONC produces the TOPCONC file containing hourly chemical concentrations at the top of the model domain, based on observations or background. Emissions preprocessors and files: UAM-IV is designed to use MOBILE5, BEIS2, and the EPS-2 emissions processing systems to convert the raw data to UAM-IV files. BEIS2 produces a gridded file of biogenic emissions. MOBILE5 is a mobile source model that creates county-based mobile source emissions data for a given scenario and domain. EPS-2 consists of many programs to produce the time-varying gridded and point source emissions files and merge them with the biogenic information into one AREA source file and one PTSOURCE file for input to UAM-IV.	
B6. Run-Time Diagnostics		***Score: 2***
	The FORTRAN code contains a number of run-time error messages and diagnostic messages. There is also a subroutine that produces the state of many variables if execution aborts prematurely. The code sometimes can crash due to floating point and other errors without any warning messages. This sometimes happen when an array dimension was unintentionally exceeded, or when the program had difficulty converging in the chemical routines. It is sometimes necessary to modify the source code to print out the maximum, minimum, and average hourly concentrations of selected pollutants to the screen for diagnostic purposes. As an option, the user can also instruct the code to dump various chemical species concentration fields by turning on the appropriate model switches.	
B7. Post-Run Diagnostics		***Score: 2***

	The UAM-IV postprocessor available from the EPA relies on SAS, which is a commercial software package. Various consulting firms also have public or in-house software available for evaluating and visualizing UAM-IV outputs. The software usually consists of FORTRAN postprocessing codes and various plotting packages such as NCAR Graphics (several thousand dollars) and SURFER (several hundred dollars). The publicly available postprocessing programs include Alpine Geophysics' MAPS software and MCNC's PAVE system; both have written documentation. Use of these programs is somewhat machine-dependent. PAVE is available on the Web (see address in Section B5). Alpine Geophysics would need to be contacted directly concerning MAPS.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 2***
	UAM-IV easily handles multiple point and area sources. However, it is very difficult to detect the effects of any one or several sources on the final pollutant concentrations.	
C2. UNIX / PC Portability		***Score: 3***
	It is very easy to port UAM-IV between the UNIX and PC platforms. Minor code changes are necessary in the job scripts and certain machine-specific FORTRAN utility functions and routines.	
C3. Run Time		***Score: 2***
	UAM-IV's run time is slower than CALGRID, UAM-V and CAMx on a per-grid-cell basis. On a 34x60x5 (in x, y, and z directions, respectively) grid, UAM-IV takes about 4 hr of CPU time to complete a 48-hr simulation on an HP 735 workstation (~ 200 times faster than a VAX 11/780 workstation, and ~ 2 times slower than a SUN Ultra 2 with a 200 MHz CPU). See Section 2.7 for more details.	
C4. Code Flexibility and Readability		***Score: 2***
	The code has some comments and is somewhat modular in the sense that it is composed of many subroutines, but it is not "user-friendly." It contains parameter files to set the maximum array sizes, but it contains some hardwired parameters and constants that are not documented. The I/O subroutines are easy to locate and change, if necessary.	
D. Cost (Non-Ranking)		
	UAM-IV and associated pre- and post-processing programs are available from EPA's SCRAM bulletin board at no charge. MCNC used to offer a user interface program called UAM-Guides, but the software is no longer on their web site. The UAM-IV user's manual set (see Section B1) must be purchased	

	from the NTIS. The cost for the entire set is several hundred dollars. Some technical support for UAM-IV is available from the EPA for free. A SAS license is required to use the EPA-supplied quality assurance and post-processing software.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	UAM-IV and all its pre- and post-processor FORTRAN codes, along with test data sets can be downloaded from EPA's SCRAM web site (http://www.epa.gov/ttn/scram/models/uam). Programs can be modified by the user without restrictions, although some changes would render the code no longer an EPA "guideline" model.	
F. Language for Model and GUI (Non-Ranking)		
	UAM-IV is written in FORTRAN (mostly 66 and some 77). The EPA post-processing software is written in SAS.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**17**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**57.8**

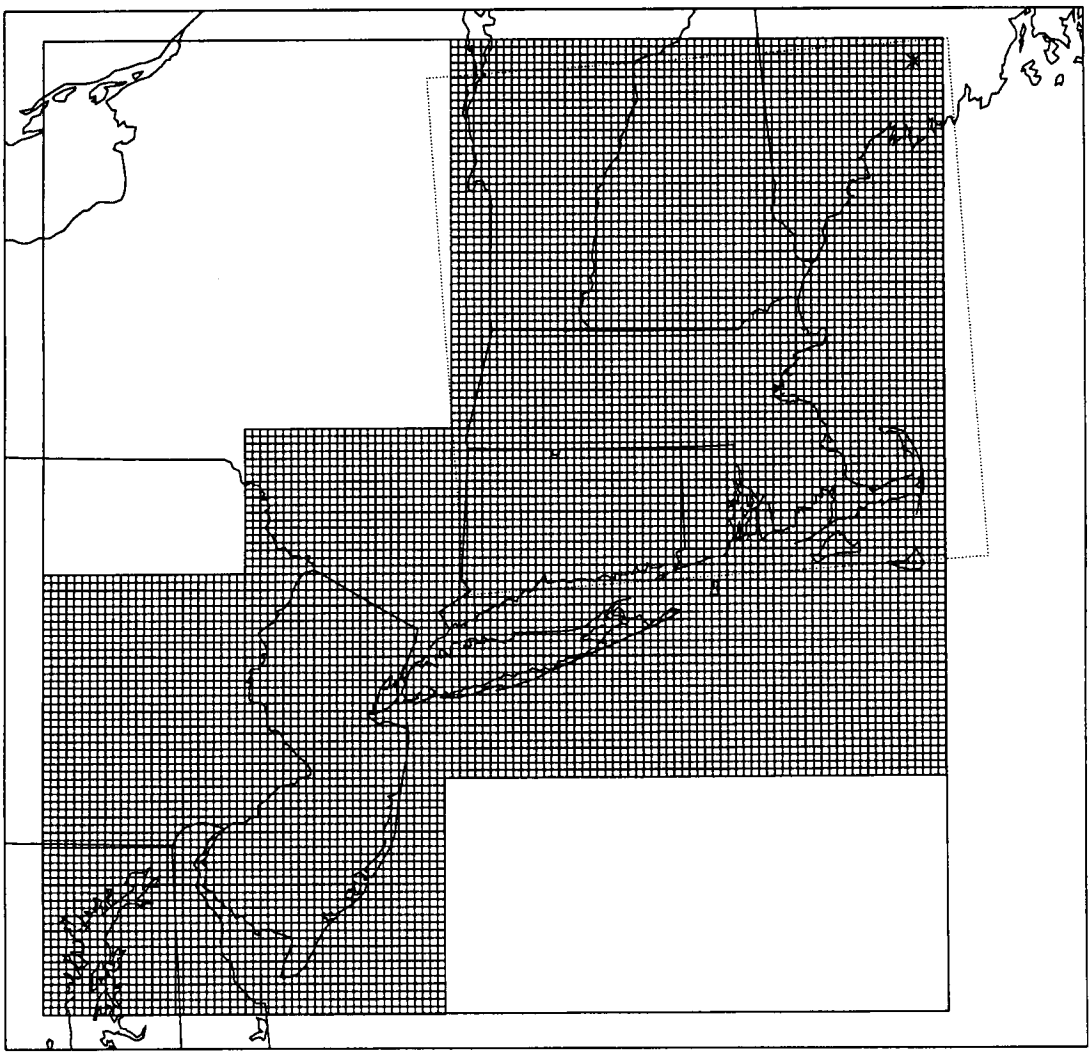

Figure 2-4 An example of a non-rectangular UAM-IV domain for the northeastern United States, comprising three different regulatory modeling domains and allowing flow between them. No chemistry or advection occurs outside the boundaries. This domain was used in the Cooperative Regional Modeling Experiment (CReME). After Hanna and Fernau (1997).

2.6 UAM-V

Model Name: Variable Grid Urban Airshed Model (UAM-V)	
Person of Contact:	
	Sharon G. Douglas Systems Applications International 101 Lucas Valley Road San Rafael, CA 94903 Tel (415) 507-7108 Fax (415) 507-7177 E-mail 02643@sainet.saiwest.saintl.com
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	***Score: 2***
	UAM-V is a comprehensive, three-dimensional, Eulerian photochemical model incorporating formulations for transport and dispersion, transformation of precursor gases to secondary species and particles, and deposition of gases and particles. Its technical formulation has been described in the user's guide (SAI, 1996a). The model is mainly designed to simulate episodes on the order of a week. Running the model on longer time scales is not yet practical. UAM-V uses the CB-IV lumped chemical mechanism (Gery et al., 1989), in which hydrocarbon species are classified, partitioned and aggregated by the number and type of carbon bonds that they contain. The user's guide mentions the support of aqueous-phase chemistry; however, a cursory code inspection showed that the option is not really available. The model has been used in regional and urban scales and in regulatory settings. The standard version of UAM-V contains two-way horizontal and vertical nesting and a plume-in-grid algorithm. SAI recently has updated the code to include: • source apportionment capability in order to identify which regions contribute to predicted concentrations, and • process analysis capability in order to examine the extent to which the various physical processes contribute to the predicted concentration fields. Formal and thorough documentation of the above two modules is not yet available. There is also an aerosol version, known as UAM-VPM, that is under development and will be available in the summer of 1998. UAM-V replaces the older UAM-IV model.	

A2. Grid Options for Eulerian and Trajectory Models		*Score: 3*
	UAM-V has a two-way nested grid option (Figure 2-1) and a plume-in-grid option (Figure 2-3). Different vertical grid resolutions are used with different horizontal grid resolutions (Figure 2-2). The coordinate system can be either Mercator (UTM) coordinates or latitude/longitude coordinates. Winds can be represented at either the cell face or the cell center.	
A3. Quality of Physical Processes Simulated		*Score: 3*
	UAM-V has not yet been peer-reviewed in the refereed literature in terms of its technical components. It contains the most up-to-date CB-IV chemistry with the new isoprene reactions, and has current photolytic reaction rates. The model conserves mass by advecting chemical species in mass concentrations rather than in volume concentrations. It has high vertical resolution near the surface and uses fixed layers. It uses three-dimensional temperature, pressure, and humidity fields, which is an improvement over UAM-IV. The plume-rise algorithm is current. The horizontal advection scheme no longer is considered state of the art.	
A4. Sparse Data Treatment		*Score: 2.5*
	The SAIMM or RAMS prognostic mesoscale meteorological models provide meteorological inputs for UAM-V. These models have been shown to perform well over water and in coastal thermal internal boundary layer (TIBL) situations. The effects of lack of data over water are minimized because the models rely on physical equations rather than data interpolation to produce three-dimensional fields. However, even with use of prognostic models, the lack of observed data may result in diminished model performance because of difficulties in assigning boundary and initial conditions and providing data for nudging.	
A5. Overwater Dispersion		*Score: 2.5*
	As mentioned above, the sophisticated treatments of the marine boundary layer and the land/water interface in the prognostic models assure relatively good performance over water, even in data-sparse situations. The lack of data, however, can lead to a degradation of performance over water because of the difficulty of calculating micrometeorological parameters and dispersion coefficients. UAM-V has been used in the Lake Michigan and Gulf of Mexico areas where overwater transport is important. Early applications of UAM-V to the New England area with SAIMM gave poor results near the land/water interface until the "nudging" coefficients were increased to let the observations have more influence on the prognostic meteorological fields. The RAMS model offers a variety of turbulence closure and lower boundary treatment options. These are summarized at http://rams.atmos.colostate.edu/detailed.html, and include Smagorinsky-type eddy viscosity, closure methods with eddy viscosity as a function of turbulent kinetic energy, constant fluxes, constant fluxes with similarity, and surface energy flux methods that depend on ground temperature.	

	SAIMM uses first-order closure to parameterize turbulent exchange. Similarity theory is used to parameterize fluxes near the lower boundary. Flux-profile relationships are used to calculate the surface fluxes in the surface layer. Two methods can be used to calculate vertical exchange coefficients and PBL heights: one involves diagnostic relationships that depend on the sign of the heat flux and the other depends on turbulent kinetic energy. The details are contained in SAI (1995c). This reference does not explain clearly how the model handles air-sea interaction among temperatures, etc. or how some of the fluxes are calculated.	
A6. Model Evaluation History		***Score: 3***
	UAM-V has been run on many different regional domains and has been reviewed by several groups (mainly for the Lake Michigan Ozone Study (LMOS) and OTAG studies). These peer reviews identified some weaknesses and performance flaws, but overall found the model to perform well in matching observed species concentrations. Its performance in the Lake Michigan domain was evaluated in a peer-reviewed journal article (Hanna et al., 1996b). The model was approved for use in several high profile regulatory and semi-regulatory uses for OTAG, in the Midwest, in Texas, in Atlanta, and elsewhere. UAM-V was compared against observations in all these applications. The model has not always been shown to perform significantly better than its simpler UAM-IV ancestor, but its superior model physics and regional capabilities increasingly have made it the model of choice for complicated regulatory situations. The latest versions of UAM-V with source apportionment, aerosol modules, and process analysis have not been peer reviewed yet.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 3***
	UAM-V's documentation is very complete and provides adequate user instructions. The documents are available for download from EPA's SCRAM bulletin board as WordPerfect files. The following volumes are available: • a guide for the model itself (SAI, 1996a), • a guide for the mesoscale model (SAI, 1995a), • a guide for mesoscale meteorological model to UAM-V interface programs (SAI, 1995c), • two guides for boundary and initial conditions preparation programs (SAI, 1996b and 1996c), • a guide for the clouds/precipitation processor (Guo et al., 1996), • a guide for other miscellaneous preprocessor and utility programs (SAI, 1995b), and • a guide for the postprocessing system (SAI, 1996d).	

	Complete documentation also exists for the process analysis version. Some documentation is available for the source-apportionment version. The RAMS user guide does not appear to be available via the Web but there is a homepage that describes the model at http://rams.atmos.colostate.edu/. The literature description of the model is contained in Pielke et al. (1992).	
B2. Model Options		***Score: 3***
	UAM-V allows options such as whether to include nested grids and whether to include plume-in-grid treatments. These options and their associated parameters are easily set in the model control file. Additional input files are usually necessary if the options are selected. There are extensive debugging switches that are set using an innovative bit-setting scheme at the command line. The user also sets file names, logical devices, output species, run information (date, time, duration, message, etc.), domain information, integration time step, deposition control information, diffusivity information, chemical integration information, and other logical switches in the control file. The user's guides clearly describe the use of these options. UAM-V outputs include hourly instantaneous concentrations for all layers, hourly average concentrations in Layer One, PiG outputs, restart files for PiG, and two diagnostic output files to monitor run progress. Restart files allow a prematurely terminated UAM-V run to resume.	
B3. Data Preparation Time		***Score: 2***
	One common problem among all photochemical models is that to prepare a model run from scratch with no existing files is not a trivial task at all. The process could take weeks to months, and usually requires some special technical skills. The process is even more involved for UAM-V compared to UAM-IV, since the former has additional input requirements and generally uses more complicated prognostic model outputs. Inputs from three different areas must be prepared: meteorological, emissions, and chemical boundary concentrations. The data preparation procedure involves acquiring raw data, running ten to 20 preprocessor programs (probably including the SAIMM or RAMS prognostic meteorological model, and the Mobile model for vehicle emissions), and validating the processed data. UAM-V has new processors for most inputs, except that it uses existing EPS-2 or EMS-95 emissions processing systems to create emissions files. To modify an existing run is generally straightforward and requires much less time than the original runs, except that the user probably still needs to develop his own utility programs to make necessary data modifications. UAM-V input and output files for the OTAG test case are available on the Internet (ftp://www.iceis.mcnc.org/pub/otagdc/testcase). The UAM-V	

	processors and the land use database included are for the OTAG regional runs with an 18-km resolution. For urban runs, land use data at a 200-m resolution are more desirable, but require new processors corresponding to the new resolution to be developed. UAM-V has a utility program that allows easy implementation of studies of emissions control strategies.	
B4. Ease of Data Acquisition		***Score: 1***
	UAM-V requires all the same types (not necessarily the same formats) of inputs as does UAM-IV plus others. The reader is referred to the corresponding section for UAM-IV for more details. UAM-V also optionally can use cloud cover and hourly precipitation data. These data are available from the National Climatic Data Center for a few hundred dollars of handling charge, or CD-ROMs from private sources at about $100 per disk. The cloud data already come with the standard meteorological data needed for UAM-IV as described in Section 2.5. The precipitation data are separate. UAM-V also needs Total Ozone Mapping Spectrometer (TOMS) gridded ozone column information. The information, used to calculate photolysis rates, is usually available for free from the National Space Science Data Center via the Internet (ftp://jwocky.gsfc.nasa.gov). Typically, the user should also contact regional EPA and state regulatory agencies, since they may already have the required data in-house.	
B5. Model Interface to Preprocessors / GUI		***Score: 1***
	UAM-V and its preprocessors do not contain a graphical user interface program. Most of the UAM-IV preprocessors also can be used for UAM-V. The additional UAM-V preprocessors are available for free from EPA's SCRAM bulletin board for government use, but they could not be modified without permission from the model developers (see Section E). In addition to the preprocessors already described under UAM-IV, the following types of UAM-V preprocessors and files exist: Albedo and rates preprocessors and files: ALHZOZ produces the ALBEDO file of albedo, turbidity, and ozone column density information for use in calculating photolysis rates. CALCJ produces the RATES file which contains the photolysis rate information for key species. READGRID reformats the TOMS data for use by ALHZOZ. Geophysical preprocessors and files: PRELND generates the SURFACE file of gridded land use information. The preprocessor also generates a gridded TERRAIN file and an optional AGGMAP cell aggregation file. Additional air quality preprocessors and files: The AIRQUL and BNDARY	

	preprocessors of UAM-IV were modified to handle the fixed vertical layer structure of UAM-V. EXTRACT_BC creates AIRQUALITY, BOUNDARY, and TOPCONC files for UAM-V from UAM-IV outputs. Additional emissions preprocessors and files: UAM-V emissions files are produced using the EPS-2 system described under UAM-IV or the EMS-95 (Wilkinson and Emigh, 1995; Wilkinson et al., 1994) emissions system. EMS-95 is publicly available, and consists of SAS, ARCINFO, and FORTRAN programs to perform the similar tasks done by EPS-2. There are also other auxiliary emissions utility programs: EMSAGG and EMSDIV aggregate or split up emissions from grids with different resolutions. RANKPTS assists in selecting sources for the PiG treatment. SYNSTK and STKLST produce listings of and merge several point source files into one file. Meteorological preprocessors and files: The user needs to apply the SAIMM or RAMS prognostic models to generate meteorological inputs to UAM-V. RAMS2UAMV and MM2UAMV convert RAMS and SAIMM, respectively, prognostic model outputs to the UAM-V format. In addition to wind and temperature, MM2UAMV produces other UAM-V files that are not found in UAM-IV, including H2O (three-dimensional water vapor fields), VDIFFUSION (vertical diffusion coefficients), and HEIGHT(height and pressure fields).	
B6. Run-Time Diagnostics		***Score: 3***
	There are many debugging switches available to monitor model progress. The user can select any subset of these options using a simple command-line switch. The code also contains many error messages.	
B7. Post-Run Diagnostics		***Score: 3***
	UAM-V comes with three post-processing programs: • an extraction program to access pollutant information of interest, • a display program that produces simple displays of the output and calculates performance statistics, and • a plotting program, based on SAI's own plotting package, to produce contour plots, time series plots and other useful output figures. The programs integrate any nested output with the coarse grid output and display it on the finest grid resolution. The display and graphical programs are still under development and should be finalized soon.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 3***
	UAM-V handles multiple point and area sources easily. A later version of UAM-V includes an innovative source attribution algorithm to identify the effects of different subregions on predicted concentrations. The version of	

	UAM-V that is on the SCRAM bulletin board does not support source attribution. SAI should be contacted directly for the newer code.	
C2. UNIX / PC Portability		***Score: 3***
	It is fairly easy to port UAM-V between the UNIX and PC platforms. For a specific platform, minor changes are necessary in the job scripts and certain machine-specific FORTRAN utility functions and routines, such as the date and time routines.	
C3. Run Time		***Score: 3***
	The fast chemical solver in UAM-V gives good computational performance compared to other photochemical models. On a 34x60x8 (in x, y, and z directions, respectively) grid, UAM-V takes slightly more than 1 hr of CPU time to complete a 48-hr simulation on an HP 735 workstation (~ 200 times faster than a VAX 11/780 workstation, and ~ 2 times slower than a SUN Ultra 2 with a 200 MHz CPU), when the plume-in-grid (PiG) option was not used. This run time is about three to four times faster than UAM-IV and CALGRID. For a limited number of PiG point sources, performance degradation is minimal. However, from the UAM-V user's manual, it is not clear how the above fast chemical solver works, and what the associated approximations are. From a cursory code inspection, it appears that the speed-up is due to combining and skipping chemical reaction steps under certain conditions.	
C4. Code Flexibility and Readability		***Score: 2***
	The UAM-V code is composed of many modular subroutines, some of which are redundant. Most of the code is extensively commented as to the purpose of each algorithm and subroutine. The programming styles are somewhat inconsistent across routines, reflecting the fact that the code was assembled from a number of existing programs over a number of years. We found some inconsistencies between the user's guide and the code. For example, some model options mentioned in the user's guide are not available in the code. There are parameter files to easily set the maximum array sizes. The I/O subroutines are easy to locate and change, if necessary.	
D. Cost (Non-Ranking)		
	UAM-V, its preprocessors, and its manuals are available for download from EPA's SCRAM bulletin board at no charge. There are licensing issues as described in Section E.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	UAM-V and all its preprocessors (including SAIMM), along with the user	

	manuals, are available for download from EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/). The copyright notice on the SCRAM version says that the UAM-V package may be used by the U.S. government for "bona fide governmental purposes," with several restrictions that involve not transmitting or disguising the code. Therefore, the MMS should be able to use the code *as is* without any problems. Permissions from the model developers, SAI, are required for any code modifications. A licensing agreement with SAI is necessary before a private user could use the UAM-V software, even though the code is "publicly available." The new process analysis, source attribution, and aerosol algorithms are not present in the SCRAM version of UAM-V. SAI must be contacted for information on these codes. A licensing agreement is necessary for access to the process analysis and source attribution codes. For the aerosol model to be released in 1998, no decision has yet been made on access issues. The UAM-V input and output files for the OTAG test case are available via ftp from: ftp://www.iceis.mcnc.org/pub/otagdc/testcase. The RAMS code does not appear to be available via the Web but there is a home page describing the model that is located at http://rams.atmos.colostate.edu.	
F. Language for Model and GUI (Non-Ranking)		
	UAM-V is written in FORTRAN 77.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**17**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**83.3**

2.7 BENCHMARK COMPARISON OF PHOTOCHEMICAL MODELS

In this comparison, an existing data set is used to compare the computational performance of several of the photochemical models evaluated in this review. The purpose of the comparison is to compare CPU time and computational requirements. We do not attempt to compare predicted chemical concentrations with observations. We emphasize that this is not a true benchmark comparison because model differences in format and application made it impossible to have identical inputs for each model. An attempt was made to make the inputs as similar as possible, given fundamental model differences and the desire to run each model in a fashion that is representative of "typical" use for that model.

In this test, the standard version of UAM-IV (available from EPA's SCRAM bulletin board), the SCRAM OTAG version of UAM-V (fast solver, new isoprene chemistry, plume-in-grid), the latest version of CALGRID (new isoprene chemistry, no PiG, Carbon Bond 4 Mechanism, no nesting), and the production version of SAQM (no PiG, no nesting, Carbon Bond 4 Mechanism, old isoprene chemistry) were compared for a 48-hour model simulation for the Lake Michigan Ozone Study (LMOS) domain using similar sets of input files. The horizontal resolution was 8 km for all models. The UAM-IV, UAM-V, and CALGRID runs were performed on identical UTM-based horizontal domains with 34 columns and 60 rows. The SAQM run was made on a slightly smaller Lambert conformal domain with 26 columns and 56 rows, because the model is designed to use that map projection. Model vertical resolution was chosen to be typical for a standard application of each model. The inputs were as identical as possible, given the differing resolutions, formats, and model input requirements. We created the inputs using a common meteorological and air quality database as part of the Cooperative Regional Model Evaluation (CReME) study (Hanna et al., 1996b). Rather than making the model configurations identical (in terms of the number of vertical layers, number of reactions, etc.), the models were run in their typical operational configurations, which the MMS is likely to use in the future. UAM-V was run both with and without 40 elevated point sources treated with plume-in-grid methods. Also, nesting was not used in the CReME implementation of UAM-V.

All models were run on an HP 735 workstation, which is about 200 times faster than a VAX 11/780 workstation, under the HP-UX operating system. The floating-point performance for a SUN Ultra 2 with a 200 MHz CPU, the machine that the MMS is currently using, is about twice that for an HP 735. The computational results are reported in Table 2-1. As mentioned above, the number of vertical layers reflects a typical application of each model. The number of grid cells is the product of the numbers of row, column and vertical layers. For this application, the Surface Layer Submodel (SLS) option of SAQM was used, in which concentrations were calculated in three sublayers within the lowest model layer. This is more computationally efficient than if two additional model layers were added to the model. The concentrations from the SLS layers feed back into the regular SAQM layer structure at each time step, and vice-versa. The model produces hourly output concentration files for both the SLS layers and the regular layers. The user can decide whether to analyze either one or both to represent the ground-level concentrations. SAQM was run in double precision according to the model developer's recommendations.

Although all models used the same types of input files (emissions, boundary concentrations, and meteorological information), the number and types of files, storage formats, and the size of the executable code all varied among the models and led to different storage requirements. The increase in input file size from UAM-IV to UAM-V was due mostly to the addition of several three-dimensional meteorological fields. The larger input file size for CALGRID and SAQM relative to the UAM models was due mostly to larger space requirements for the meteorological and horizontal boundary condition files. Note that CALGRID has an option to use a much simplified boundary condition file that would save considerable

disk space (perhaps almost 17 MB). The input file requirements listed in Table 2-1 are for all files, including meteorological files, but do not include raw data files, preprocessor program inputs, or prognostic meteorological program inputs.

Table 2-1. Comparison of Model Storage Requirements and CPU Performance for a 48-Hour Run for the Lake Michigan Ozone Study Domain, 15-16 July 1991 Episode. The CPU Times are Based on an HP 735 Workstation with 256MB of RAM. The floating-point performance for a SUN Ultra 2 with a 200 MHz CPU, the machine that the MMS is currently using, is about twice that for an HP 735.

Model	No. of vertical levels	Total no. of grid cells	Input file storage (MB)	Output file storage (MB)	CPU time (day 1) (hr)	CPU time (day 2) (hr)
UAM-IV	5	10,200	31	98	1.37	1.64
UAM-V	8	16,300	45	80	0.42	0.69
UAM-V/PiG	8	16,320	45	142	0.49	0.82
CALGRID	10	20,400	79	19	1.90	2.17
SAQM-SLS	15+3	21,840	63	377	7.30	7.68

The disk space requirements for the model outputs again varied considerably among the models. CALGRID was most efficient because for this application (and most other routine applications) the hourly averages for only a few species and at only a few levels are saved. In addition, the restart or instantaneous concentrations files only contain two hours of data, rather than all hours. The large disk space requirements of SAQM were partly due to the use of the SLS option, which produces a second parallel but smaller set of output files, and partly due to the fact that separate restart files are created for both instantaneous and hourly average concentrations. For this application, a total of 16 output files were produced by SAQM, although according to the model developers not all of them are used or needed. The outputs from UAM-V without the PiG treatment were somewhat smaller than that for UAM-IV, even though UAM-V had more layers. This is because the hourly average concentrations are saved only in the first layer in UAM-V. Adding PiG increased storage needs by about 60 percent. If deposition amounts are wanted, the storage requirements for each model will increase by a small percentage. Note that since disk storage is relatively cheap (~ $1000 per 10GB) nowadays, the storage requirements mentioned above for each model are not likely to be a limiting factor.

The CPU time also varied from model to model. CALGRID was somewhat slower than UAM-IV, but had twice as many grid cells. SAQM with SLS was much slower than any of the other models. For various technical reasons, the California Air Resources Board no longer recommends the use of the SLS option. When run without SLS, SAQM probably will run at least twice as fast. However, the model developers report that when the vertical resolution near the ground is increased in order to compensate for the absence of SLS, the model performance falls off quickly, to as much as four to ten times slower (Chang et al., 1997). This is due to the need for a smaller time-step in the model.

UAM-V with the "fast chemical solver" was the fastest model, and the addition of 40 plume-in-grid sources only decreased performance by about 20 percent. However, it has been reported that the fast chemical solver can give maximum ozone concentrations that are higher than those from the standard chemical module. This difference has been reported to be larger than 10 ppb at times. However, the model developers claim that the latest version of the solver gives differences of only several ppb (about three percent) at most (Morris et al., 1994). Neither a summary nor details of the fast solver is provided in the user's manual. The unsettling fact about photochemical models: that a change in inputs,

parameterizations, or computational methods can lead to a variation in predicted concentrations that is on the order of that seen with emissions control strategy simulations, is something that all modelers and policy makers must accept, given the current state of the art.

Table 2-2 shows model computational performance as the ratio of the total CPU seconds for the 48-hour run divided by the number of grid cells. The SAQM number is biased high because the SLS cells are not included in the ratio. (Not all calculations are done in the SLS cells.) One can see that, on a per grid cell basis, CALGRID was more efficient than UAM-IV. The UAM-V fast solver was three times more efficient than CALGRID, and lost little efficiency with 40 PiG sources. Note that no nesting was done in these UAM-V runs. Although budget constraints prevented us from testing CAMx using this data set, the model developers report that CAMx also contains a fast chemical solver that results in a speed increase of a factor of three to four over the standard solver (Environ, 1997).

Table 2-2. Comparison of CPU Performance Ratio (Seconds/Cell) for a 48-Hour Run for the Lake Michigan Ozone Study Domain, 15-16 July 1991 Episode.

Model	Total no. of grid cells	Total CPU time (sec)	Ratio (sec/cell)
UAM-IV	10,200	10,832	1.06
UAM-V	16,320	3,989	0.24
UAM-V/PiG	16,320	4,744	0.29
CALGRID	20,400	14,672	0.72
SAQM-SLS	21,840	53,944	2.47

2.8 SUMMARY AND RECOMMENDATIONS

In this task, five regional photochemical models were rated and compared. The models are the Urban Airshed Model-Version 4 (UAM-IV), CALGRID, the SARMAP Air Quality Model (SAQM), the Comprehensive Air Quality Model with Extensions (CAMx), and the Variable Grid Urban Airshed Model (UAM-V). These models are designed and used primarily for simulating short-term (on the order of a week) urban and regional ozone episodes. Their large data input requirements and CPU demands make it impractical to use them to simulate longer periods of time on a routine basis. Therefore, the models are of limited use for annual average calculations. They possess treatments of sulfur and aerosol chemical and physical processes, but to date the emphasis has been on their use for ozone regulatory studies. All models except UAM-V are completely in the public domain. The UAM-V code is freely available to the public, but its use is somewhat restricted. UAM-V's copyright allows government agencies to use the model for "bona fide government purposes" without any code modifications. The use of the model by private users requires special licensing agreements from the model developers, Systems Applications International (SAI).

In addition to these well-known and relatively available models, there are several other photochemical models that have been used recently for urban and regional studies. These were developed in university settings, and are more research-oriented. They include the Georgia Tech Urban-to-Regional Multiscale Model (Harley et al., 1993) and the UCLA Surface Meteorology and Ozone Generation Model (SMOG) (Lu and Turco, 1996). These two models were not reviewed as part of this study.

Under active research and development with the support of the EPA are the Models-3 program and the Multiscale Air Quality Simulation Platform (MAQSIP) of MCNC (http://www.envpro.ncsc.org/EDSS/, contact Neil Wheeler (919) 248-1819; see also http://www.iceis.mcnc.org). The MAQSIP is part of the Environmental Decision and Support System (EDSS), which is an attempt to build a comprehensive framework to conduct the next generation of air modeling. EDSS includes the Package for Analysis and Visualization (PAVE) that allows outputs from air quality models to be graphically displayed in a number of ways. PAVE can read directly and produce plots for all UAM-IV input and output files and some UAM-V (and CAMx) files, including the coarse grid output files. The rest of the UAM-V (CAMx) files (mostly those that are not in UAM-IV format), including the nested output, need to have an associated metafile created that contains certain information about the file. CALGRID and SAQM need to have their output first reformatted into UAM-IV, UAM-V, or IO/API (netCDF) format before input to PAVE. An example conversion program for SAQM is provided on the website. EDSS also includes the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System, which is an alternative to the more wellknown EPS-2 and EMS-95 emissions modeling systems to be described below. Because of their unfinished nature, these models also were not reviewed.

EPS-2 and EMS-95 are the two most popular packages to create emissions files for regional photochemical models. EPS-2 (U.S. EPA, 1992a) is available via the SCRAM bulletin board and uses FORTRAN codes. The somewhat more sophisticated EMS-95 (Wilkinson et al., 1994; Wilkinson and Emigh, 1995) is publicly available from Alpine Geophysics and requires both SAS and ARC-INFO commercial software packages to function.

Before presenting the results of the model evaluation, it must be mentioned that several other versions of the basic photochemical models reviewed here also exist. SAI has a version of UAM-IV that calculates concentrations of additional toxic species (Ligocki and Whitten, 1992). This version is not publicly available and was not reviewed. It is available from SAI upon request, and may or may not have a licensing fee depending on the nature of the request. SAI also has a long-term, long-range transport model (REMSAD) with simplified particulate chemistry to examine the transport and deposition of

toxics, acidic species, and particulates and to consider visibility issues (Emery et al., 1996). This development work is being sponsored by the EPA, which may make the model public as part of Models-3. SAI or the EPA should be contacted regarding REMSAD's status and availability. It is likely to suit some of MMS's needs.

The SAQM-AERO and UAM-AERO versions of SAQM and UAM-IV have a comprehensive, state-of-the-art aerosol module developed by Sonoma Technologies Incorporated (STI). The aerosol module and its application to UAM-IV are described in Wexler et al. (1994) and Lurmann et al. (1997). It is very CPU-intensive and is suitable mainly for episodic studies. Additional data requirements, usage complexities, and model uncertainties would arise due to the aerosol module. In addition, STI developed a simplified version of UAM-AERO to do annual average aerosol studies. It is called UAM-LC and can simulate an entire year in about 24 hours of CPU time on a typical UNIX workstation. These codes and the documentation are publicly available upon request from the funding agencies that sponsored the model development work. The codes are still being assessed and evaluated. As a result, we did not acquire and review them for this study. The UAM-LC and possibly the UAM-AERO models would be appropriate for further investigation by the MMS for regulatory applications. The contacts for the models and documentation are:

UAM-LC and UAM-AERO
Henry Hogo
South Coast Air Quality Management District
(909) 396-3184
hhogo@aqmd.gov

SAQM-AERO
Nahzat Motallebi
California Air Resources Board
(916) 324-1744

In addition, SAI is planning to release an aerosol version of UAM-V in the summer of 1998.

Table 2-3 contains a summary of the ratings for the five models. The models split into two groups: (1) UAM-IV and SAQM, and (2) CALGRID, CAMx, and UAM-V. UAM-IV scores low because of its technical shortcomings: it no longer is state of the art and it is not particularly suited for MMS applications. (However, its derivative, UAM-LC, may be of interest.) SAQM is considered to be a state-of-the-art model, but its relative difficulty in use, slow run time, and a few technical shortcomings make it score lower compared to its peers.

At first glance, UAM-V appears to have done better than CAMx and CALGRID, and CALGRID appears to be rated on a par with CAMx. However, these results are due to the nature of the scoring system. In fact, CAMx and UAM-V are more nearly identical in their overall usefulness and both are somewhat technically superior to CALGRID, because of their support of two-way nesting, plume-in-grid, source apportionment, and process analysis. However, the importance and need for technical superiority clearly depends on the application. The scoring system causes CAMx to get a lower relative rating mainly because the model has not been extensively reviewed and lacks a comprehensive user's guide and pre-and post-processing software; all are typical for a new model.

The three models scored almost identically in the Computation Requirements category, but it is important to note that CALGRID runs slower than UAM-V and CAMx. We emphasize that we were unable to

determine the degree to which the source-apportionment methodology increases CPU requirements for CAMx or UAM-V.

CAMx was penalized relative to UAM-V in the Ease of Use category for the following three reasons. (1) It does not contain the voluminous run-time diagnostics option that UAM-V provides. (2) It does not have its own pre- and post-processing system so that one must acquire the UAM-V system and documentation even if using CAMx. (3) Its documentation, although good, is not as comprehensive as that of UAM-V, since it contains no information at all on the procedures or data formats for the pre- and post-processing activities. On the other hand, the CAMx documentation contains information regarding its source apportionment methods, whereas the UAM-V documentation in that area has not yet been released and is not as complete. We think the lack of discussions of data formats and preparation outweighs the inclusion of a discussion of source apportionment methods. CAMx was also penalized relative to CALGRID because CALGRID's meteorological processor CALMET has a very good GUI, which might be important for inexperienced users.

CAMx scored slightly lower than UAM-V in the Science and Credibility category because it has a shorter and less thorough evaluation history. However, the evaluations that have been done to date have shown little difference in technical characteristics and performance between the two models. The actual difference between the two models may be small or nonexistent, since the CAMx developers also participated in the original design of UAM-V. In the scoring system, CALGRID's longer and broader evaluation history offset its shortcomings in regard to nesting, source apportionment, and plume-in-grid treatments compared to CAMx.

In summary, we recommend that the MMS acquire CAMx and UAM-V. Both are state-of-the-art models. CAMx is in the public domain. The UAM-V code is freely available but its use is restricted. However, since the MMS is a government agency, a special licensing agreement concerning the use of the model is not necessary, as long as code modifications are not involved. Both models require, as does any photochemical modeling exercise, major time and effort to acquire and develop input data, except in the trivial case of applying the test case. The usefulness of UAM-V will be enhanced if the MMS negotiates additional licensing agreements with SAI to allow source code changes and model access to meet MMS's special needs, particularly in the areas of process analysis and source apportionment. Whether the available documentation and support are sufficient to make those components useful and understandable is also important. Despite its shorter regulatory track record, CAMx also is worthy of acquisition. Its source apportionment code at this point appears to be more accessible and user friendly than that of UAM-V.

We also recommend the acquisition of the CALMET/CALGRID/CALPUFF modeling system (see Section 3 concerning CALPUFF). CALGRID's lack of two-way nesting, plume-in-grid, aerosol, and source apportionment capabilities render it less powerful than UAM-V and CAMx. However, the system is very easy to use and produces credible results for regional ozone and puff applications. The CALMET meteorological processor, when used with observed data only, is much easier to apply than the prognostic models that are necessary to create inputs for UAM-V and CAMx, and still yields good performance over water and near land/water boundaries.

Finally, we also recommend that if the MMS is interested in particulate modeling, then the UAM-LC and UAM-AERO models, and perhaps the aerosol version of UAM-V when it becomes available, should be further investigated and acquired, if necessary.

Table 2-3. Ratings for the (a) Science and Credibility, (b) Ease of Use, and (c) Computational Requirements Categories for Five Photochemical Grid Models. Note That the Ratings for (a) and (b) Have a Weight That is Twice That for the Ratings for (c). Each Individual Rating Can be Between 1 and 3, and is not Adjusted According to the Weight in the Table. See Section 1 for a Description of Evaluation Methodology and Criteria.

	UAM-IV	SAQM	CALGRID	UAM-V	CAMx
Tech & Gen	1	1.5	1.5	2	2
Grid Options	1	2	2	3	3
Qual of Phys	1	2	3	3	3
Sparse Data	1.5	2.5	2.5	2.5	2.5
Overwater	1	2.5	2.5	2.5	2.5
Model Eval	3	3	3	3	2
S & C Score	17	27	29	32	30
User Guide	3	2	2	3	1.5
Options	2	2	3	3	3
Data Prep	2	1	2	2	2
Data Acq	1	1	1	1	1
GUI	1	1	2	1	1
Run Diag	2	2	2	3	2
Post Diag	2	2	2	3	2
Ease Score	26	22	28	32	25
Mult Source	2	2	2	3	3
UNIX/PC	3	1	3	3	3
Run Time	2	1	2	3	3
Code flex	2	1	3	2	3
Comp Score	9	5	10	11	12
Overall Score	52	54	67	75	67
Percent Score	57.8	60.0	74.4	83.3	74.4

3 LAGRANGIAN TRAJECTORY MODELS

3.1 INTRODUCTION

Lagrangian trajectory (puff) models are used to model instantaneous and short-duration emission sources, or when temporal and spatial variations in meteorological fields are important. With adequate configuration, the models are also appropriate for long-term (e.g., seasonal and annual) simulations. Depending on the formulation and physical processes treated, the model spatial scales can be from tens of meters (local-scale) up to several hundred kilometers (meso-scale). In this section, we reviewed the following five Lagrangian puff models:

- CALPUFF
- HYSPLIT_4
- INPUFF
- MESOPUFF II
- SLAM

The above models represent a larger degree of variation in terms of the formulation, physical processes treated, input data requirements, intended applications, and the design concept than do the models reviewed in Sections 2 (Eulerian regional-scale dispersion models) and 4 (toxic release models) where they are more similar.

We stress that there are many puff models that have been developed, and that our review is not intended to be comprehensive because of budget constraints. The above five models were selected as "representative." Our omission of a model does not imply that the model is inferior or less desirable in any way.

The review of each model is presented in Sections 3.2 through 3.6. Refer to Section 1 for a description of the evaluation methodology. A summary and our recommendations are given in Section 3.7.

3.2 CALPUFF

Model Name: CALPUFF, Version 5.0	
Person of Contact:	
	Joseph S. Scire Earth Tech, Inc. 196 Baker Avenue Concord, MA 01742 Tel (978) 371-4270 Fax (978) 371-2460 E-mail jss@src.com
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	***Score: 3***
	CALPUFF (Scire et al., 1998) is a multi-layer, multi-species non-steady-state puff dispersion model that simulates the effects of time- and space-varying meteorological conditions on pollutant transport, transformation, and removal. It produces predictions of ambient pollutant concentrations, wet deposition fluxes, dry deposition fluxes, and visibility effects such as extinction coefficients. CALPUFF is intended for use on scales from tens of meters from a source to hundreds of kilometers. It includes algorithms for near-field effects such as building downwash, transitional buoyant and momentum plume rise, partial plume penetration, subgrid scale terrain and coastal interaction effects, and terrain impingement. It also treats longer range effects such as pollutant removal due to wet scavenging and dry deposition, chemical transformation, vertical wind shear, overwater transport, plume fumigation, and visibility effects due to particulate matter. CALPUFF contains a set of computationally efficient puff sampling algorithms that makes its use for simulating long time periods (one or more years) computationally practical. The model can be run in a mode to reproduce the results of straight-line regulatory models such as ISCST3 in steady-state conditions, but CALPUFF offers the advantage of accounting for non-steady-state effects when they exist. CALPUFF includes parameterized gas phase chemical transformation of SO_2, SO_4, NO, NO_2, HNO_3, NO_3, and organic aerosols. A model for aqueous phase chemical transformation of SO_2 to SO_4 is included. CALPUFF can treat primary pollutants such as PM_{10}, toxic pollutants, ammonia, and other pollutants. The model includes a resistance-based dry deposition model for both gaseous pollutants and particulate matter. Wet deposition is treated using a scavenging coefficient approach.	

	The model has detailed parameterizations of complex terrain effects, including terrain impingement, side-wall scrapping, and steep-walled terrain influences on lateral plume growth. A gridded field of terrain elevations is used to determine multiple hill effects on plume transport and dispersion. A subgrid-scale complex terrain module based on a dividing streamline concept divides the flow into a lift component traveling over the subgrid-scale feature and a wrap component traveling around the feature. Plume dispersion can be treated using turbulence-based dispersion curves. Measured values of turbulence can be used in the model, or estimated values of turbulence will be produced by the model based on similarity theory. There is also an option to use ISCST3 (Pasquill-Gifford for rural areas or McElroy-Pooler for urban areas) dispersion coefficients. The gridded meteorological fields used by CALPUFF are produced by the CALMET meteorological model. CALMET includes a diagnostic wind field model containing objective analysis and a divergence minimization procedure. Effects such as slope flows, valley flows, terrain blocking, and lake and sea breeze circulations are treated. An energy-balance scheme is used to compute sensible and latent heat fluxes and turbulence parameters over land surfaces. A profile method is used over water. CALMET contains interfaces to prognostic meteorological models such as Versions 4 and 5 of the Penn State/NCAR Mesoscale Model (MM4 and MM5). Many pre-processor programs are available with the CALPUFF modeling system that allow standard meteorological, terrain, and land use data bases to be used directly by the models. Postprocessing programs (PRTMET and CALPOST) provide options for analysis and display of the modeling results. A set of PC-based graphical user interface (GUI) programs can be used to define the model control files.	
A2. Grid Options for Eulerian and Trajectory Models		***Score: 2.5***
	CALPUFF has an arbitrary vertical structure defined by the user. The number of horizontal grid cells is also specified by the user. The domain must be rectangular in shape (i.e., NX × NY cells), and each grid cell is the same length in the x and y directions. There are no limits on the number of vertical layers or horizontal grid cells imposed by the model. The maximum array dimensions are set by the user in PARAMETER statements, so they are limited only by the amount of computer memory available. CALPUFF has three grid systems: a meteorological grid defining the domain on which the winds and other meteorological variables are defined; a computational grid defining the domain on which transport and dispersion of pollutants are tracked; and a sampling grid specifying the network of gridded receptors. The sampling grid can be nested within the computational grid using a user-specified nesting factor. The model also accepts randomly-spaced receptors.	

A3. Quality and Physical Processes Simulated		*Score: 3*
	As described in Section A1, CALPUFF includes many state-of-the-art algorithms to treat different physical processes. These processes also provide the user with great flexibility. For example, CALPUFF contains options to treat dispersion on different levels of sophistication depending on the data available. The highest level is to use observed turbulence measurements of σ_v and σ_w (or σ_θ and σ_φ) to compute σ_y and σ_z. Other options include the use of similarity theory to estimate σ_v and σ_w as a function of height based on gridded surface heat and momentum fluxes derived from CALMET. The third option is to use the regulatory Pasquill-Gifford (PG) dispersion coefficients (rural areas) or McElroy-Pooler dispersion coefficients (urban areas). Vertical wind shear can sometimes be important for plume transport and dispersion. CALPUFF explicitly models wind shear effects on different puffs by independently advecting each individual puff by its local average wind speed and direction. Moreover, CALPUFF optionally allows a single well-mixed puff to split into two or more pieces when across-puff shear becomes important. A single puff may be split multiple times if it remains in the model domain long enough. The user can control the frequency at which a puff is split. Unlike models such as HYSPLIT_4 and SLAM, CALPUFF also treats many subgrid-scale effects such as terrain, building downwash, and the land-sea interface.	
A4. Sparse Data Treatment		*Score: 2.5*
	CALPUFF and CALMET accept a hierarchy of different data sets as inputs, depending on data availability. The simplest, minimum data requirements are the same as the ISCST3 model. That is, single-station data are sufficient. More sophisticated inputs include the use of surface, upper air, precipitation, and overwater data from multiple meteorological stations. Since CALMET can take the outputs from the prognostic MM4 or MM5 models as inputs, the effects of lack of data over water are reduced. The approach of using prognostic model outputs is technically sound. However, the lack of observed data has so far made a comprehensive assessment difficult of CALMET's performance over areas of sparse data. Furthermore, it is still possible that the lack of observed data may lead to diminished model performance because of difficulties in assigning boundary and initial conditions and providing data for nudging for prognostic models.	
A5. Overwater Dispersion		*Score: 2.5*
	The overwater boundary layer methods in CALMET are the same as those used in the OCD model. Effects such as plume fumigation and the thermal internal boundary layer (TIBL) are treated in the model. For the Lake Michigan and New England areas, CALGRID produced realistic ozone concentrations over water and near the land/water interface with meteorological fields prepared by CALMET. This good performance is likely due to its high vertical resolution	

	near the ground and CALMET's good handling of overwater meteorological conditions. CALMET uses a different set of equations to calculate mixing height and surface layer micrometeorological parameters over water as opposed to over land. The user's manual has omitted some of these equations and some appear to be different in the code from what appears in the manual. The mixing height equation in the manual is based on neutral barotropic scaling, which is adequate for mid-latitude open ocean purposes as suggested by Garratt (1995). CALMET has a mixing height advection algorithm that can transport mixing heights from coastal areas into the near-shore area. Prognostic model outputs can be introduced into the model as "pseudo buoy data" if necessary.	
A6. Model Evaluation History		***Score: 2.5***
	CALPUFF has been evaluated with the Kincaid and Lovett data sets (Strimaitis et al., 1998), the CAPTEX tracer data set (Scire et al., 1995b), and by Irwin (1997). A coastal dispersion model evaluation, sponsored jointly by Jersey Central Power & Light and the California Energy Commission, is currently in progress by the model developers.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 3***
	A comprehensive set of user's guides is available for the model. The CALMET user's guide (Scire et al., 1995a) describes the technical basis for the meteorological model and provides user's instructions for the meteorological model as well as a set of preprocessing and postprocessing programs for CALMET. The CALPUFF user's guide (Scire et al., 1998) describes the technical formulation of the dispersion model and provides user instructions for the model and its postprocessing programs. Regular training courses are offered by the model developers to help users learn the modeling system. A course notebook with case study example problems and data sets is provided in the course.	
B2. Model Options		***Score: 3***
	The main model options are for overwater transport and dispersion, buoyant and momentum plume rise, partial plume penetration, subgrid scale terrain and coastal interaction effects, terrain impingement, dry deposition, wet removal, chemical transformation, plume fumigation, building downwash, and vertical puff splitting. See Section A1 for more details.	
B3. Data Preparation Time		***Score: 2.5***
	The time required to prepare a CALPUFF simulation varies depending upon the model options selected. In its ISCST3 mode where gridded meteorological fields are not required, CALPUFF requires about the same level of effort as a simple steady-state model. If CALMET is used to create three-dimension wind fields, about a week of data preparation effort is normally required. This	

	depends on the number of meteorological stations to be included in the simulation, and the quality of the data sets. However, many pre-processor programs are available with the CALPUFF modeling system that allow the user to process standard meteorological, terrain, and land use data bases.	
B4. Ease of Data Acquisition		***Score: 3***
	CALMET and CALPUFF are designed to use standard terrain and land use data sets available from the U.S. Geological Survey (USGS), meteorological data sets available from the National Climatic Data Center (NCDC), and optional MM4 data using the EPA MM4 CD-ROM data base (available from NTIS). Special non-routine data sets can also be used by the modeling system, as long as they are properly reformatted.	
B5. Model Interface to Preprocessors / GUI		***Score: 3***
	The CALMET meteorological preprocessor is a state-of-the-art diagnostic model that generates mass-consistent wind fields. CALMET treats phenomena such as slope flows, valley flows, terrain blocking, and lake and sea breeze circulations. The wind fields generated by CALMET have been successfully used to study transport and dispersion up to several hundred kilometers. CALMET has an option of using the results from a prognostic meteorological model. Winds derived from the prognostic model can be introduced as the initial guess field, the Step 1 field, or simply as observations. The modeling system comes with the graphical user interface (GUI) programs for the main components of the model (CALMET, CALPUFF, and CALPOST). Through the GUI programs, the user can prepare, execute, and analyze a model run. Comprehensive on-line help system is available, so that the user rarely has to consult to written documentation. A full package of preprocessors provides all the software needed to interface the programs to the standard geophysical, meteorological, and overwater data bases available from the federal government. Note that the GUI programs are an integral component for the CALMET/CALPUFF/CALPUFF modeling system. When the model codes are changed, the GUI programs are also changed. This is because model enhancements often lead to additional input requirements. It is crucial that consistent versions of the models, control files, and GUIs are always used. If the control files for earlier versions of the models were used, the current version of the GUIs will warn the user about the deficiency in the control files and prompt the user to enter the additional information required.	
B6. Run-Time Diagnostics		***Score: 3***
	The CALPUFF model and its CALMET processor have diagnostic checks within the FORTRAN code to identify inconsistent model options or parameter selections. The GUI programs also perform extensive checking of model inputs.	

B7. Post-Run Diagnostics		***Score: 2.5***
	The CALPOST module processes the output form CALPUFF, producing tables of pollutant concentrations, wet deposition fluxes, dry deposition fluxes, threshold exceedances, and extinction coefficients for visibility applications. The user configures the analysis period, averaging time(s), and processing options. The PRTMET module extracts and displays fields produced by CALMET. These modules provide options to create plot files that are easily interfaced to commercially-available plotting software such as SURFER. The model output can be displayed as vector plots (for winds), contour plots (most other scalar fields), or tile plots (e.g., land use).	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 2.5***
	The model can treat an unlimited number of point, area, volume, and line sources. The source array dimensions are specified by the user in the model PARAMETER files. The point, area, and line sources can be buoyant or non-buoyant. Volume sources are assumed to be non-buoyant. All source types allow arbitrarily time-varying emission parameters. CALPUFF does not directly treat source attribution. Separate model runs and additional post-processing are necessary if the user wants to investigate the impacts due to certain sources.	
C2. UNIX / PC Portability		***Score: 3***
	The models and the processor programs, developed in FORTRAN, can be run on PC or Unix platforms. The GUIs are PC-based only.	
C3. Run Time		***Score: 2.5***
	The model run time varies considerably depending on the model application. A full year simulation with a few sources in ISCST3 mode requires less than five minutes on a Pentium-II PC. However, a full three-dimensional modeling with CALMET and CALPUFF on large domains with hundreds or thousands of sources may require several days of computer time.	
C4. Code Flexibility and Readability		***Score: 3***
	The code has extensive internal documentation and comments. It is designed to be flexible and modular.	
D. Cost (Non-Ranking)		
	An earlier version of the code is freely available for download from EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/). The latest version of the code, with many technical enhancements, is also available at no or low cost from the model developers. Note that since model enhancements often require	

	additional inputs, as a result, the control files and GUIs for later versions of CALPUFF/CALMET are not fully backward compatible. See Section B5 for more details.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	The FORTRAN source code is available for CALMET, CALPUFF, CALPOST, and the major processor programs. The user can make code changes if necessary. Copyright restrictions exist against redistribution of the code by third parties.	
F. Language for Model and GUI (Non-Ranking)		
	CALPUFF, CALMET, and all processor programs are written in FORTRAN 77. The GUI programs are developed in Visual Basic.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**17**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**91.7**

3.3 HYSPLIT_4

Model Name: HYSPLIT_4 (Hybrid Single-Particle Lagrangian Integrated Trajectory, Version 4)	
Person of Contact:	
	Dr. Roland Draxler Air Resources Laboratory National Oceanic and Atmospheric Administration 1315 East West Highway Silver Spring, MD 20910 Tel (301) 713-0295 Fax (301) 713-0119 E-mail roland.draxler@noaa.gov
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	***Score: 2.5***
	The HYSPLIT_4 model (Draxler and Hess, 1997) is a modeling system for computing simple trajectories to complex dispersion and deposition simulations using either puff or particle approaches. The model was originally developed by NOAA's Air Resources Laboratory, with recent contributions from Australia's Bureau of Meteorology. The model consists of a modular library structure for each process. There are separate main programs for each application. The generic version of HYSPLIT_4 has one model that calculates concentration and deposition/settling, and one model that calculates trajectories. Multiple pollutant species may be defined from the same emission source, where each species may behave differently for deposition calculations. Customized versions of HYSPLIT_4 have been developed to handle gridded area source emissions and nonlinear sulfur chemistry. (The generic version includes linear chemistry in the form of a pollutant decay rate.) The model accepts gridded meteorological inputs from various numerical models, such as the RAMS (Regional Atmospheric Modeling System) model and NCEP's (National Centers for Environmental Prediction) ETA model. HYSPLIT_4 supports multiple nested meteorological grids. Calculations can start on a high resolution grid and then switch to a coarser resolution when the pollutant expands beyond the domain of the fine grid. Meteorological grids can be defined at different temporal and spatial resolutions. Concentration grids have similar flexibility (see Section A2). Pollutant dispersion is calculated by assuming either a Gaussian or Top-Hat	

	(i.e., uniform distribution within a certain range and zero outside the range) horizontal distribution within a puff or from the dispersal of a fixed number of particles. In the puff model, puffs expand until they exceed the size of a meteorological grid cell (either horizontally or vertically) and then split into several new puffs, each with its share of the pollutant mass. In the particle model, a fixed number of initial particles are advected about the model domain by the wind field. However, a disadvantage is that at longer time periods too few particles can be left in a grid cell to adequately define the pollutant concentration. An alternative approach combines both puff and particle methods by assuming a puff distribution in the horizontal direction and particle dispersion in the vertical direction. This leads to a greater accuracy of the vertical dispersion parameterization of the particle model, combined with the advantage of having an expanding number of puffs represent the pollutant distribution as the spatial coverage of the pollutant increases. The model does not treat near-field effects such as building downwash and plume rise. HYSPLIT_4 does not handle terrain directly. All terrain effects are parameterized in meteorological models. HYSPLIT_4 has been previously applied to calculate seasonal and annual concentrations. As a result, the model is appropriate for EIS (environmental impact study). One unique feature for HYSPLIT_4 is that anyone can perform calculations on-line to predict the impacts due to a certain episode through ARL's READY web site at http://www.arl.noaa.gov/ready.html. Once connected to the web site, the user selects a meteorological data set (forecast or archived); and defines other modeling information such as the source location, the simulation start time, the run duration, the averaging period, and the concentration grid. HYSPLIT_4 will then be executed at ARL's server, and the user can directly view the trajectory and the time series of concentration contours via a web browser. All data processing steps are transparent to the user. The above feature makes HYSPLIT_4 appropriate for an emergency response program, since the model can project the concentration and trajectory of a release up to 48 hours with forecast meteorological data.	
A2. Grid Options for Eulerian and Trajectory Models		***Score: 3***
	HYSPLIT_4 considers two types of grids: • *The meteorological grid* is dictated by the type of gridded meteorological input data used and requires no user intervention. • *The concentration grid* is defined by the user in the model control file. The user may define multiple or nested concentration grids. Depending on the concentration grids selected, the model internally decides the optimal integration time step. The concentration grids are expressed in latitudes and longitudes. Each grid may have different sampling start/stop times and concentration averaging time. The averaging time can be as short as a few minutes.	

A3. Quality of Physical Processes Simulated		*Score: 3*
	The quality of various physical processes treated by HYSPLIT_4 appears to be state-of-the-art. The advection algorithms have been updated to include temporal interpolation. There are two options to estimate the boundary layer stability: one based on the calculated heat and momentum fluxes, and the other one based on the temperature and wind gradients. A three-dimensional particle dispersion routine has been added that computes air concentrations from the dispersion of an initial fixed number of particles. Dispersion and deposition can be calculated using either puff or particle approaches. Pollutant vertical mixing is assumed to follow the mixing coefficients for heat, which in turn are based on recent boundary layer theories. Puff and particle dispersion equations are formulated in terms of the turbulent velocity components and the Lagrangian time scales, which is state-of-the-art. The model treats three types of removal mechanisms: dry deposition, wet removal, and radioactive decay. Dry deposition is either explicitly defined as a deposition velocity, or for particles it may be computed as being the equivalent to the gravitational settling velocity; or it may be computed using the resistance method. Wet removal consists of two processes, one in which the polluted air is continuously ingested into a cloud from a polluted boundary layer, and the other one in which rain falls through a polluted layer. The model also treats pollutant resuspension in case the winds are sufficiently strong and the deposited pollutants are not bound to the surface.	
A4. Sparse Data Treatment		*Score: 2.5*
	HYSPLIT_4 requires gridded meteorological data prepared by models such as RAMS and ETA. The effects of lack of data over water are minimized because these prognostic meteorological models rely on physical equations, rather than data interpolation, to produce three-dimensional fields. However, the lack of observed data may still lead to diminished model performance because of difficulties in assigning boundary and initial conditions and providing data for nudging. The ETA model uses data from many different sources, such as geostationary satellites, where data availability is the same for both over land and over water. Sophisticated initialization methods also further reduce reliance on observed data. At present, the highest spatial resolution for the ETA model is 40 km, and RAMS can be run with a grid resolution on the order of a few kilometers.	
A5. Overwater Dispersion		*Score: 1.5*
	There are no special algorithms in the model to deal with overwater dispersion. The effects of overwater dispersion would have been treated in the meteorological models that provide inputs to HYSPLIT_4. As a result, more detailed (subgrid-scale) phenomena such as the Thermal Internal Boundary Layer (TIBL) and plume fumigation are not likely to be properly treated.	
A6. Model Evaluation History		*Score: 3*

	The model has been evaluated against various inert tracer experiments, including CAPTEX (Cross Appalachian Tracer Experiment; Ferber et al., 1986), ANATEX (Across North America Tracer Experiment; Draxler et al., 1991), and ETEX (European Tracer Experiment (Hess et al., 1997). The model was also used to simulate the Chernobyl accident that occurred in the former USSR (ATMES,1992).	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 3***
	The latest technical descriptions of the model can be found in Draxler and Hess (1997). Draxler (1992) provides user's instructions for version 3 of the model. A draft 1998 user's guide, in the Adobe PDF format, for version 4 of the model is distributed with the HYSPLIT_4 package, available from the Internet at http://www.arl.noaa.gov/ss/models/hysplit.html. The first document is also available from the same web site in the Adobe PDF format. The technical documentation includes detailed descriptions of various algorithms such as advection, dispersion, deposition, and meteorological data fields. The two user's guides provide detailed descriptions of various input data files, including necessary steps to run the test cases.	
B2. Model Options		***Score: 2***
	The generic HYSPLIT_4 system has two major models, one for concentration and deposition, and one for trajectories. Model options are specified in the corresponding control files. Major options for the concentration model include: the simulation start time, pollutant starting locations, the total run time, the vertical motion calculation method (i.e., the vertical coordinates of choice), the top of the model domain, meteorological input data grids, the pollutant emission rate, concentration grids, deposition parameters, the pollutant half-time, and the pollutant resuspension rate. The trajectory model has fewer model options, since information regarding the pollutant (except for starting locations) and concentration grids is not required. The options for the concentration model can be further modified according to the settings in the *NAMELIST* file, where code recompilation is not necessary. For example, the user can decide (1) if the model is configured as a puff or particle model, (2) the maximum age that any puff or particle is permitted to attain, (3) the maximum number of puffs or particles permitted during a simulation, and (4) the number of hours between emission cycles. Code recompilation is usually necessary for any non-typical applications of HYSPLIT_4. For example, a library routine to treat gridded area source emissions is included in the package but not activated. If that routine is to be used, then the user needs to modify and recompile the code.	
B3. Data Preparation Time		***Score: 3***

	Meteorological fields accepted by HYSPLIT_4 either have already been gridded, such as outputs from a meteorological model, or are prepared by the user himself. The first option is more typical (see Section B4 for more details), in which case all the user has to do is to convert the model outputs to the HYSPLIT format. There are some example conversion programs available to convert data from NOAA or ECMWF (European Center for Medium Range Forecast) sources. Note that NOAA, ECMWF, and HYSPLIT data files are all compressed in WMO's (World Meteorological Organization) GRIB (Gridded Binary) format. GRIB is highly efficient in packing binary information while retaining a relatively high degree of accuracy. A typical compression ratio for binary data is 4:1. A GRIB data file is platform-independent; however, platform-specific I/O library routines are required. These I/O routines are available at various sites, such ftp://ncardata.ucar.edu/libraries/grib at NCAR (National Center for Atmospheric Research).	
B4. Ease of Data Acquisition		***Score: 3***
	As mentioned previously, HYSPLIT_4 requires gridded input data from various meteorological models. NCEP runs a series of computer analyses and forecasts operationally. Gridded NCEP meteorological data archives include MRF (Medium Range Forecast, for 1991-1996), NGM (Nested Grid Model, for 1991-1997), and EDAS (ETA Data Assimilation System, since 1997). These data are available from the Climate Services Branch of the National Climatic Data Center (NCDC, http://www.ncdc.noaa.gov), or directly from ARL for recent months. The cost for obtaining archived model outputs from NCDC is roughly $210 for two months of MRF data, or six months of NGM data. ARL also archives recent (since 1997) gridded outputs from RAMS (Regional Atmospheric Modeling System). HYSPLIT_4 can be further customized to treat gridded area source emissions. If there are gridded emissions files already prepared for photochemical models such as CALGRID (Section 2. 2), CAMx (Section 2.3), and UAM-V (Section 2.6), then these files can be simply reformatted for use in HYSPLIT_4.	
B5. Model Interface to Preprocessors / GUI		***Score: 2.5***
	HYSPLIT_4 has a graphical user interface (GUI) program that performs the following tasks: (1) set up the model control file, (2) run the model, (3) invoke the plotting program to draw concentration contours and trajectories, and (4) convert compressed binary output to ASCII. Due to HYSPLIT_4's simple control file structure, Task (1) of the GUI has only two screens. On-line help is also available from the GUI. The GUI program runs on both the PC and UNIX environments (see Section C2).	
B6. Run-Time Diagnostics		***Score: 3***
	HYSPLIT_4 includes many diagnostics in the code to trap potential run-time errors.	

B7. Post-Run Diagnostics		***Score: 2***
	HYSPLIT_4 comes with graphical software that displays the results (e.g., pollutant trajectories and concentration contours for each averaging period) once the model simulation is completed. HYSPLIT_4 also writes gridded concentrations to a separate file for each averaging period. The user needs to develop his own software to conduct further analysis.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 2***
	The generic version of HYSPLIT_4 can simulate multiple point sources from different locations *but with the same emission rate*. Code recompilation is necessary if different emission rates are to be specified for each point source. HYSPLIT_4 comes with a library routine to treat gridded area source emissions, which have direct relevance to MMS' EIS applications. All that the user has to do in order to use that feature is to "uncomment" the CALL statement and recompile the code.	
C2. UNIX / PC Portability		***Score: 3***
	The computational portion of the HYSPLIT_4 code is written in FORTRAN, and thus can be freely ported between the PC and UNIX environments. More importantly, HYSPLIT_4's graphical user interface (GUI) program, developed with the Tcl scripting language and Tk tool box (Tcl/Tk), can also run on the PC (i.e., Windows 95 and NT) and UNIX environments. Tcl/Tk is in the public domain and is freely available. It is automatically loaded when the GUI program for HYSPLIT_4 is installed. Complete package and other technical information for Tcl/Tk can be downloaded from http://www.scriptics.com.	
C3. Run Time		***Score: 2.5***
	The model run time mainly depends on the concentration grids, the number of sources, and the integration time period. For a 41×61×1 (in x, y, and z direction, respectively) grid, HYSPLIT_4 took less than 30 seconds on a Pentium-II 300MHz PC to simulate one source for 48 hours.	
C4. Code Flexibility and Readability		***Score: 3***
	The HYSPLIT_4 code is quite flexible and modular, since the model has been extended and applied to scenarios such as radiological calculations, volcanic ash, gridded area source emissions, and sulfur chemistry. Most of the array limits and other parameters that affect model's memory allocation are specified in the *DEFSIZE.INC* INCLUDE file. If necessary, the user can easily modify some parameters and recompile the code.	
D. Cost (Non-Ranking)		

	The HYSPLIT_4 modeling system is in the public domain, and is available (see below) free of charge.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	The PC version (requires Windows 95 or NT) of HYSPLIT_4 is available from ARL's web site at http://www.arl.noaa.gov/ss/models/hysplit.html. The package includes the executable code, the graphical user interface, documentation, a test case, and the source code for the post-processing graphical display programs. The model source code is not included in the package, but is available through special arrangement with the model developers. The complete UNIX version of HYSPLIT_4 is also available from the model developer. HYSPLIT_4 is in the public domain. Thus, the user can freely make changes to the code. The modular design of the system facilitates the development of different customized versions for different applications.	
F. Language for Model and GUI (Non-Ranking)		
	The HYSPLIT_4 model is written in FORTRAN 77. The post-processing graphical display routines require the use of the NCAR Graphics package, which is also in FORTRAN 77. The graphical user interface (GUI) is developed with the Tcl scripting language and the Tc tool box (Tcl/Tk), which are supported in many machine platforms, including PC and UNIX.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**17**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**85.0**

3.4 INPUFF

Model Name: INPUFF, Version 2.3

Person of Contact:

Dr. William B. Petersen
Environmental Protection Agency
MD-80
Research Triangle Park, NC 27711
Tel (919) 541-1376
E-mail petersen.william@epa.gov

A. Science and Credibility (Ranking)

A1. Technical and General Descriptions — ***Score: 2***

INPUFF (Petersen and Lavdas, 1986) is designed for episodic simulations of concentrations resulting from emissions from point sources. These sources may exhibit both time-variable and space-variable properties (i.e., moving point sources are simulated), and the wind field may vary in both time and space. Gaussian puffs are released, tracked, and sampled at high rates to resolve important variations in the emissions. Much of the flexibility of this model arises from the control allowed the modeler in configuring the source, dispersion, transport, and sampling parameters to match the needs of a particular simulation.

The INPUFF features include: multiple point sources; arbitrary variation of source data in time; optional 2-D wind speed and direction field (user-supplied); wind speed extrapolated to release height; stacktip downwash option; particle deposition and settling option; buoyancy induced dispersion option; choice of PG, turbulence-based, or user-supplied dispersion rates; transition to $t^{1/2}$ growth at large time (user-supplied σ_y); and choice of Briggs or user-supplied plume rise formulas.

On the other hand, INPUFF does not include: spatial variation in dispersion characteristics, treatment for source-induced effects (e.g. building downwash), treatment for area or line sources (volume sources are points with initial σ_y and σ_z), puff-splitting to simulate wind shear, chemical transformations, complex terrain adjustments other than the 2-D wind field option, and wet deposition. The model does not come with any pre-processor programs.

INPUFF is applicable to simulating "simple" source types possessing complex emissions characteristics, resolving concentrations of inert compounds on scales of tens of meters to several kilometers across substantially uniform terrain, when vertical wind shear in the atmospheric surface layer is weak.

A2. Grid Options for Eulerian and Trajectory Models		*Score: 1.5*
	The standard configuration allows up to 100 receptors, specified at discrete (x, y, z) locations. Wind speed and direction may, as an option, be specified on a single Cartesian grid. These wind data are supplied for a single layer in the vertical.	
A3. Quality of Physical Processes Simulated		*Score: 2*
	Puff tracking and sampling in INPUFF follows robust procedures. However, the model does not resolve the effects of wind shear, and does not include spatial changes in *all* meteorological variables used in the simulation. This limits the applicability of the model to relatively simple meteorological situations. INPUFF uses the standard PG curves as well as turbulence-based functions to calculate dispersion coefficients. This is consistent with the current practice. The model also allows the user-supplied dispersion option for special situations and an experienced modeler. No probability-density-function (PDF) option for dispersion in the convective boundary layer is offered. The model uses Briggs equations for simulating the rise from point sources where the vertical structure of the surface layer is prescribed by a single wind speed, stability class, and mixing height. This is an accepted practice. Highly buoyant releases that partially penetrate an elevated inversion are not treated. INPUFF uses the K-theory model of Rao (1982) to treat the mass depletion due to gravitational settling and deposition. This is strictly valid for σ_z growth laws that follow the $x^{1/2}$ form. For other forms, correction factors are typically applied to restore mass conservation. It appears that INPUFF does not provide these correction factors. Furthermore, the user needs to specify the deposition velocities.	
A4. Sparse Data Treatment		*Score: 1*
	Meteorological data are explicitly entered into the input (model control) file as domain averages, or into a 2-D wind field file. No preprocessor is provided. The modeler must somehow construct these data from other sources. This might be problematic for data-sparse areas.	
A5. Overwater Dispersion		*Score: 1*
	There is no explicit treatment for coastal environments. The overwater boundary layer must be simulated/measured by the modeler, and resulting wind and turbulence data provided to INPUFF. Winds may change spatially, but the mixing height and turbulence are characterized for the modeling region by single values at each time step, so the treatment of a coastal thermal internal boundary layer (TIBL) is precluded.	
A6. Model Evaluation History		*Score: n/a*

	Unknown	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 2.5***
	The user's guide (Petersen and Lavdas, 1986) for INPUFF provides an overview of model's technical features, lists the content and format of its input file, and provides a few examples. Because the input file is not self-documenting, this guide is essential when setting up a run, even for experienced modelers. Information on the optional input file (gridded wind field) and the optional output file is incomplete. An experienced modeler will not have a problem in using these options, but an example for each should be listed for less experienced users. Details for implementing user-supplied diffusion and plume rise algorithms are found in the sample subroutines provided. This is appropriate, as novice modelers will not attempt to use these options.	
B2. Model Options		***Score: 2***
	The following model options are configured within the input file by setting logical (True or False) or integer variables: - User-supplied 2-D wind field (T/F) - Binary concentration output file (T/F) - Dispersion option (1=PG curves; 2=Irwin curves; 3=user-specified, distance-dependent; 4=user-specified, time-dependent) - Debug option for puffs (T/F) - Debug option for intermediate data (T/F) - Stacktip downwash (T/F) - Buoyancy-induced dispersion (T/F) - Deposition and settling (T/F) - User-supplied plume rise module (T/F) - Puff combination (T/F) Proper selection requires careful editing of the input file, with the users guide close at hand.	
B3. Data Preparation Time		***Score: 1.5***
	Data preparation for long or complex runs can be tedious, because of the way the input file is structured. The meteorological data are placed within the source loop, so they must be repeated for each source in the simulation. If many sources or periods are simulated, the modeler may want to modify the code to streamline the way the meteorological data are read, or create preprocessing software to construct the INPUFF input file. Otherwise, the source and meteorological data needed are common to other dispersion model applications, and can be as simple as that used for typical plume models such as ISCST3, requiring a day or less preparation time.	

	If highly variable periods are simulated with specialized data, more time may be needed to properly sort out interrelationships between transport wind data and turbulence data. Complex land use patterns also require more care (and time) in constructing the simulation. A single dispersion regime is used for the entire region, making coastal simulations particularly tricky. Finally, when deposition is modeled, both the settling and deposition velocities must be provided for each source and each period. This may require the preparation of yet another preprocessor.	
B4. Ease of Data Acquisition		***Score: 2***
	Minimum data requirements for a simulation can be as simple as that used in standard plume modeling applications (e.g. ISCST3). Because no preprocessors are provided for characterizing either the sources or the dispersion meteorology, much is left to the user to design the simulation.	
B5. Model Interface to Preprocessors / GUI		***Score: n/a***
	INPUFF does not include preprocessors, or a GUI. (The BREEZE HAZ SUITE commercial software reviewed in Section 4.8 provides a GUI to INPUFF.)	
B6. Run-Time Diagnostics		***Score: 3***
	INPUFF performs many checks on the options selected and the data provided (e.g. source data), with detailed error-reporting to the list file. In addition, a debug mode is provided that lists much intermediate data to the list file for review.	
B7. Post-Run Diagnostics		***Score: 1.5***
	A plotting postprocessor is included in the INPUFF system. It allows the user to produce puff trajectory (and size) plots and concentration time series plots at specified receptors. However, the program is designed to run on a UNIVAC 1110 with the CALCOMP plotting software, which is obsolete (and of limited use) according to today's standards.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 2.5***
	INPUFF treats multiple point sources. Concentrations for all sources combined can be written to a binary file for each period, so that a postprocessor could be written to perform further averaging for multiple period analyses. The standard list file also reports the concentrations due to each source for each period simulated, as well as the total concentrations from all sources.	
C2. UNIX / PC Portability		***Score: 3***
	Portability is not an issue because INPUFF is based on standard FORTRAN,	

	with ASCII input/output files.	
C3. Run Time		***Score: 2***
	Because INPUFF uses the "snap-shot" sampling approach, many puffs are used to resolve the spatial and temporal cloud distribution from each source. Puff merging is employed to reduce the computational requirements of this method. However, the design of the model focused on detailed simulations of limited-duration episodes, so that optimizations for long-period simulations are not present. This might cause problems to applications such as the environmental impact study (EIS). The standard configuration allows up to 100 receptors, and no more than 144 meteorological periods. If the code were modified to accept more receptors and longer simulations, run-times may become substantial.	
C4. Code Flexibility and Readability		***Score: 2***
	The code is structured insofar as major functions are isolated as subroutines, and indenting is used to visually identify blocks of code. However, array sizes are numerically defined in each routine. Although not as modular as it might be, the code is small enough so that making changes to array sizes or implementing subroutine substitutions remains feasible.	
D. Cost (Non-Ranking)		
	The cost of obtaining INPUFF from NTIS is $50.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	INPUFF is available from NTIS, order number PB90-500752 (one disk and two documents). The NTIS numbers for the two documents are PB86-242468 and PB86-242450. The EPA publication number for the user's guide is EPA/600/8-86/024. There are no restrictions on its use.	
F. Language for Model and GUI (Non-Ranking)		
	INPUFF is written in FORTRAN 77.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**15**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**63.5**

3.5 MESOPUFF II

Model Name: MESOPUFF II, Version 5.1 (Mesoscale Puff Model)	
Person of Contact:	
	Joseph S. Scire Earth Tech, Inc. 196 Baker Avenue Concord, MA 01742 Tel (978) 371-4270 Fax (978) 371-2460 E-mail jss@src.com
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	***Score: 2***
	MESOPUFF II (Scire et al., 1984a and 1984b; USEPA, 1994a) is a regional-scale, Gaussian, variable-trajectory, puff superposition model designed to account for the spatial and temporal variations in transport, diffusion, chemical transformation and removal mechanisms. The model calculates concentrations of up to five pollutants (SO_2, SO_4, NO_x, HNO_3, and NO_3). With the puff superposition approach, a continuous plume is modeled as a series of discrete puffs, where each puff is independently transported. At travel distances up to 10 km, dispersion is calculated with the traditional PG (Pasquill-Gifford) curves that are functions of stability class and downwind distance. MESOPUFF II uses the virtual source approach to account for spatial variations of stability class. At travel distances greater than 10 km, the model switches to time-dependent puff growth equations that are functions of vertical diffusivity, K_z (also a function of stability class). MESOPUFF II uses a resistance model to account for dry deposition. The model has two options for treating the removal of pollutant from the puff. The first option assumes that material deposited is removed from the full depth of the puff (a single-layer model). The second option accounts for the effect of boundary layer mixing with a three-layer model. Wet deposition is treated using a scavenging coefficient approach. MESOPUFF II is one element of an integrated modeling system, which also includes meteorological pre-processors such as: • READ62: Extracts and processes upper air data in NCDC TD-6201 format. • PXTRACT: Extracts and processes precipitation data in NCDC TD-3240	

	format. • PMERGE: Reformats the precipitation data files created by PXTRACT to a form suitable to MESOPUFF II. • MESOPAC II: Develops gridded fields of interpolated winds, mixing heights, surface friction velocities, and Monin-Obukhov lengths required by MESOPUFF II. The concentration, dry deposition, and wet deposition files generated by MESOPUFF II can be further processed with the MESOFILE II post-processor. The model is optimized for mesoscale (> 50 km) transport. As a result, it does not treat near-field effects such as building downwash, transitional plume rise, or partial plume penetration. MESOPUFF II does not treat terrain and visibility effects. MESOPUFF II has been approved for regulatory applications by the EPA and other government agencies. For example, MESOPUFF II is listed as one of the "Appendix B" models (alternative air quality models) in EPA's *Guideline for Air Quality Models* (USEPA, 1986a). The model was recommended by IWAQM (Interagency Workgroup on Air Quality Modeling) to estimate air quality impacts associated with prevention of significant deterioration (PSD) due to sources farther than 50 km from a Class I area (USEPA, 1993b and 1995a). PSD applications typically involve multi-year model simulations. The IWAQM members include the EPA. U.S. Forest Service, National Park Service, and U.S. Fish and Wildlife Service. The code, although having achieved regulatory status, is to be superseded by the CALPUFF model also reviewed in this study (see Section 3.2).	
A2. Grid Options for Eulerian and Trajectory Models		***Score: 2***
	A Cartesian coordinate system in the horizontal is employed in MESOPUFF II and MESOPAC II. Three grid systems are used by MESOPUFF II: a meteorological grid, a computational grid, and a sampling grid. The maximum size for grids is easily set with PARAMETER statements. Discrete receptors are also supported. MESOPUFF II always uses two vertical layers, one within and one above the mixed layer.	
A3. Quality of Physical Processes Simulated		***Score: 2***
	As described in Section A1, MESOPUFF II treats deposition and chemistry. However, MESOPUFF II treats NO and NO_2 as a single species (NO_x). The dry deposition scheme in MESOPUFF is also simpler and more highly parameterized when compared to CALPUFF. MESOPUFF uses PG (Pasquill-Gifford) curves to calculate dispersion coefficients. It does not have an option to use more state-of-the-art, turbulence-based method. The model has limited vertical resolution with only two layers. The MESOPAC II meteorological pre-processor does not consider terrain effects. Refer to Section A1 for other limitations of the model.	

A4. Sparse Data Treatment		***Score: 1***
	MESOPUFF II might have problems in data-sparse areas. This is because the MESOPAC II meteorological processor mainly interpolates meteorological variables from discrete, available stations to the grid points.	
A5. Overwater Dispersion		***Score: 1***
	MESOPUFF II does not treat overwater dispersion.	
A6. Model Evaluation History		***Score: 3***
	Because of its regulatory status, MESOPUFF II has been extensively evaluated with field data (e.g., Scire et al., 1995b; Carhart et al., 1989; Godowitch, 1989; and USEPA, 1986b).	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 3***
	The original user's guide (Scire et al., 1984a) was recently updated and expanded (USEPA, 1994a). The new user's guide is comprehensive and of high quality. It clearly explains file formats and model parameters, lists sample files, and provides technical discussions for each module.	
B2. Model Options		***Score: 2.5***
	The model allows considerable flexibility in conducting simulations. Some of the technical model options include: the concentration averaging time, the minimum puff sampling rate, whether to use variable sampling rate that depends on wind speed, the option for the vertical concentration distribution (with reflection or fumigation), whether to consider chemical transformation / dry deposition / wet removal, whether to print intermediate puff data, the time interval at which intermediate puff data are printed, whether to save necessary data for restarting purpose, and whether to use user-specified dispersion coefficients / dry deposition parameters / wet removal parameters / chemical transformation parameters.	
B3. Data Preparation Time		***Score: 2.5***
	Once raw meteorological data are acquired (see next section), it will take a few days up to a week to process the data so that they can be used to run the model. Since the MESOPUFF II package already comes with many pre-processors, it is usually not necessary for the user to write additional programs.	
B4. Ease of Data Acquisition		***Score: 3***
	MESOPUFF II is designed to run with routine meteorological data that are readily available from the National Climatic Data Center (NCDC) at http://www.ncdc.noaa.gov. The required data include surface data (CD-144), upper air data (TD-6201), and precipitation data (TD-3240). The typical cost	

	for data would be several hundred dollars for about five years of data.	
B5. Model Interface to Preprocessors / GUI		***Score: 2.5***
	As described in Section A1, MESOPUFF II has a suite of pre-processors that help the user prepare input files. In particular, MESOPAC II is the meteorological pre-processor that computes time and space interpolated fields of meteorological variables required by MESOPUFF II. MESOPAC II constructs hourly gridded wind fields within two user-specified vertical layers: *a lower level wind field* representing the boundary layer flow, and *an upper level wind field* representing the flow above the boundary layer. The lower level winds are used to advect puffs within the mixed layer and to determine the plume rise of newly released puffs. The upper level winds are used to advect puffs above the boundary layer. The position of the puff center relative to the mixing height (which varies with time and space) determines which wind field is used to advect the puff. Considerable flexibility is allowed in choosing the most appropriate level or vertically-averaged layer for each wind field. The default is to use the winds averaged through the mixed layer for the lower level wind field, and the winds averaged from the top of the mixed layer through the 700 mb level for the upper level wind field. Spatial interpolation is done according to $1/R^2$, where R is the distance between the station and the grid point. MESOPUFF II does not have a graphical user interface (GUI) program.	
B6. Run-Time Diagnostics		***Score: 3***
	MESOPUFF II together with its processors have diagnostic checks to identify inconsistent model options and potential user errors. MESOPUFF II also optionally prints out intermediate puff data (puff height, σ_y, σ_z, location, transformation rate, deposition velocity, wet removal rate, etc.) for debugging.	
B7. Post-Run Diagnostics		***Score: 2***
	The model tabulates predicted concentrations and deposition fluxes. The MESOFILE II post-processor provides further file manipulation functions and calculates some statistics (e.g., averages, highest, second highest, etc.) for the modeling results. There are no provisions in MESOPUFF II to assist the user to visualize the results.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 2.5***
	MESOPUFF II handles multiple point (buoyant and non-buoyant) and area (non-buoyant only) sources. The model offers the capability to model the large number of stationary and mobile sources within an urban area as one or more area sources. It is assumed that the emission distribution can be adequately described as Gaussian. The user needs to specify initial sizes (σ_y and σ_z) and heights.	

C2. UNIX / PC Portability		*Score: 3*
	Since the complete modeling system is written in FORTRAN, it can be easily ported between the PC and UNIX platforms. Minor code changes are necessary for machine-specific FORTRAN utility functions and routines (e.g., the date and time routines).	
C3. Run Time		*Score: 2.5*
	MESOPUFF II should run faster than CALPUFF (see Section 3.2), since the model has only two vertical layers and fewer near-field simulation features.	
C4. Code Flexibility and Readability		*Score: 3*
	The MESOPUFF II code is quite flexible and modular with extensive internal documentation and comments.	
D. Cost (Non-Ranking)		
	The code, test case, and documentation for MESOPUFF II can be downloaded from EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/) at no cost.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	Since the code is in the public domain, it can be modified without restrictions.	
F. Language for Model and GUI (Non-Ranking)		
	MESOPUFF II together with all the processor programs are written in FORTRAN 77.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**17**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**77.8**

3.6 SLAM

Model Name: SLAM (Short-Range Layered Atmospheric Model)	
Person of Contact:	
	William L. Steorts, Jr. Applied Research and Systems Division ENSCO, Inc. 445 Pineda Court Melbourne, FL 32940 Tel (407) 254-4122 Fax (407) 254-3293 E-mail bills@fl.ensco.com
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	*Score: 2*
	SLAM (Short-Range Layered Atmospheric Model; ENSCO, 1997b) is a U.S. Air Force model that treats multiple sources, multi-layer splitting trajectory, time-varying transport layer depth, and Gaussian diffusion. The model accepts meteorological data from many sources, including conventional surface and upper air observations and gridded outputs from meteorological models (see Section B2 for more details). All meteorological data are managed by a "Local File Server" (e.g., an Oracle server) in a client-server environment. SLAM has a graphical user interface (GUI) program with many I/O functions that allow the user to prepare, execute, and analyze a model run. The technical aspects of SLAM are in many ways similar to the HYSPLIT_4 model also reviewed in this study. SLAM starts the calculations with a single trajectory. Trajectory splitting (with a redistribution of the pollutant mass into different transport layers) is controlled by the mixing depth that varies twice daily (i.e., day and night). SLAM treats multiple point sources. However, all sources have the same emission rate and stack height. Typical spatial and temporal scales for the model are 1000 km and a week, respectively. The model has not been tested with EIS-type (environmental impact study) applications with long time periods (e.g., ≥ one year) and hundreds of sources. Although there is nothing inherent to prevent the model from being applied to this type of application, practical memory, computation, and storage requirements may cause problems. Additional code customization is also required so that different emission attributes can be assigned to different sources.

	SLAM does not treat dry or wet deposition. Linear chemistry in the form of a half-life decay is included. The model can be interfaced to ORCHID, a photochemical model that includes CB-IV photochemistry. The model does not treat near-field effects such as plume rise and building downwash. SLAM is flexible in terms of its meteorological data inputs. Almost any combination of surface observations, upper observations, and numerical model analyses and forecasts are supported. For example, SLAM accepts wind fields generated by: • the Winds On Critical Streamline Surfaces (WOCSS) model, • the Higher Order Turbulence Model for Atmospheric Circulation (HOTMAC) model, • the Regional Atmospheric Modeling System (RAMS), • Navy Operational Global Atmospheric Prediction System (NOGAPS), • National Center for Atmospheric Research (NCAR) Re-Analysis Fields, • the Nested Grid Model (NGM), and • the Medium Range Forecast (MRF) model. Meteorological models do not have to run locally. SLAM mainly takes outputs generated by the models and reformats them for later use. Surface observations can be from conventional airport data and offshore observations such as buoys and CMAN (Coastal Marine Automated Network) stations, as long as they have been properly reformatted by the user. Observations typically have a larger weighting than gridded model outputs in spatial interpolation. It appears that the installation of SLAM is highly site-specific, as indicated by the high installation costs (see Section D). We also tried to obtain a copy of the SLAM code from Patrick Air Force Base, Florida. However, due to the great dependence of SLAM on other software and hardware infrastructure, a "self-contained" SLAM model could not be made available to us for review. As a result, our comments below were mainly based on reviews of the user's guide (ENSCO, 1997a) and technical documentation (ENSCO, 1997b), and interviews with the model developers.	
A2. Grid Options for Eulerian and Trajectory Models		***Score: 2.5***
	SLAM considers two types of grids: *the meteorological grid* controlled by the type of gridded meteorological input data used, and *the concentration grid* defined by the user in the model control file. The concentration grid is in latitudes and longitudes. SLAM also allows the user to specify randomly-spaced concentration receptors, and accepts meteorological data from randomly-spaced surface and upper air stations. However, randomly-spaced user receptors cannot be used in conjunction with a latitude/longitude concentration grid. Multiple or nested concentration grids are not supported.	
A3. Quality of Physical Processes Simulated		***Score: 2***
	The horizontal and vertical dispersion in SLAM is based on traditional, discrete stability class. Turbulence intensities are not used. The vertical dispersion coefficient, σ_z, is based on the K-theory. Vertical diffusivity, K_z, varies with	

	stability class, and is independent of height. The horizontal dispersion coefficient, σ_y, is based on the algorithms in MESOPUFF (Scire et al., 1984) until 100 km. Beyond 100 km, a user-defined scheme (essentially $\sigma_y \propto$ travel time) is used. The model uses a constant power-law exponent to extrapolate surface winds to a user-defined constant height (e.g., 300 m). This approach is questionable since both the wind profile in the atmospheric boundary layer and the height to which the extrapolation is applicable vary with atmospheric stability (i.e., time of day) and land use type. The default value, 0.14, of the power-law exponent recommended in the user's guide (ENSCO, 1997a) is representative of rural areas under neutral conditions. SLAM can calculate the mixing depth based on (1) the potential temperature gradient information, (2) the gradient Richardson number, or (3) the observed sounding as compared to the moist adiabatic lapse rate. The user selects which method use. SLAM does not contain an explicit treatment for terrain. All terrain effects are treated by meteorological models that provide inputs. Therefore, if SLAM were run with only surface and upper air observations, terrain effects would not be considered. The user needs to specify SLAM's integration time step, which should be a function of data density and run duration. Recommendations on the integration time step are not provided in the current user's guide. SLAM is still under active development. According to the model developers, some of the new features to be added include increased vertical resolution in the lower atmosphere for the mixing depth procedures, wet and dry deposition, horizontal splitting for older puffs, the use of turbulence fields generated by meteorological models to estimate the mixing depth, and improved vertical dispersion estimates.	
A4. Sparse Data Treatment		***Score: 2.5***
	Since SLAM can optionally use gridded meteorological data prepared by models such as RAMS, NOGAPS, HOTMAC (see Section A1), the effects of lack of data over water are minimized because these prognostic meteorological models rely on physical equations, rather than data interpolation, to produce three-dimensional fields. Some models use data from sources such as geostationary satellites, where there is no difference between over water and over land in data availability.	
A5. Overwater Dispersion		***Score: 1.5***
	SLAM has simple algorithms for overwater stability (based on the Monin Obukhov length) and mixing height. However, from the limited available documentation, it is not clear exactly how dispersion parameters are calculated. The effects of overwater dispersion can be further treated in the meteorological models that provide inputs to SLAM. Phenomena such as the Thermal Internal	

	Boundary Layer (TIBL) and plume fumigation for coastal areas are not treated in SLAM.	
A6. Model Evaluation History		***Score: 2***
	SLAM has been evaluated with data from the SEADEX (Johnson et al., 1987; Atchison et al., 1996), SIESTA (Gassman et al., 1986; Evans, et al., 1998), and ACE (Atchison, et al., 1998) experiments. However, most of the evaluation studies are qualitative in nature, and do not include a full-scale statistical performance evaluation.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 2.5***
	SLAM's user guide (ENSCO, 1997a) is an HTML (hyper-text mark-up language) document. Therefore, it can be viewed with web browsers such as Netscape's Navigator and Microsoft's Internet Explorer. Various "hyperlinks" exist in the document allowing the reader to quickly move to a section of interest. The user's guide provides information on the system design and features, model options, and the use of the graphical user interface (GUI) and various post-processing display programs. The section layout in the user's guide is logical. However, the descriptions of model options should be more comprehensive. For example, the meanings and effects of certain model options are not always clear to the reader. We also notice that the specification of variable emission rates, although a model option, is not explained at all in the user's guide.	
B2. Model Options		***Score: 2.5***
	SLAM has three tiers of model options: primary, secondary, and advanced. The *primary options* group specifies basic run information, including the hemisphere for the application, the method of entering source locations, sources of meteorological data (see Section A1), trajectory start/end times, names of input files, and receptor locations (randomly-spaced locations or a latitude/longitude grid). The *secondary options* group includes the run duration, the trajectory step interval, the vertical influence height for surface data (i.e., the capping height for the vertical extrapolation of surface winds), the domain top height, the weather data selection method, the minimum and maximum values for the mixing height, default values for the day and night mixing heights, the method by which the mixing height is determined, coefficients for defining the horizontal dispersion coefficient, the stack height, and the release rate. Note that the same stack height and release rate apply to all sources. The *advanced options* group includes modification of the default stability class	

	for each hour, input of user-specified vertical diffusivity (K_z), whether to calculate surface stability or to use the default value, whether to persist the stability from the previous hour if the model cannot calculate the stability for the current hour, the daytime start hour (the time at which the split test occurs), the wind-profile power-law exponent, the off-centerline distance (in terms of number of σ) beyond which concentration calculations are not performed, the gridded data weighting (through which observations can have more influence during data interpolation), and whether to create a concentration output file.	
B3. Data Preparation Time		***Score: 2.5***
	As mentioned above, SLAM accepts gridded outputs from meteorological models. As long as these models have been previously executed and the output files are available, SLAM can directly accept and reformat the data with little user intervention. However, to run SLAM from scratch with observed data would require a week to a month of effort to reformat the data. SLAM does not come with a set of formal pre-processors to reformat observed meteorological data in popular formats, such as TD-1440 for surface observations (from the National Climatic Data Center), TD-6201 for upper air observations (from the National Climatic Data Center), and F291 for buoy data (from the National Oceanographic Data Center).	
B4. Ease of Data Acquisition		***Score: 3***
	Observed meteorological data can be obtained from the National Climatic Data Center (NCDC, http://www.ncdc.noaa.gov) and the National Oceanographic Data Center (NODC, http://www.nodc.noaa.gov). NCDC also maintains archives of model outputs at roughly $210 for two months of MRF data, or six months of NGM data. NCAR re-analysis fields (http://www.scd.ucar.edu/dss/pub/reanalysis/index.html) can be obtained from NCAR at $10 per CD-ROM. It is not likely that archives of model outputs from HOTMAC exist, since the code is proprietary.	
B5. Model Interface to Preprocessors / GUI		***Score: 2.5***
	Because we had no access to SLAM's graphical user interface (GUI) program, the comments listed below are mainly based on our review of the user's guide (ENSCO, 1997a), which includes sample images of some of GUI's menu screens. The GUI program, or Control Panel (CP), of SLAM appears to be state-of-the-art. It includes many features, such as: • Allows the user to display surface and upper air meteorological observations on a map background. The GUI can plot various weather symbols, contours, time series for surface data, and skew T log-P diagrams for upper air data. • Allows the user to interactively screen and edit suspect surface and upper air observations. • Enters and validates model control parameters. • Executes the SLAM model in the foreground (with the Tracker option) or	

	in the background (without the Tracker option). • Executes various post-processing graphical programs to display the results. Although SLAM's GUI program is quite powerful, it lacks an on-line help system. That is, each menu screen does not have a "Help" button through which information on a certain input parameters is provided.	
B6. Run-Time Diagnostics		***Score: 2***
	According to the model developer, SLAM includes diagnostics in the code to trap potential run-time errors. We did not actually review the source code to verify. The GUI program validates all user inputs before running the model.	
B7. Post-Run Diagnostics		***Score: 3***
	A host of post-processing display programs provides an interactive environment to view the results of a SLAM model run. The "Trajectory Display" program shows multi-layer trajectories by source release time on a map background. The user can click on the trajectory markers to view specific information on the trajectory segment of interest. The "Concentration Analysis Display" program shows concentration contours and time series for multiple samplers (receptors). The "Data Viewer" program tabulates all model output files, and allows the user to screen the information according to time, source, and sampler.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 1.5***
	SLAM treats multiple point sources at different locations; however, all sources share the same emission rate and the same stack height. This is not appropriate for EIS applications. Additional code changes are necessary in order to treat variable source attributes.	
C2. UNIX / PC Portability		***Score: 1***
	SLAM is designed to run on a SUN/Solaris platform. The model does not directly run a PC, except in an X-Window client-server environment where the PC is simply treated as an X-terminal.	
C3. Run Time		***Score: 2***
	According to the model developer, SLAM takes roughly ten minutes to simulate one source for 96 hours on a Sun Ultra 1 UNIX workstation. An annual simulation with one source can take 4 to 24 hours.	
C4. Code Flexibility and Readability		***Score: n/a***
	Not available, since the model developers did not provide source codes for review, and we did not have enough information to make further inference.	

D. Cost (Non-Ranking)		
	SLAM's source code is available free of charge, since the model was originally developed with funding from the U.S. Air Force. However, because the model also relies on numerous other software packages and data ingestion sources, it is not trivial to install and customize SLAM . ENSCO provides a complete turnkey software/hardware system where the SLAM model is installed on a SUN workstation (a SPARC 5 or 10). This offering is unique among all the models reviewed in this study. The total cost for the turnkey system is around $90,000, plus additional costs for necessary customization in order to access external data services.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	Since the code is in the public domain, the user should be able to modify the code without restrictions. However, given the complex interface between SLAM and its supporting infrastructure (i.e., files, databases, and data ingestion systems) , considerable technical expertise is necessary for code changes.	
F. Language for Model and GUI (Non-Ranking)		
	Ada for SLAM; and X11, Motif, agX/Toolmaster for the graphical user interface (GUI) and the display programs. The display programs also use the geopolitical boundary information included in NCAR (National Center for Atmospheric Research) Graphics software package. The new GUI currently under development is based on Java that can be accessed by web browsers such as Netscape's Navigator and Microsoft's Internet Explorer.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**16**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**77.6**

3.7 SUMMARY AND RECOMMENDATIONS

In this section, we reviewed five Lagrangian puff models: CALPUFF, HYSPLIT_4, INPUFF, MESOPUFF II, and SLAM. The scores for all models are summarized in Table 3-1. Section 1 describes the evaluation methodology and criteria.

All models are in the public domain, and thus can be customized by the user. They are available at no cost or nominal cost. The SLAM model is not designed to be run as a stand-alone program unit. It requires considerable supporting infrastructure, such as an Oracle file server, a data ingestion unit to retrieve data from external archives, and the Motif and agX/Toolmaster packages, to run. The cost to purchase a complete turnkey system from ENSCO with SLAM installed and configured on a SUN Sparc workstation would be around $90,000. This is significant given the fact that the SLAM code can be obtained for free.

All models except SLAM treat deposition. However, INPUFF requires the user to directly enter information such as deposition and settling velocities, which requires additional expertise. CALPUFF has the most up-to-date scheme to treat dry deposition, and is the only model that deals with impacts to regional visibility due to particulate matter.

All models except INPUFF treat chemical transformation. CALPUFF and MESOPUFF II include non-linear chemistry for sulfates and nitrates. SLAM and the generic version of HYSPLIT_4 include linear chemistry in the form of a half-life decay. A special version of HYSPLIT_4 has been developed to treat nonlinear sulfur chemistry.

HYSPLIT_4, MESOPUFF II, and SLAM are optimized for regional transport and dispersion. As a result, these models are not concerned with near-field effects such as downwash and plume rise, and are not appropriate for studying near-field impacts. INPUFF treats stacktip downwash and plume rise. CALPUFF includes comprehensive building downwash algorithms and treats plume rise (final and transitional) and partial plume penetration. Both INPUFF and CALPUFF are appropriate for spatial scales from tens of meters to several hundred kilometers.

MESOPUFF II and CALPUFF have been routinely used to conduct annual simulations to support EIS (environmental impact study) and PSD (prevention of significant deterioration) applications. Typical applications of HYSPLIT_4, SLAM, and INPUFF involve simulations of a few days to a week. HYSPLIT_4 has been applied to calculate seasonal and annual concentrations. SLAM has not been fully tested with long-term simulations. It is impractical to use INPUFF to conduct long-term modeling with multiple sources, since the current input file structure requires that the meteorological data entered within the source loop. In other words, if there are 100 sources to be modeled, then the same meteorological data would have to be repeated 100 times. Of course, this problem could be solved with additional code modifications.

All models will run with gridded meteorological fields. CALPUFF and INPUFF provide the option of using single-station data. SLAM can also run with data from discrete surface and upper air stations only. Gridded meteorological fields are usually created with meteorological models. HYSPLIT_4 and SLAM can directly use outputs generated by prognostic models such as RAMS (Regional Atmospheric Modeling System), MRF (Medium Range Forecast), NGM (Nested Grid Model) and ETA. CALPUFF requires the user to run CALMET, a diagnostic wind field model that can optionally use outputs from the prognostic model MM5 (Penn State/NCAR Mesoscale Model). In order to run MESOPUFF II, the user needs to run

MESOPAC II, also a diagnostic model, to create necessary gridded wind fields. INPUFF simply includes the option of reading a 2-D wind field. It is up to the user to decide how this 2-D wind field should be created. Treatment of sparse data (e.g., overwater) will be adequate as long as prognostic model outputs are used. This is because these models use physical relationships, rather than straight data interpolation, to produce gridded meteorological fields.

There are different levels of treatment for terrain in the models. The most common approach is through the adjustment of the wind field to large-scale (i.e., greater than a grid cell) terrain features. This is usually done in meteorological models and not in dispersion models. All meteorological models, except MESOPAC II, mentioned in the above paragraph produce wind fields that are consistent with terrain. Note that, however, resolutions for these models range from less than one kilometer to 2.5° in latitude/longitude. So, the resolvable terrain features will vary greatly. CALPUFF is unique among the models reviewed in that it provides another level of treatment where the puff-terrain interaction is explicitly provided, altering the vertical distribution of the puffs due to subgrid-scale terrain features.

For models such as HYSPLIT_4 and SLAM that directly use gridded fields generated by other meteorological models, the user typically only has to reformat these model output files for later use and the processor programs often already exist. There is no need to obtain observed meteorological data. On the other hand, applications of CALPUFF and MESOPUFF II typically use observed data, and include a comprehensive suite of processors to retrieve and process raw data from various government data archives such as the National Climatic Data Center and U.S. Geological Survey. Although SLAM also accepts observations from conventional surface stations, upper air stations, offshore buoys, and CMAN (Coastal Marine Automated Network) stations, it is the user's responsibility to reformat the raw data and no processors are provided.

HYSPLIT_4, INPUFF, and MESOPUFF II do not have special treatment for overwater dispersion. (Note that some effects of overwater dispersion could be incorporated in gridded meteorological fields prepared by the meteorological models, but spatial resolution is determined by the grid size.) SLAM has a simple algorithm (based on the Monin-Obukhov length only) to calculate overwater stability class. CALPUFF contains a special overwater boundary layer module based on the profile method. CALPUFF is also the only model that treats the thermal internal boundary layer (TIBL) in coastal areas.

All models except HYSPLIT_4 can use the traditional PG (Pasquill-Gifford) curves to calculate dispersion coefficients. CALPUFF, INPUFF, and HYSPLIT_4 also can use more state-of-the-art turbulence-based method to calculate dispersion coefficients.

All models treat multiple sources, but with different degrees of complexity. CALPUFF, INPUFF, and MESOPUFF II allow each source to have its own characteristics. SLAM and the generic version of HYSPLIT_4 assume that all sources have the same emission rate. This will severely limit the usefulness of these models for EIS-type applications. However, HYSPLIT_4 does come with a library routine to treat gridded area source emissions. The user only has to change one statement to activate the call to that routine and recompile the code.

INPUFF accepts only discrete receptors. CALPUFF and MESOPUFF II accept both Cartesian and discrete receptors. HYSPLIT_4 accepts multiple, nested receptor grids in latitudes and longitudes. SLAM accepts either a receptor grid in latitudes and longitudes, or discrete receptors, but not both.

CALPUFF, HYSPLIT_4, and SLAM have graphical user interface (GUI) programs to assist the user to set up, execute, and analyze a model run in a menu-driven environment. These GUI programs all perform extensive error-checking. SLAM's GUI does not have on-line help that is easily accessible from each

menu screen, and runs only on a UNIX platform. CALPUFF's GUI is PC-based. HYSPLIT_4's GUI runs on both PC and UNIX platforms. The user can also visualize the modeling results (e.g., contour plots) within HYSPLIT_4 and SLAM's GUIs, where a separate plotting package is required for CALPUFF.

All models have adequate user's guides, although they range from about 50 pages (e.g., SLAM and HYSPLIT_4) to several hundred pages (e.g., CALPUFF). There is a trend for on-line publication. For example, the user's guide for HYSPLIT_4 is in the PDF format, which can be viewed on different computer platforms with a PDF Reader. The user's guide for SLAM is in the HTML format, which can be viewed with web browsers such as Netscape's Navigator and Microsoft's Explorer. CALPUFF's documentation is also being converting to the PDF format.

The run time for Lagrangian puff models varies greatly depending on applications (e.g., the number of sources, the run duration, and the resolution for the meteorological and concentration grids) and machine platforms. In general, it would take a few days to a week on a Pentium II PC (~ 300 MHz) to make an annual simulation with hundreds of sources. This is still much faster than Eulerian grid models reviewed in Section 2, where the ratio of model time to CPU time is between 10 and 1 on a typical UNIX workstation. Storage requirements might also be considerable for long simulation periods, mainly due to the model input data. 3-D meteorological fields for one year could easily exceed 10 GB in size.

INPUFF and MESOPUFF II are older models and have been widely used by many users (both public and private sectors). HYSPLIT_4 has been used by many government agencies, universities, and national laboratories. CALPUFF, destined to replace MESOPUFF II, has been gaining popularity among various Regions of the EPA, and has been used in many regulatory applications. The use of SLAM has been mainly limited to the U.S. Air Force community.

CALPUFF, HYSPLIT_4, INPUFF, and MESOPUFF II are written in FORTRAN. SLAM is written in ADA. All models except SLAM are easily portable between the PC and UNIX platforms. As mentioned in Section 3.6, the installation of SLAM is highly site-specific because of model's great dependence on other file management and data ingestion functions.

In summary, we recommend that the MMS acquire CALPUFF and HYSPLIT_4. CALPUFF has state-of-the-art treatments of overwater dispersion, terrain, chemistry, and deposition. There are numerous model options. The model is suitable for regional-scale as well as local-scale applications. HYSPLIT_4 is also a model with good technical merits. It uses either puff or particle approaches to calculate dispersion and deposition. It is flexible in that meteorological and concentration grids can all be nested. The code is quite modular and many customized versions have been developed to simulate interesting cases such as the Chernobyl accident, volcanic ash, and gridded area source emissions.

MESOPUFF II and SLAM basically ranked the same. MESOPUFF has achieved regulatory status, is well tested, and is still actively used (e.g., USEPA, 1995a and 1993a). However, we do not recommend the model since it does not treat overwater dispersion, and is to be replaced by the newer CALPUFF model, which includes all the features in MESOPUFF plus numerous new features. SLAM's system design reflects the most current development in software engineering, e.g., a client-server environment, a web-based user's guide, and powerful display functions in the GUI program. However, we do not recommend the model since it received only moderate scores in the "Science and Credibility" category. For example, the model does not treat deposition, dispersion coefficients are not turbulence-based, a constant power-law exponent is used to extrapolate winds vertically, and a constant emission rate is used for all sources. Furthermore, the model has not been fully tested for environment impact studies that involve annual simulations.

Table 3-1. Ratings for the (a) Science and Credibility, (b) Ease of Use, and (c) Computational Requirements Categories for Five Lagrangian Puff Models. Note That the Ratings for (a) and (b) Have a Weight That is Twice That for the Ratings for (c). Each Individual Rating Can be Between 1 and 3, and is not Adjusted According to the Weight in the Table. See Section 1 for a Description of Evaluation Methodology and Criteria.

	CALPUFF	HYSPLIT_4	INPUFF	MESOPUFF II	SLAM
Tech & Gen	3	2.5	2	2	2
Grid Options	2.5	3	1.5	2	2.5
Qual of Phys	3	3	2	2	2
Sparse Data	2.5	3	1	1	3
Overwater	3	1.5	1	1	2
Model Eval	2.5	3	n/a	3	2
S & C Score	16.5	16	7.5	11	13.5
User Guide	3	3	2.5	3	2.5
Options	3	2	2	2.5	2.5
Data Prep	2.5	3	1.5	2.5	2.5
Data Acq	3	3	2	3	3
GUI	3	2.5	n/a	2.5	2.5
Run Diag	3	3	3	3	2
Post Diag	2.5	2	1.5	2	3
Ease Score	20	18.5	12.5	18.5	18
Mult Source	2.5	2	2.5	2.5	1.5
UNIX/PC	3	3	3	3	1
Run Time	2.5	2.5	2	2.5	2
Code flex	3	3	2	3	n/a
Comp Score	11	10.5	9.5	11	4.5
Overall Score	47.5	45	29.5	40.5	36
Percent Score	93.3	88.3	63.5	77.8	77.6

4 TOXIC RELEASE MODELS

4.1 INTRODUCTION

Toxic release models are used for analysis of the potential effects of accidental releases of hazardous air pollutants. The temporal and spatial scales for the models are typically less than an hour and a few kilometers, respectively. In this section, we reviewed the following seven toxic release models:

- AFTOX
- ARCHIE
- CANARY
- DEGADIS
- HGSYSTEM
- SLAB
- TSCREEN

In addition, we also reviewed the following three graphical user interface (GUI) programs:

- BREEZE HAZ SUITE
- SLAB View
- SLAB for Windows

The first GUI program supports AFTOX, DEGADIS, and SLAB. However, we reviewed only the interface to DEGADIS. The second and third GUIs work with the SLAB model.

In Sections 4.2 through 4.11, each program is critically reviewed. Section 1 describes the evaluation methodology. A summary and our recommendations are given in Section 4.12.

4.2 AFTOX

Model Name: AFTOX, Version 3.1	
Person of Contact:	
	Air Force Weather Technical Library (for distribution only, no technical support provided) Scott AFB, IL 62225 Tel (618) 256-4024 Fax (618) 256-4819
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	***Score: 1.5***
	The U.S. Air Force Toxic Chemical Dispersion (AFTOX) model (Kunkel, 1988) is an interactive Gaussian puff/plume model. The model treats steady-state or instantaneous releases. The duration of a steady-state release can be finite, due to the puff algorithms included in the model. However, AFTOX does not accept a time-varying emission rate. The release can be either gas or liquid. The model determines whether the release is a gas or liquid based on whether the ambient temperature is above or below the boiling point temperature of the chemical. Gas releases are assumed to be point sources and liquid releases are assumed to be area sources. The model does not account for dense-gas and momentum effects. Predicted concentrations are adjusted for the effect of averaging time on the degree of plume meandering through the lateral dispersion coefficient. The model assumes default values of averaging time for quasi-continuous releases. The default averaging time is 15 minutes for release duration equal to or longer than 15 minutes. The default averaging time is equal to the actual release duration for shorter releases. The averaging time is one minute for instantaneous releases. AFTOX can calculate the mass emission rate for an evaporating pool release. The user needs to specify the source strength for other types of releases. AFTOX has a database that includes properties for about 80 chemicals, including hydrogen sulfide (sour gas). The database is ASCII, and can be upgraded by the user with the CHFIL utility or with a text editor directly. AFTOX also has a station database that includes information such as latitude, longitude, surface roughness, elevation, anemometer height, and time zone for various stations. Like most other dispersion models, AFTOX predicts ensemble average hazard	

	distance and area. Therefore, in theory, 50% of the time the model will underpredict the above hazard information. AFTOX includes an algorithm to extrapolate ensemble averages to values with 90% confidence limits (Kahler, et al., 1980) The model has not been under active development in the past ten years. The Air Force Weather Technical Library is responsible for software distribution only, and provides no technical support. Note that the commercial BREEZE HAZ SUITE software (also reviewed in this study) developed by Trinity Consultants includes a graphical user interface for the AFTOX model. Therefore, one possible way of obtaining technical support for AFTOX is through the purchase of the software package.	
A2. Grid Options for Eulerian and Trajectory Models		***Score: n/a***
	Not applicable	
A3. Quality of Physical Processes Simulated		***Score: 2***
	AFTOX is based on the well-tested conventional Gaussian puff/plume model. The source model for a pool release is based on Shell's SPILL model (Fleischer, 1980). The model uses boundary layer theory to calculate parameters such as the friction velocity and the Monin-Obukhov length. AFTOX uses classical Briggs' (1975) plume rise formulas for buoyant plumes.	
A4. Sparse Data Treatment		***Score: n/a***
	Not applicable	
A5. Overwater Dispersion		***Score: n/a***
	Not applicable	
A6. Model Evaluation History		***Score: 3***
	The conventional Gaussian puff/plume model used in AFTOX has been benchmarked in numerous evaluation studies. For example, Kunkel (1988) evaluated the model with data from the Prairie Grass (SO_2), Green Glow (ZnS), Ocean Breeze (ZnS), and Dry Gulch (ZnS) field experiments.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 3***
	AFTOX has a concise, informative user's guide (Kunkel, 1988) that includes the theory, user instructions, and evaluation for the model. The user's guide also includes several model run examples.	
B2. Model Options		***Score: 2***

	As mentioned above, AFTOX treats steady-state (possibly with a finite duration) and instantaneous releases. The model can treat a release with or without initial buoyancy. The model has two options to determine atmospheric stability, Golder's (1972) method based on the surface roughness length (z_0) and the Monin-Obukhov length (L), and Mitchell's (1982) method based observed σ_θ and wind speed. Golder's method is a nomogram with z_0 and 1/L as its y and x axes, respectively. There are curves on the nomogram that delineate different stability classes. Give the values of z_0 and L, one can determine the corresponding stability class.	
B3. Data Preparation Time		***Score: 2***
	It will take less than 15 minutes to prepare an AFTOX run due to simple input data requirements and the chemical database. However, the model does not have the option of saving the information for previous runs. Thus, the user will have to repeat the same data preparation effort each time for similar runs.	
B4. Ease of Data Acquisition		***Score: n/a***
	Not applicable	
B5. Model Interface to Preprocessors / GUI		***Score: 2***
	AFTOX has a rudimentary text-based user interface, which essentially prompts the user for a series of question in order to define a release scenario and output options. There is no need to specify properties of the chemical of interest owing to the chemical database.	
B6. Run-Time Diagnostics		***Score: 2***
	AFTOX has only a few run-time warning messages to indicate potential problems, e.g., when the code fails to find a convergent solution for the vapor pressure (using the Frost-Kalkwarf equation), and when the user enters a stack height that is above the inversion base.	
B7. Post-Run Diagnostics		***Score: 2***
	AFTOX can generate the following three types of output: contour plot for a given concentration and elapsed time concentration at specified location and elapsed time, and maximum concentration at given height and elapsed time. AFTOX does not generate other statistics such as concentrations at a receptor grid and the maximum concentration at a given location, which limits the usefulness of the model.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 1***

	AFTOX treats only one source at a time.	
C2. UNIX / PC Portability		*Score: 1*
	AFTOX runs only on the PC platform.	
C3. Run Time		*Score: 2*
	The AFTOX model performs dispersion calculations rather quickly (in a few seconds) due to the simple Gaussian puff/plume dispersion algorithms. However, as explained below, depending on the type of the release and the answer required by the user, the actual model run time sometimes can be quite lengthy. When running AFTOX, the user must specify the elapsed time after the spill as an input parameter for dispersion calculations. In order to find the maximum concentration at a fixed location for a finite-duration or instantaneous release, the user usually has to try many different elapsed times before obtaining the answer. Since AFTOX runs only in interactive mode, these repeated runs are time-consuming.	
C4. Code Flexibility and Readability		*Score: 1*
	The AFTOX code is marginally readable with limited comments. The abundance of the GOTO statements sometimes makes the code difficult to follow and customize.	
D. Cost (Non-Ranking)		
	The AFTOX code plus the user's guide can be obtained from the Air Force Weather Technical Library free of charge. However, the library primarily provides services to the Department of Defense and its contractors.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	The software is distributed only by mail. The source code of AFTOX is in the public domain, and the user can make code changes for personal use.	
F. Language for Model and GUI (Non-Ranking)		
	AFTOX was written in Microsoft's QuickBASIC language, which was made obsolete by Visual BASIC many years ago.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**13**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**66.7**

4.3 ARCHIE

Model Name: ARCHIE, Version 1.0	
Person of Contact:	
	ARCHIE (DHM-15/Room 8104) U.S. Department of Transportation 400 7th Street, S.W. Washington, DC 20590 Tel (202)366-4900 Model mainly developed by: John H. Hapogian Hazmat America, Inc. 9 Browning Road Arlington, MA 02174 Tel (781)646-4564
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	***Score: 2.5***
	The ARCHIE (Automated Resource for Chemical Hazard Incident Evaluation) model (FEMA, 1989) was originally developed by scientists at Arthur D. Little, Inc. for the Federal Emergency Management Agency (FEMA), the U.S. Department of Transportation (DOT), and the U.S. Environmental Protection Agency (EPA). The primary purpose of the software is to provide emergency preparedness personnel several integrated estimation methods to assess the vapor dispersion, fire, and explosion impacts associated with accidental releases of hazardous materials into the atmosphere. In addition to performing dispersion calculations, ARCHIE includes various simple empirical models for estimating (1) the discharge rate and duration of a gas or liquid release from a tank or a pipeline; (2) the evaporation rate, duration, and size of a liquid pool; (3) thermal radiation hazards for a flammable release; (4) the pollutant mass within flammability limits; (5) consequences of an explosion arising from ignition, internal overpressurization, external heating, or internal reaction. Although ARCHIE can estimate the size of an evaporating pool, the pool size is not subsequently used in dispersion calculations, where a point source is always assumed. ARCHIE does not include algorithms to model denser-than-air releases. ARCHIE does not include a chemical data base. As a result, all physical properties of the pollutant have to be entered manually.

A2. Grid Options for Eulerian and Trajectory Models		*Score: n/a*
	Not applicable.	
A3. Quality of Physical Processes Simulated		*Score: 2.5*
	ARCHIE includes the following source term modules: liquid discharge models for tanks with different shapes, gas discharge from a tank, gas discharge from a pipeline, two-phase flow from a tank, pool size estimation methods for a liquid discharge, and emission rates from liquid pools. ARCHIE uses a traditional Gaussian plume model with well-known Pasquill-Gifford dispersion coefficients to perform dispersion calculation. Effects of finite source duration are treated. In addition to dispersion, ARCHIE also uses the following models to appropriately characterize the fate of an accidental release: a pool fire model to estimate the radiant heat dose to an observer, a fireball model to describe the maximum diameter, height, and duration of a fireball resulting from a large liquefied hydrocarbon (e.g., propane) release, a flame jet model to estimate the length of a flaming jet, a vapor cloud fire model to determine the length and width of a hazard zone for a flammable vapor cloud, and a vapor cloud explosion model to characterize the effects of an unconfined explosion in terms of an equivalent TNT charge. Thus, ARCHIE contain a suite of models that enable the user to model the complete history of an accidental release. The source, dispersion, fire, and explosion models mentioned above are all based on well-known published literature. Since ARCHIE is primarily used in an emergency response setting where it is crucial to obtain modeling results quickly, all models, except for the Gaussian dispersion model, are highly empirical and are designed to obtain rough, first-order estimates. In the ARCHIE user's guide (FEMA, 1989), it is suggested that the use of a neutral buoyancy (or passive) dispersion model would be adequate for denser-than-air releases. The argument was made based on running a limited number of test cases, and comparing the penetration distances (i.e., the downwind distances to certain concentrations of interest) predicted by ARCHIE against those predicted by a dense gas dispersion model (Mudan, 1983). However, the test cases considered are all pressurized two-phase releases, and do not include other common dense gas releases such as evaporating pools. Moreover, while a passive dispersion model might yield a penetration distance similar to that given	

	by a dense gas dispersion model, the predicted toxic area will certainly be quite different between the two types of models. Therefore, it is concluded that the approach of modeling a denser-than-air release with a passive model as adopted in ARCHIE is not fully justified.	
A4. Sparse Data Treatment		***Score: n/a***
	Not applicable.	
A5. Overwater Dispersion		***Score: n/a***
	Not applicable.	
A6. Model Evaluation History		***Score: 1.5***
	To the reviewer's knowledge, ARCHIE has not been subjected to thorough evaluation. However, all modules included in ARCHIE are derived from well-known theories published in peer-reviewed journals, and these theories are often based on laboratory and field data. Therefore, it is believed that the model should perform in a satisfactory manner.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 3***
	The user's guide (FEMA, 1989) includes user's instructions and technical descriptions of various modules. The document clearly explains what ARCHIE does and does not model, and points out common user errors. One minor shortcoming of the user's guide is that it does not include tutorials and sample inputs and outputs. The user's guide also includes vast amount of background information for chemical hazard analysis procedures in general, thus making it a valuable reference even if the reader is not interested in ARCHIE.	
B2. Model Options		***Score: 3***
	As described above, ARCHIE includes (1) modules to estimate the source terms for different types of releases. (2) a dispersion module to calculate pollutant concentrations after the release, and (3) modules to estimate the impacts associated with fire and explosion for flammable liquids and vapors. Depending on the source configuration, different modules will be used to perform a complete analysis. This comprehensive approach is usually found in expensive commercial software packages only.	
B3. Data Preparation Time		***Score: 3***
	The primary purpose of ARCHIE is to provide emergency preparedness personnel with tools to estimate the consequence of an accidental release. Therefore, getting the results quickly is assured, and it generally takes about 15	

	minutes to prepare an ARCHIE run. One factor that usually lengthens the preparation time is the lack of a built-in chemical database.	
B4. Ease of Data Acquisition		***Score: n/a***
	Not applicable, since ARCHIE does not require data from external data archives.	
B5. Model Interface to Preprocessors / GUI		***Score: 2.5***
	ARCHIE has a text-based, menu-driven interface, through which all the modules are connected. The interface is not "fancy" according to today's standards; however, it is straightforward and practical. Limited on-line help is available. The software reminds the user if certain inputs, such as the pool area and the emission rate, required by the current module can be calculated by other modules in ARCHIE. In a typical ARCHIE session, about half of the questions faced by the users are to confirm input data. This is probably too excessive, especially for an experienced user.	
B6. Run-Time Diagnostics		***Score: 2.5***
	ARCHIE has a number of diagnostic checks implemented to prevent inconsistent or inappropriate use of the model.	
B7. Post-Run Diagnostics		***Score: 2***
	The vapor dispersion module in ARCHIE provides tabular outputs that list contaminant concentrations, recommended evacuation zone widths, contaminant arrival and departure times as a function of downwind distance. Other source, fire, and explosion modules usually give simple statistics, such as (1) the pool area, (2) the evaporation rate, (3) the maximum diameter and height of a fireball, and (4) the radius from the center of a liquid pool fire in which exposed people might experience second-degree burns. ARCHIE does not generate graphical outputs.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 1***
	ARCHIE treats one source at a time.	
C2. UNIX / PC Portability		***Score: 1***
	ARCHIE runs only on the PC platform.	
C3. Run Time		***Score: 3***

	ARCHIE takes only a few seconds to run on a Pentium PC.	
C4. Code Flexibility and Readability		***Score: n/a***
	Not applicable, since ARCHIE's source code is not available.	
D. Cost (Non-Ranking)		
	The software and user's guide for ARCHIE can be obtained free of charge from the U.S. Department of Transportation, 400 7th Street, S.W., Washington, DC 02590. Tel (202) 366-4900.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	The software is available to the public free of charge (see above). In addition to from the Department of Transportation, the software (but not the user's guide) can also be downloaded from the Internet from places such as the Canadian Centre for Occupational Health and Safety (CCOHS) at the Internet address http://www.ccohs.ca/ccohs/hazard.htm.	
F. Language for Model and GUI (Non-Ranking)		
	ARCHIE was written in Microsoft's Quick BASIC language, which has been superseded by Visual BASIC many years ago.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**12**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**79.4**

4.4 CANARY

Model Name: CANARY by QUEST, Version 3.0	
Person of Contact:	
	John B. Cornwell Quest Consultants, Inc. P.O. Box 721387 Norman, OK 73070-8069 Tel (405)329-7475 Fax (405)329-7734 E-mail jbc@questconsult.com
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	*Score: 3*
	The CANARY (Quest Consultants, 1997) model is used to model (1) vapor dispersion (from pressurized gases, superheated liquids, subcooled liquids, and refrigerated liquefied gases); (2) fire radiation (from liquid pool fires, flares, torch fires, and BLEVE fireballs); and (3) explosions (from vapor cloud explosions and confined space explosions). The CANARY model also has modules to estimate source terms for releases from pipes and vessels, and evaporating pools. Comprehensive thermodynamic calculations are included in CANARY to account for two-phase mixtures of up to ten components. CANARY has a database that contains properties for about 300 chemicals, including hydrogen sulfide (sour gas). The database cannot be expanded by the user, which is an important limitation. CANARY treats steady-state (possibly with a finite duration), instantaneous, and transient releases. For a transient release, the time-varying source information is internally calculated by the model and cannot be directly specified by the user. A pressurized liquid release will sometimes result in one portion of the pollutant enters the atmosphere directly, and the remaining pollutant forms a liquid pool at the ground and then evaporates into the atmosphere. CANARY can simultaneously track the fate of momentum jet and liquid pool streams. The CANARY model replaces the older QuestFOCUS model.	
A2. Grid Options for Eulerian and Trajectory Models	*Score: n/a*
	Not applicable.	

A3. Quality of Physical Processes Simulated		***Score: 3***
	The heavy-gas dispersion module in CANARY is redeveloped from the base equations used in the well-known SLAB model (Ermak, 1990). This is different from other software packages such as BREEZE, BEE-Line or SLAB View where the original SLAB model is directly used. The fire and radiation models in CANARY are based on theories that appear in peer-reviewed technical journals. These models are of high-quality and defensible. Moreover, CANARY has state-of-the-art thermodynamic treatments for two-phase mixtures with up to ten components, while most other similar models, except for HGSYSTEM, do not even explicitly treat single-phase mixtures.	
A4. Sparse Data Treatment		***Score: n/a***
	Not applicable.	
A5. Overwater Dispersion		***Score: n/a***
	Not applicable.	
A6. Model Evaluation History		***Score: 3***
	The CANARY model and its predecessor FOCUS have been subjected to extensive review and evaluation. For example, Hanna et al. (1993) evaluated an *earlier* version of the FOCUS model with data from the Burro (LNG), Coyote (LNG), Desert Tortoise (NH_3), Goldfish (HF), Maplin Sands (LNG and LPG), and Thorney Islands (mixture of CFC-12 and N_2) field experiments. They found that this earlier version of FOCUS tends to overpredict concentrations. The user's guide of CANARY also provides a detailed description of the evaluation history of different modules in the model.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 2***
	The user's guide (Quest Consultants, 1997) provides only brief instructions concerning the use of the model. The main text (i.e., not including appendices) has only 17 pages. This does not appear to be consistent with the flexibility of CANARY to treat many kinds of hazards, including vapor dispersion, fire radiation, and explosions. In addition, more detailed descriptions of the consequences of selecting various model options should be available. For example, from the user's guide, it is not clear what types of text and graphical outputs are available for different types of releases. Appendix D of the user's guide provides brief technical discussions of various modules included in the CANARY model. The discussions also include solution methodology, module validation history, and references. The user's guide has a section that describes some CANARY sample cases. The	

	text description for each hypothetical scenario is clear. However, the corresponding CANARY model inputs are not mentioned in the user's guide. A step-by-step tutorial should also be included.	
B2. Model Options		***Score: 2.5***
	Hazard scenarios treated by CANARY include vapor dispersion, fire radiation, and explosions. For vapor dispersion, CANARY calculates vapor cloud concentrations as a function of downwind distance, and the maximum amount of vapor within flammability limits for flammable gases. For fire radiation, CANARY calculates the steady-state radiative heat flux as a function of distance. CANARY estimates, two types of explosion hazards: overpressure and the maximum size of the fireball	

	The CANARY model provides various types of tabular and graphical outputs, with which the user can determine whether the results appear reasonable and correct. Graphical outputs include x-y and contour plots. There are sometimes "kinks" in the distribution of the centerline concentration with downwind distance. This is a result of the fact that predictions, from two different models are patched together. For example, a pressurized jet touching down the grounds requires the Ooms et al. (1974) momentum jet model coupled with the SLAB model.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 1***
	The software models one source at a time.	
C2. UNIX / PC Portability		***Score: 3***
	The software can be ported from the PC to UNIX platform, as long as codes are recompiled.	
C3. Run Time		***Score: 2***
	On a Pentium Pro 200MHz PC, CANARY typically takes less than one minute to finish a model run. However, if the user wants to calculate the source information, such as the mass release rate from a breach of containment, and the associated time-dependence of physical state of the release of a fluid stream, the model run time can be considerably longer, e.g., about ten minutes. In this case, it would be helpful if the CANARY could print out some messages on the screen so that the user will not suspect whether the program has "crashed" or is still running.	
C4. Code Flexibility and Readability		***Score: n/a***
	Not applicable, since the source codes are not available.	
D. Cost (Non-Ranking)		
	For government agencies and universities: $5,000 for software purchase and technical support (software service contract) for the first year. $500 for technical support for each ensuing year. For commercial clients, the costs are $17,500 and $1,500, respectively.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	The software is available from the model developer in diskettes. Only	

	executable codes are included in the package. As a result, the end user cannot make code changes and then recompile the code.	
F. Language for Model and GUI (Non-Ranking)		
	FORTRAN 77 and C for both numerical models and the interface program.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**12**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**84.1**

4.5 DEGADIS

Model Name: DEGADIS, Version 2.1

Person of Contact:

Dr. Thomas O. Spicer
Chemical Hazards Research Center
University of Arkansas Engineering Research Center
700 West 20th Street
Fayetteville, AR 72701
Tel (501) 575-6516
Fax (501) 575-8718
E-mail tos@engr.uark.edu

A. Science and Credibility (Ranking)

A1. Technical and General Descriptions — *Score:2.5*

The DEGADIS model was first developed, by Havens and Spicer (1985) to model LNG spills from tankers over water. It is designed to model the dispersion of a dense gas cloud released at ground-level with zero initial momentum. The release can be either steady-state (with finite duration) or transient. The model approaches a Gaussian model for tracer (neutrally-buoyant) releases. The Ooms et al. (1974) model for a vertical jet release was later on added to DEGADIS as a "front-end" module. The jet module is independent and will make transition to DEGADIS when the jet touches down to the ground.

DEGADIS uses the concept of atmospheric take-up rate, the rate at which source material can be taken up or absorbed by the atmosphere, to determine the possible formation of a so-called secondary source blanket. The take-up rate is assumed to increase with increasing friction velocity and decreasing cloud density excess. If the gas release rate does not exceed the potential take-up rate, the model assumes that the gas is taken up directly by the atmospheric flow and dispersed downwind. If the gas release rate exceeds the potential take-up rate, the model assumes the formation of a "secondary source blanket" over the primary source. The blanket is represented as a cylindrical gas volume that spreads laterally as a gravity flow, with entrainment from the top of the source blanket by wind shear and air entrainment into the advancing front edge. The blanket spreads until the take-up rate balances the release rate.

Once the secondary source blanket, if any, stops growing, DEGADIS proceeds to calculate the downwind dispersion. The model treats the dispersion of gas from the secondary vapor cloud as if it were emitted from an area source.

	Lateral concentration profile is assumed to have a horizontally homogeneous central core with Gaussian edges. Vertical concentration profile is similar to Gaussian, but with an exponent of 1+α (rather than 2), where α is the best-fit vertical wind profile exponent. Note that the lateral and vertical profiles assumed by DEGADIS are identical to those assumed by HGSYSTEM (Post,1994a). The air entrainment is assumed to be from the cloud top, with an entrainment rate proportional to the cloud Richardson number (a function of cloud density excess, friction velocity, and effective cloud height). DEGADIS does not directly treat two-phase releases. The user's guide (Spicer and Havens, 1990) recommends that the *isothermal* option in the model be selected for a two-phase release, where the user needs to specify a set of "triplets" that define the relationships among the density of the vapor-aerosol-air mixture, the mass concentration of the vapor-aerosol mixture in the cloud, and the mole fraction of vapor-aerosol mixture in the cloud. DEGADIS comes with a sample database called EXAMPLE.GAS, where properties for seven chemicals are included. Hydrogen sulfide (sour gas) is not included. The user must specify the source strength for DEGADIS.	
A2. Grid Options for Eulerian and Trajectory Models		***Score: n/a***
	Not applicable.	
A3. Quality of Physical Processes Simulated		***Score: 3***
	The transport and dispersion algorithms included in DEGADIS are the same of those included in HGSYSTEM. These algorithms are of high quality, demonstrated by the fact that DEGADIS is one of the best-performing toxic release models in predicting ground-level centerline concentrations for field data (Hanna et al., 1993). However, the model does tend to predict a shallower cloud height, and thus a wider cloud width. The treatment of along-wind dispersion appears to be outdated, since it is based on neutrally-buoyant, rather than denser-than-air, releases and the reference (Beals, 1971) is not easily accessible and somewhat obscure.	
A4. Sparse Data Treatment		***Score: n/a***
	Not applicable.	
A5. Overwater Dispersion		***Score: n/a***
	Not applicable.	
A6. Model Evaluation History		***Score: 3***
	DEGADIS has been subjected to extensive review and evaluation. For example, Hanna et al. (1993) evaluated DEGADIS with data from the Burro (LNG), Coyote (LNG), Desert Tortoise (NH_3), Goldfish (HF), Maplin Sands (LNG and	

	LPG), and Thorney Islands (mixture of CFC-12 and N_2) field experiments. They found that DEGADIS is one of the best-performing models, with a slight tendency to overpredict concentrations for continuous dense-gas releases. Touma et al. (1995) also independently evaluated DEGADIS with data from the Burro, Desert Tortoise, and Goldfish field experiments.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 3***
	The user's guides for DEGADIS (Spicer and Havens, 1990, for the VAX/VMS version; and Spicer, 1990, for the PC version) provide a detailed description of the theory and formulation used in the model. Sample model inputs and outputs, diagnostic messages, and partial listing of source codes are also included in the user's guides. The user's guides also provide recommendations concerning the limitations of the model. This information is very valuable and is rarely provided in the user's guides for other models. The user's guides are only available as hard copies. On-line (or electronic) versions do not exist.	
B2. Model Options		***Score: 2***
	DEGADIS mainly treats ground-level evaporating pool releases, which can be either steady-state (finite duration) or transient. The JETPLU front-end module (Ooms et al. 1974) can be used to simulate a release that is initially pointed upward. JETPLU will make transition to DEGADIS once the jet touches down the ground. The release can be pure or diluted. DEGADIS internally determines the value of the Monin-Obukhov length (L) based on stability class and surface roughness. If necessary, the user can also enter a value for L. The model optionally treats heat and water transfers from the surface, where the user can either use the default transfer coefficients or specify his own.	
B3. Data Preparation Time		***Score: 3***
	It will take less than one man-hour to prepare a DEGADIS run. Tasks that require more time are (1) source characterization and (2) specification of pollutant properties. The sample database, EXAMPLE.GAS, that comes with the DEGADIS code includes properties for only seven common pollutants. As mentioned above, DEGADIS does not directly treat a two-phase release. In order to conduct an accurate simulation, the user needs to specify up to 25 "triplets" that define the relationships among the density of the vapor-aerosol-air mixture, the mass concentration of the vapor-aerosol mixture in the cloud, and the mole fraction of vapor-aerosol mixture in the cloud, based on adiabatic	

	mixing of ambient air with the chemical. This can be time-consuming if the user does not have a separate program to generate the information required. (By default, DEGADIS assumes a linear concentration-density relationship that is based on only two triplets, pure vapor-aerosol mixture and pure air.)	
B4. Ease of Data Acquisition		***Score: n/a***
	Not applicable, since DEGADIS does not require data from external data archives.	
B5. Model Interface to Preprocessors / GUI		***Score: 2***
	Although the public-domain version of the DEGADIS model does not have a Graphical User Interface (GUI) program, it does have a text-based utility program called DEGINP that can assist the user in creating new and editing existing DEGADIS input files. DEGINP will also create the necessary batch file to run DEGADIS.	
B6. Run-Time Diagnostics		***Score: 2***
	DEGADIS has a procedure to trap errors that occur during run-time. More than 30 error messages can be generated by the code. The user's guides provide a detailed listing of the meaning and possible solution for each error message. Note, however, that most error messages are concerned with the computational, rather than the physical, aspect of the model. For example, many messages are devoted to errors that might occur during root-finding and integration operations.	
B7. Post-Run Diagnostics		***Score: 2***
	DEGADIS generates only tabular outputs of cloud properties. However, the output listing does include all the necessary information for the user to visualize the results (after some necessary postprocessing) in different forms (e.g., 2- and 3-D) with external plotting packages. For transient releases, DEGADIS yields snapshots (i.e., at different times after the release) of spatial distributions of the cloud. A post-processor is available where the user can sort the outputs so that concentration time series at different downwind distances can be obtained.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 1***
	DEGADIS models one source at a time.	
C2. UNIX / PC Portability		***Score: 2***
	DEGADIS was originally developed with the FORTRAN language in a VAX/VMS environment. As a result, the code can be ported between the UNIX and PC environments, but with some potential problems listed below. There are frequent uses of FORTRAN extensions (e.g., using DATA statements to	

	initialize variables that are declared by COMMON statements), which may not be supported by other compilers. The user should also be aware of the different syntax for batch files, directly generated by the DEGADIS code, between the UNIX and PC environments.	
C3. Run Time		***Score: 3***
	DEGADIS takes less than a minute to run on a Pentium PC for a steady-state release. The run time will be longer (e.g., up to 10 minutes) for a transient release.	
C4. Code Flexibility and Readability		***Score: 3***
	The DEGADIS code is relatively complex with close to 70 subroutines. However, the code is flexible and modular, and has ample comments. For example, if the user decides to use a different numerical solver to integrate the governing equations, then all is required is to replace a subroutine and re-compile the code. Some important constants that appear repeatedly in various subroutines are defined in INCLUDE files, making it relatively easy to make changes.	
D. Cost (Non-Ranking)		
	The DEGADIS code can be downloaded from EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/) with no cost. There are commercial versions of the Graphical User Interface (GUI) programs available for DEGADIS. These GUI programs always use the basic code that is available from SCRAM.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	The source code is available to the public domain, and the user can customize the code. The user's guides can be ordered through the National Technical Information Service (NTIS), telephone (800)553-6847, publication number PB90-213893,	
F. Language for Model and GUI (Non-Ranking)		
	DEGADIS was written in FORTRAN 77. The public-domain version of DEGADIS does not have a GUI program.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**13**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**81.8**

4.6 HGSYSTEM

Model Name: HGSYSTEM, Version 3.0	
Person of Contact:	
	Mr. Peter Roberts Shell Research Limited Thornton Research Centre P.O. Box 1, Chester, CH1 3SH, U.K. Tel 44-151-3735893 Fax 44-151-3735845 E-mail p.t.roberts@msmail.trctho.simis.com
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	*Score: 3*
	The HGSYSTEM software package (Post, 1994a and 1994b) is based on the NTIS version of the HEGADAS (Witlox, 1988) dense gas dispersion model, with many enhancements to account for HF (hydrogen fluoride) chemistry and thermodynamics, aerosol thermodynamics, jet/plume modeling, gravity spreading, time-varying emissions from evaporating pools, and multi-component releases. While considerable efforts have been made to correctly simulate the HF chemistry and thermodynamics, HGSYSTEM is also applicable to other non-reactive chemicals. HGSYSTEM can treat aerosol mixtures with up to eight chemicals. The HGSYSTEM software package consists of more than a dozen of stand-alone modules, each having its unique function, including: • the SPILL and LPOOL modules for evaporating pools, • the AEROPLUME and HFPLUME modules for high momentum, arbitrarily oriented jets (one- or two-phase), • the steady-state and transient versions of the HEGADAS module for ground-level dense or tracer gas area-sources, • the HEGABOX module for instantaneous releases of an initially stagnant, dense cloud, and • the PGPLUME module for the passive far-field dispersion of elevated plumes. HGSYSTEM can calculate the source information for a pressurized jet, a transient liquid spill from a pressurized vessel, and an evaporating pool. HGSYSTEM allows spatial variations in surface roughness, which is unique among the models reviewed.

	HGSYSTEM was mainly designed to run in interactive mode. Batch mode execution is only recommended for an experienced user. HGSYSTEM has probably the most complicated input data requirements among the seven models reviewed. This problem arises because the modules in HGSYSTEM are designed to run in succession. The upstream module provides only part of the input data required by the downstream module. Additional efforts are required to prepare the remaining input data for the downstream model. The dispersion algorithms used in the HEGADAS module of HGSYSTEM are very similar to those used in the DEGADIS model (Spicer and Havens, 1990), where HEGADAS was first developed at an earlier date. For example, both models use the same concept of the atmospheric take-up rate to parameterize a secondary source blanket. Both models also use the same concentration profiles. HGSYSTEM has a chemical database that includes properties for 30 chemicals, not including hydrogen sulfide (sour gas). Each chemical has 52 numerical entries included in the database. More than half of the entries were derived from Shell's proprietary PEPPER database. As a result, it will be difficult to upgrade HGSYSTEM's chemical database.	
A2. Grid Options for Eulerian and Trajectory Models		***Score: n/a***
	Not applicable.	
A3. Quality of Physical Processes Simulated		***Score: 3***
	HGSYSTEM contains state-of-the-art treatments of various physical processes. For example, it includes complex routines to treat a two-phase aerosol mixture with up to eight components. HGSYSTEM also has a separate set of routines to treat complex HF thermodynamics and chemistry. The LPOOL module uses energy balance methods to calculate time-varying source information for an evaporating pool. The AEROPLUME module for the near-field dispersion of a pressurized jet release explicitly accounts for the different stages (i.e., airborne, touchdown, and slumped) of plume development, where each stage involves different physical processes. Parameterizations of these physical processes rely on the results from a vast number of field and wind tunnel experiments. However, the down side of the above advanced treatments of physical processes is that the code becomes less robust and more prone to "crashes." The numerical solvers used in the model are also quite sophisticated. For example, the proprietary NAESOL solver used in AEROPLUME can integrate a stiff set of simultaneous ordinary differential and algebraic equations.	
A4. Sparse Data Treatment		***Score: n/a***
	Not applicable.	
A5. Overwater Dispersion		***Score: n/a***

	Not applicable.	
A6. Model Evaluation History		***Score: 3***
	HGSYSTEM has been subjected to extensive review and evaluation, particularly the HEGADAS far-field dispersion module for ground-level area-source releases. For example, Hanna et al. (1993 and 1996b) evaluated an earlier and the most recent versions of HGSYSTEM with data from the Burro (LNG), Coyote (LNG), Desert Tortoise (NH_3), Goldfish (HF), Maplin Sands (LNG and LPG), Prairie Grass (SO_2), and Thorney Islands (mixture of CFC-12 and N_2) field experiments. They found that HGSYSTEM is one of best-performing models with a slight tendency of overpredicting concentrations for continuous dense gas releases. There is no systematic bias in model performance with independent variables such as wind speed, downwind distance, and stability.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 3***
	HGSYSTEM has a comprehensive technical reference manual (Post 1994a) and a user's manual (Post 1994b). There are also numerous internal Shell reports documenting different components of HGSYSTEM. The technical reference manual contains in-depth technical information. However, since the document is essentially a collection of chapters written by different authors at different times, the level of discussion and the format of presentation for each module are not consistent. Discussions are sometimes not properly integrated, making it difficult to locate the right section for a topic of interest. For example, there is very little information on LPOOL, the module to calculate time-varying source information for an evaporating pool, other than citations to two technical papers. Technical discussions of HEGADAS, the module to calculate atmospheric dispersion of a ground-level area source, consists of three major sections: one section for the basic discussions of the model, and other two sections for the "new" algorithms added to the model. Discussions in the last two sections should be appropriately included in the first section. The user's manual provides adequate discussions for each module. All input parameters are systematically explained, including the meaning, the allowed range, and the default value (if appropriate). The user's manual also includes discussions of intended applications and limitations for each module, which helps reduce potential user errors.	
B2. Model Options		***Score: 3***
	HGSYSTEM is very flexible in terms of model options. For example, there are various input parameters that control the selections of lateral dispersion	

	algorithms, thermodynamics models (inert vs. HF), output options, convergence criteria, and transition criteria.	
B3. Data Preparation Time		***Score: 2***
	It will take about one man-hour to prepare a HGSYSTEM run for a novice user. As mentioned above, HGSYSTEM includes a host of modules that are run in sequence. Each module has its own input file. For any "downstream" module, the required inputs are partly prepared by the "upstream" module, and partly specified by the user. This sometimes leads to confusion.	
B4. Ease of Data Acquisition		***Score: n/a***
	Not applicable, since HGSYSTEM does not require data from external data archives.	
B5. Model Interface to Preprocessors / GUI		***Score: 2***
	There is a text-based interface program for HGSYSTEM. The program asks the user a series of questions in order to decide the possible run sequence for modules, invokes a user-selected text editor to edit input files when necessary, creates batch files, and then runs batch files. However, the interface program does not allow as much flexibility as manual execution of HGSYSTEM. HGSYSTEM does not have a graphical user interface.	
B6. Run-Time Diagnostics		***Score: 3***
	HGSYSTEM can generate many warning and error messages during run time so that the user can monitor the progress of a model run. Messages are printed on the screen and written to a file for later review. It seems that some less severe error messages, which will halt the model execution, should be reclassified as warning messages, so that the model can run to completion.	
B7. Post-Run Diagnostics		***Score: 2.5***
	HGSYSTEM contains a number of postprocessors to further analyze the results. Postprocessors mainly retrieve and process text information already included in existing model output files. The user needs to use a separate plotting package with the files created by postprocessors in order to generate any graphical outputs. The POSTHT postprocessor for the transient version of HEGADAS performs time-averaging correction on predicted centerline concentrations to account for the intermittency (i.e., zeros) in a concentration time series. This is done through the numerical integration of a concentration time series and then divided by a time period. This is *in addition to* the traditional approach of treating averaging time via a change in the lateral dispersion coefficient . The steady-state version of HEGADAS does not directly treat a finite-duration release. The finite release duration is treated in the POSTHS postprocessor.	

C. Computation Requirements (Ranking)		
C1. Multiple Sources		*Score: 1*
	HGSYSTEM simulates only one source at a time.	
C2. UNIX / PC Portability		*Score: 2.5*
	HGSYSTEM was developed with the FORTRAN language. Thus, the code can be ported between the UNIX and PC environments. One issue that should be addressed during code porting is the different syntax for the batch files that are used to control the run sequence and manage data files.	
C3. Run Time		*Score: 2.5*
	As mentioned above, HGSYSTEM is a collection of many modules. In general, all modules take less than a minute to run on a Pentium PC, except for (1) the AEROPLUME module, which might progress slower initially due to a much smaller step size to ensure numerical stability near the source, and (2) the transient version of the HEGADAS module since it involves making many steady-state HEGADAS runs.	
C4. Code Flexibility and Readability		*Score: 3*
	The HGSYSTEM codes, although complex, are also quite modular with plenty of comments. An experienced user can easily customize the codes if necessary.	
D. Cost (Non-Ranking)		
	The HGSYSTEM software package can be ordered through the National Technical Information Service by calling (800)553-6847, order number PB96-501960INC. The price is $152 for U.S., Canada, and Mexico; and $304 for other countries.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	HGSYSTEM source codes are available; however, the user is not allowed to make code changes without explicit licensing agreements with Shell U.K.	
F. Language for Model and GUI (Non-Ranking)		
	HGSYSTEM was developed with the FORTRAN 77 language.	

Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)	**13**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes	**87.9**

4.7 SLAB

Model Name: SLAB	
Person of Contact:	
	Original model developer: Donald L. Ermak Physics Department, Atmospheric and Geophysical Sciences Division Lawrence Livermore National Laboratory P.O. Box 808 Livermore, CA 94550 The software is licensed to: BEE-LINE Software (Contact: Thomas Bowman) 56 Central Avenue, Suite 205 Ashville, NC 28801 Tel (704)258-1895 Fax (704)258-1821
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	*Score: 2.5*
	SLAB (Ermak, 1990) is a model that simulates the dispersion of denser-than-air releases. The model also approaches a Gaussian model for tracer (neutrally-buoyant) releases. The types of releases treated by the model include (1) a ground-level evaporating pool, (2) an elevated horizontal jet, (3) an elevated vertical jet or stack, and (4) an instantaneous or short-duration volume source. The source must be all vapor for release types (1) and (4), but can be two-phase (i.e., a mixture of vapor and liquid droplets) for release types (2) and (3). Transport and dispersion are calculated by solving the conservation equations of mass, momentum, energy, species, and the cloud half-width. The cloud is modeled as either, a steady-state plume, a transient puff, or a combination of both depending on the release duration. In the steady-state plume mode, the cross-wind averaged conservation equations are solved, and all variables depend on the downwind distance. In the transient puff mode, the volume-averaged conservation equations are solved, and all variables depend on the travel time of the puff center of mass. The instantaneous ensemble-averaged concentration is obtained as a solution to the basic conservation equations. The time-averaged concentration at any given

	location is then calculated using the instantaneous ensemble averaged concentration, the concentration averaging time, and the assumed cloud lateral and vertical profiles, accounting for effects such as meandering and along-wind dispersion. In addition to the vertical entrainment rate included in many other dense gas dispersion models, SLAB also includes a crosswind entrainment rate. SLAB uses an equilibrium thermodynamics model to treat liquid droplet formation and evaporation. The model allows droplet formation for both the released pollutant and the entrained ambient water vapor. Plume rise is treated by SLAB for a vertical jet or stack release. The user must specify the source strength for SLAB. SLAB does not have a built-in chemical database. The user needs to manually specify all properties of the chemical of interest in the input data file. However, the user's manual (Ermak, 1990) does include properties for 14 common pollutants, including hydrogen sulfide (sour gas).	
A2. Grid Options for Eulerian and Trajectory Models		***Score: n/a***
	Not applicable.	
A3. Quality of Physical Processes Simulated		***Score: 3***
	The transport and dispersion algorithms included in SLAB are state-of-the-art. In fact, previous model evaluation studies (e.g., Hanna et al., 1993) show that SLAB is among the best-performing toxic release models when compared against field data. Treatments of a finite release duration and along-wind dispersion are also of high quality, and are adopted in other models such as HGSYSTEM (Post, 1994a).	
A4. Sparse Data Treatment		***Score: n/a***
	Not applicable	
A5. Overwater Dispersion		***Score: n/a***
	Not applicable	
A6. Model Evaluation History		***Score: 3***
	SLAB has been subjected to extensive review and evaluation. For example, Hanna et al. (1993) evaluated SLAB with data from the Burro (LNG), Coyote (LNG), Desert Tortoise (NH_3), Goldfish (HF), Maplin Sands (LNG and LPG), and Thorney Islands (mixture of CFC-12 and N_2) field experiments. Touma et al. (1995) also independently evaluated SLAB with data from the Burro, Desert Tortoise, and Goldfish field experiments. They found that SLAB is one of the best-performing models with minimal trend in residual plots, i.e., there is no	

	systematic bias of model performance with independent variables such as downwind distance, wind speed, and atmospheric stability. The model occasionally underpredicted concentrations.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 3***
	SLAB has a user's guide (Ermak, 1990) that includes (1) comprehensive descriptions of technical aspects of the model, (2) user's instructions to run the model, and (3) four representative test cases. The user's guide is available only in hard copy.	
B2. Model Options		***Score: 2.5***
	SLAB treats the following four types of releases: (1) a ground-level evaporating pool, (2) an elevated horizontal jet, (3) an elevated vertical jet or stack, and (4) an instantaneous or short-duration volume source. Depending on the source duration and the pollutant travel time, the model automatically decides whether to use the plume or puff dispersion algorithm without any user intervention. The user has the option of using the Monin-Obukhov length or the conventional stability class to define atmospheric stability.	
B3. Data Preparation Time		***Score: 3***
	It will take less than one man-hour to prepare a SLAB run. Regardless of the release type, the user always needs to deal with one input file with the same file structure. Tasks that are more time-consuming include source characterization, and the specification of pollutant properties. The user's manual (Ermak, 1990) includes properties for 14 common pollutants, including hydrogen sulfide (sour gas).	
B4. Ease of Data Acquisition		***Score: n/a***
	Not applicable, since SLAB does not require data from external data archives.	
B5. Model Interface to Preprocessors / GUI		***Score: n/a***
	Not applicable.	
B6. Run-Time Diagnostics		***Score: 2***
	It appears that SLAB generates only one run-time diagnostic message when the model determines that the source height is greater than the calculated mixing layer height minus the stack half width. The program execution will stop when such condition exists. However, the model does perform many checks internally to verify that the user inputs are physically valid. For example, if the user specifies a source temperature (TS) that is lower than the boiling point temperature of the material (TBP), SLAB then sets TS = TBP. For a two-phase release with a finite initial liquid mass fraction, SLAB always sets TS = TBP	

	regardless of the value of TS specified by the user. The SLAB code is quite robust and rarely "crashes." Program crashes, if any, are usually associated with numerous integration of the conservation equations. The code does not explicitly trap such errors. Using a different (higher) value of NCALC, a numerical substep parameter, often solves the problem.	
B7. Post-Run Diagnostics		***Score: 2***
	The SLAB model generates only tabular outputs of instantaneous and time-averaged cloud properties. However, the output listing includes all the necessary information to recreate the three-dimensional cloud distribution so that the user can visualize the results with external plotting packages.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 1***
	SLAB models one source at a time.	
C2. UNIX / PC Portability		***Score: 3***
	SLAB was developed with standard FORTRAN language. As a result, the code can be easily ported between the UNIX and PC environments.	
C3. Run Time		***Score: 3***
	SLAB takes only a few seconds to run on a Pentium PC.	
C4. Code Flexibility and Readability		***Score: 3***
	Compared to other accidental release models such as HGSYSTEM and DEGADIS, the SLAB code is compact with all modules nicely integrated into a single program unit. (DEGADIS and HGSYSTEM each has about a dozen separate program units, where communication is achieved via intermediate data files.) The code is well documented and clearly written. The code is also modular, thus flexible to include other algorithms.	
D. Cost (Non-Ranking)		
	The SLAB code can be downloaded from EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/) with no cost. There are commercial versions of the Graphical User Interface (GUI) programs available for SLAB. These GUI programs always use the basic numerical code that is available from SCRAM.	
E. Availability / Restrictions / Terms (Non-Ranking)		

	As mentioned above, the source code is available to the public. The user can make code changes for personal use. Bowman Environmental Inc. owns the commercial software license of SLAB.	
F. Language for Model and GUI (Non-Ranking)		
	SLAB was written in FORTRAN 77. The public-domain version of SLAB does not have a GUI program.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**12**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**86.7**

4.8 TSCREEN

Model Name: TSCREEN (Version 95260)	
Person of Contact:	
	Mr. Jawad S. Touma Office of Air Quality Planning and Standards MD-14 U.S. Environmental Protection Agency Research Triangle Park, North Carolina 27711 Tel (919)541-5381 E-mail touma.joe@epa.gov
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	*Score: 2*
	TSCREEN (USEPA, 1994b) is a screening tool for toxic air pollutant concentrations. It is intended to be used in conjunction with EPA's *Workbook of Screening Techniques for Assessing Impacts of Toxic Air Pollutants* (USEPA, 1992d). Since TSCREEN is mainly used for screening, it will automatically select meteorological conditions based on the criteria given in the EPA Workbook. This is different from all other models reviewed in this section where the user specifies meteorological conditions. TSCREEN is a modeling system that consists of the following components: • A front-end (or user-interface) module • Four distinct dispersion modules (SCREEN2, PUFF, RVD, and B&M) • A chemical database The front-end module is mainly used to (1) provide a user-interface where data are entered via a series of menus and screens, (2) perform the source term calculations according to the formulas listed in the Workbook (USEPA, 1992d), (3) provide enough information to run the dispersion modules listed below, and (4) display the final model results in text and graphics. The SCREEN2 model (USEPA,1988) is for continuous releases of non-dense pollutants. The model treats building downwash and terrain effects. The PUFF model (Petersen, 1982) is for instantaneous releases of non-dense pollutants, where terrain effects are treated. The RVD model (USEPA, 1989) is for continuous and instantaneous releases of denser-than-air gases from vertical jets. The B&M model (Britter and McQuaid, 1989) is for continuous and

	instantaneous releases of denser-than-air gases. RVD and B&M do not treat terrain. Each dispersion module still maintains its own identity and modeling assumptions. There was no attempt to make these modules more consistent with one another. Therefore, it is possible that two very similar release scenarios, because of the way the release types are categorized, might be simulated by two different dispersion modules, thus leading to results that are quite different. The default chemical database that comes with TSCREEN contains only seven chemicals. The database can be updated if necessary.	
A2. Grid Options for Eulerian and Trajectory Models		***Score: n/a***
	Not applicable.	
A3. Quality of Physical Processes Simulated		***Score: 1.5***
	SCREEN2 (USEPA, 1988) and PUFF (Petersen, 1982) are will known Gaussian dispersion models that have been used in the past decades. In essence, SCREEN2 and PUFF are simplified versions of the USEPA regulatory models ISC3 (USEAP, 1995b) and INPUFF (Petersen and Lavdas, 1986), respectively. (INPUFF is also reviewed in this report.) The RVD model (USEPA, 1989) is based on empirical formulas derived from a series of wind tunnel experiments on elevated, vertically-oriented momentum jets (Hoot et al., 1973). The RVD model predicts the highest plume rise, the plume touchdown distance and the associated concentration, and the ground-level concentration farther downwind. The B&M model is an implementation of the nomograms presented in the workbook by Britter and McQuaid (1989). The nomograms were developed based on data from field and wind tunnel experiments. At distances far away from the source where dense gas effects are not important, a dense cloud should behave like a neutrally-buoyant cloud. However, it is not clear whether these nomograms are asymptotic to the passive SCREEN2 and PUFF dispersion modules at neutral limit. For a continuous two-phase saturated liquid release from a pressurized storage, the front-end module of TSCREEN calculates the vapor fraction after depressurization (flashing). This fraction in turn is used to calculate the aerosol density. Therefore, due to the presence of aerosols, a cloud could still be denser than air even if the molecular weight of the released material is smaller than that of air. In this case, the TSCREEN front-end module will invoke the RVD module for dispersion calculations if the release is vertically-oriented. In RVD, however, we found that the information just obtained regarding aerosols was completely ignored, and the module again determines whether the cloud is	

	denser than air based on only the molecular weight and temperature of the released material. If RVD thinks the release is buoyant, zero concentrations will be predicted. TSCREEN does not treat multi-component releases.	
A4. Sparse Data Treatment		***Score: n/a***
	Not applicable.	
A5. Overwater Dispersion		***Score: n/a***
	Not applicable.	
A6. Model Evaluation History		***Score: 3***
	The SCREEN2 and PUFF modules are based on well-known Gaussian plume and puff models, respectively, that have been extensively evaluated in the past. The RVD module was developed and validated with many wind tunnel experiments. Hanna et al. (1993) evaluated the B&M model with dense-gas dispersion data from the Burro (LNG), Coyote (LNG), Desert Tortoise (NH_3), Goldfish (HF), Maplin Sands (LNG and LPG), and Thorney Islands (mixture of CFC-12 and N_2) field experiments. Good model performance was found.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 3***
	The user's guide of TSCREEN (USEPA, 1994b) is brief but complete. It provides instructions on how to define a new release scenario, revise an existing scenario, execute the dispersion module, use the HELP system, and inspect the results. The interface between the front-end module of TSCREEN and various dispersion modules is achieved via ASCII data files. An experienced modeler might be interested in the formats of these files for the purpose of batch processing. However, the user's guide does not provide such information. The *Workbook of Screening Techniques for Assessing Impacts of Toxic Air Pollutants* (USEPA, 1992d) provides detailed descriptions of how to calculate the source term for more than 20 kinds of release scenarios plus worked examples.	
B2. Model Options		***Score: 1.5***
	TSCREEN can treat more than 20 types of release scenarios. These release scenarios eventually lead to continuous or instantaneous releases of buoyant or denser-than-air gases. (Note that a vapor cloud might originally come from a liquid release.)	

	As mentioned above, since TSCREEN is a screening tool, it will automatically select worst-case meteorological conditions based on the criteria given in the EPA Workbook. Therefore, the user does not have the option of specifying a particular meteorological condition.	
B3. Data Preparation Time		***Score: 2.5***
	It will take less than one-hour to prepare a TSCREEN run. However, the procedure where the user moves through a series of screens in order to specify the input data is a little tedious, because excessive number of keystrokes are needed. The source term calculations performed by the front-end module TSCREEN are helpful when the release rate is unknown.	
B4. Ease of Data Acquisition		***Score: n/a***
	Not applicable, since TSCREEN does not require data from external data archives.	
B5. Model Interface to Preprocessors / GUI		***Score: 1.5***
	To start a simulation, TSCREEN presents a series of questions arranged in a logical fashion in order to identify the appropriate type of scenario. The user provides information such as the source geometry and chemical properties of the pollutant that are required for the source term calculations. TSCREEN then decides which dispersion module to use and prepares the data necessary to run that module. Chemical properties of the pollutant can be directly specified by the user or retrieved from a chemical database, which includes only seven chemicals. Retrieval of chemical properties is very inefficient, since only one property can be retrieved at a time. Thus, the chemical database will have to be consulted repeatedly in order to retrieve all properties associated with a pollutant. To make things even worse, it generally takes five to eight keystrokes to move between menus (or screens) in order to retrieve a value from the database. As a result, using the chemical database is almost counter-productive. TSCREEN's chemical database should have been implemented like most other models, where the user first selects a chemical. Once a chemical is selected, all properties for that chemical are simultaneously retrieved.	
B6. Run-Time Diagnostics		***Score: 2***
	If an error occurs while the TSCREEN user-interface is running, an error message window will be displayed showing the error number, and the subroutine and line number where the error occurred. The error information will also be saved to a disk file called ERROR.OUT. If an error occurs while one of the dispersion modules is running, then the ERROR.OUT file will contain the data that were used to run the module, but not the reason why the error occurred.	
B7. Post-Run Diagnostics		***Score: 2***

	After the dispersion module completes its calculations, the model output listing will be displayed on the screen, including tabulation of predicted concentrations as a function of downwind distance. The same information can also be plotted. Because TSCREEN is still DOS-based software, the number of output devices (i.e., printers and plotters) supported is limited. Since TSCREEN includes four distinct dispersion modules, different types of information will be predicted depending on which module was used. For example, for SCREEN2, the plume width information is calculated and output; for PUFF, the puff width information is calculated but not output. RVD and B&M do not calculate the plume or puff width information. This inconsistency in model outputs is sometimes confusing.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: 1***
	TSCREEN treats one source at a time.	
C2. UNIX / PC Portability		***Score: 1***
	TSCREEN runs only on the PC platform.	
C3. Run Time		***Score: 3***
	TSCREEN takes only a few seconds to run on a Pentium PC.	
C4. Code Flexibility and Readability		***Score: 2.5***
	The source code for the four dispersion modules in TSCREEN is quite flexible and has many comments. Modifying the code is relatively straightforward.	
D. Cost (Non-Ranking)		
	TSCREEN can be downloaded from EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/) at no cost.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	The source code of TSCREEN is available to the public. The user can make code changes for personal use. However, since the interface of TSCREEN was developed with an outmoded version of the FoxFro database management system, and requires the commercial INGRAF graphical library (see below), any changes that involve the interface might be difficult to implement.	

F. Language for Model and GUI (Non-Ranking)		
	The user-interface of TSCREEN was developed with the DOS version of the FoxPro database management system, which has been superseded by Microsoft's Visual FoxPro for Windows. Graphics in TSCREEN was developed with Microsoft C Version 5.1, where routines in the INGRAF C library by Sutrasoft are called. The SCREEN2, PUFF, and B&M dispersion modules were developed with FORTRAN 77. The RVD dispersion module was developed with BASIC.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**13**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**68.9**

4.9 BREEZE HAZ SUITE

Model Name: BREEZE HAZ SUITE (DEGADIS+/EXPERT) - Release 1.0

Person of Contact:

Brian Harvey (or Thomas Grosch)
Trinity Consultants, Inc.
P.O. Box 14205
Research Triangle Park, NC 27709-4205
Tel (919)549-0499
Fax (919)549-0273
E-mail bharvey@trinityconsultants.com (or tgrosch@trinityconsultants.com)

A. Science and Credibility (Ranking)

A1. Technical and General Descriptions — *Score: 3*

BREEZE HAZ SUITE (Trinity Consultants, 1997) unites a suite of publicly-available toxic release models, including AFTOX (Kunkel, 1988), DEGADIS (Spicer and Havens, 1990), INPUFF (Petersen and Lavdas, 1986), and SLAB (Ermak, 1990), by providing a common graphical user interface with standardized menus, commands, and toolbars. Common data such as station, meteorological, and chemical can be shared among different models. The software also includes a proprietary tool, EXPERT, to perform source-term calculations, which greatly increases the usefulness of the software. The software runs under Microsoft's various Windows environments.

The reader is referred to the corresponding review tables concerning the technical information on the AFTOX, DEGADIS, INPUFF, and SLAB models. Only the interface to DEGADIS (called DEGADIS+) and the EXPERT source-term module are reviewed in the following.

EXPERT estimates the source terms (e.g., rate, temperature, partition of vapor and liquid, concentration and density) for the following types of release:

two-phase (gas and liquid, choked and unchoked),
single-phase gas,
single-phase high-volatility liquid, and
single-phase low-volatility liquid.

The source term information calculated by EXPERT is then used to drive dispersion models such as DEGADIS+ and SLAB. Although the source terms might be time varying for certain types of releases, EXPERT applies a conservative approach by assuming the maximum emission rate over the release

	duration. Therefore, EXPERT does not support transient releases. BREEZE HAZ SUITE includes station, meteorological, chemical, and source databases. The station database contains information such as location, anemometer height, and surface roughness for different stations. The meteorological database contains information such as wind speed, temperature, atmospheric stability for different weather conditions. The chemical database includes properties for over 200 chemicals, including hydrogen sulfide (sour gas). The source database contains information such as geometry and storage state for different release configurations. All databases can be updated by the user. The user can use the information previously entered to various databases to define a new scenario. This is very useful if, for example, the user wants to model a number of releases with the same meteorological conditions.	
A2. Grid Options for Eulerian and Trajectory Models		***Score: n/a***
	See discussions for the generic DEGADIS model.	
A3. Quality of Physical Processes Simulated		***Score: 3***
	See also technical discussions for the generic DEGADIS model. The DEGADIS+ code is slightly expanded from the original DEGADIS code to allow more observers for numerical integration for transient releases and one additional concentration level of interest (with a total of three levels). Some of the array limits in the original DEGADIS model were also relaxed. The EXPERT source module treats a wide range of release types, such as two-phase (both choked and unchoked), single phase gas, and single phase liquid (both low and high volatility). The source term algorithms are comparable to those included in, for example, the AIChE (1996) workbook and the proprietary CANARY (Quest Consultants, 1997) model. The EXPERT module can also conduct sensitivity analysis, through which the user can study the effects of variations in source term parameters on the emission rate.	
A4. Sparse Data Treatment		***Score: n/a***
	See discussions for the generic DEGADIS model.	
A5. Overwater Dispersion		***Score: n/a***
	See discussions for the generic DEGADIS model.	
A6. Model Evaluation History		***Score: n/a***
	See discussions for the generic DEGADIS model.	
B. Ease of Use (from User's Perspective) (Ranking)		

B1. User's Guide		*Score: 3*
	BREEZE HAZ SUITE has a comprehensive user's guide (Trinity Consultants, 1997) that includes user instructions for various modules and technical discussions of source-term estimation and dispersion modeling concepts. The technical discussions are detailed and up-to-date. There are adequate discussions of model limitations and assumptions, which should further prevent misuse of models. The user's guide has an index, which is unique among all the user's guides reviewed. The index is found to be extremely helpful.	
B2. Model Options		*Score: n/a*
	See discussions for the generic DEGADIS model.	
B3. Data Preparation Time		*Score: 3*
	See discussions for the generic DEGADIS model. It takes even less time to prepare a DEGADIS+ run, mainly because the built-in chemical database and the EXPERT source module.	
B4. Ease of Data Acquisition		*Score: n/a*
	See discussions for the generic DEGADIS model.	
B5. Model Interface to Preprocessors / GUI		*Score: 3*
	BREEZE HAZ SUITE provides an integrated environment with standardized menus for dispersion models such as AFTOX, DEGADIS, INPUFF, and SLAB. The layout of menus is intuitive, logical, and structured. All dispersion codes require the user to explicitly specify the source term. (The only exception is for AFTOX where it can calculate the evaporation rate for a liquid pool.) For that purpose, BREEZE HAZ SUITE also includes the EXPERT module that estimates the source term. All dispersion codes share common databases, including station, chemical, meteorological, and source. As a result, it is efficient to model the same scenario with different dispersion codes, or to conduct sensitivity studies for the same scenario. After the EXPERT source module is run, depending on the release type, BREEZE HAZ SUITE recommends which dispersion model to use. For example, DEGADIS+ is recommended for a vertical jet release and a denser-than-air evaporating pool release, SLAB is recommended for a horizontal jet release, and AFTOX is recommended for a neutrally buoyant release. The model selection is somewhat arbitrary. For example, DEGADIS+, SLAB, and AFTOX all treat neutrally buoyant releases; DEGADIS+ and SLAB both treat denser-than-air evaporating pool releases. The user could override the recommendation if necessary.	

	The original DEGADIS code does not directly treat aerosol (two-phase) releases. Spicer and Havens (1990) recommend that the *isothermal* option in the model be selected for a two-phase release, where the user needs to specify a set of "triplets" of the chemical concentration and mixture density as a function of the chemical mole fraction. The user usually has to perform their own calculations based on adiabatic mixing of ambient air with the chemical in order to obtain the necessary data. This is the area where the GUI program could excel and greatly speed up data preparation. Unfortunately, DEGADIS+ does not provide additional help in this area. BREEZE HAZ SUITE has a comprehensive on-line help system. There is a "Help" button on the main tool bar, and on each menu screen. The software has value-added tools that help the user calculate parameters such as the Richardson number, the flash ratio, and the mixture bulk density. The software also allows the user to edit the parameter files for DEGADIS, although this is recommended for advanced users only.	
B6. Run-Time Diagnostics		***Score: 2.5***
	See also discussions for the generic DEGADIS model. All error messages generated by the original DEGADIS code will be displayed by DEGADIS+ in a dialog box. DEGADIS+ also provides additional information such as which subroutine issued the error message and suggestions to correct the problems.	
B7. Post-Run Diagnostics		***Score: 3***
	After a DEGADIS+ run is completed, the software automatically displays (1) the output listing generated by the DEGADIS+ code, (2) a plot of ground-level centerline concentration as a function of downwind distance, and (3) a contour plot with three concentration levels of interest. The output listing generated by DEGADIS+ is essentially the same as the generic DEGADIS code, except that the width information for a third concentration of interest is added. DEGADIS+ accepts base maps in the AutoCAD DXF or Windows bitmap format. For example, the user can import an AutoCAD drawing of the area of interest, identify the source location on the drawing by a mouse click, DEGADIS+ will then automatically position the plume contours on the base map.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: n/a***
	See discussions for the generic DEGADIS model.	
C2. UNIX / PC Portability		***Score: 1***

	The software runs only on the PC platform.	
C3. Run Time		***Score: n/a***
	See discussions for the generic DEGADIS model.	
C4. Code Flexibility and Readability		***Score: n/a***
	Not applicable, since the source codes are not available.	
D. Cost (Non-Ranking)		
	As mentioned above, BREEZE HAZ SUITE includes five modules, AFTOX, DEGADIS+, INPUFF, SLAB, and EXPERT. The complete package can be purchased at $2,900. Each module can also be purchased separately, with AFTOX: $400; DEGADIS+: $1,500; INPUFF: $500; SLAB: $1,500; and EXPERT: $900. Technical support is free. Software upgrade is available through the maintenance plan, which is free for the first three months, and then with the following annual fees: AFTOX: $100; DEGADIS+: $380; INPUFF: $130; SLAB: $380; EXPERT: $230; and the complete BREEZE HAZ SUITE: $730. Federal and state agencies can obtain the software for free. Universities can obtain the software at 50% discount.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	The software is distributed in diskettes, CD-ROMs, or E-mail. The option of downloading the software through the World Wide Web will be available in a few months. The package includes executable codes only. Source codes for the graphical user interface program (i.e., BREEZE HAZ SUITE) and the EXPERT model are proprietary. Source codes for public-domain dispersion models such as AFTOX, INPUFF, DEGADIS, and SLAB are available from the EPA SCRAM bulletin board (http://www.epa.gov/ttn/scram/). If necessary, the user can make changes to these models. An example would be DEGADIS+, an enhanced version of DEGADIS .	
F. Language for Model and GUI (Non-Ranking)		
	BREEZE HAZ SUITE and the EXPERT model were developed using Microsoft's Visual BASIC. The SLAB, DEGADIS, and INPUFF models were developed in FORTRAN 77. The AFTOX model was developed in Quick	

	BASIC.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**8**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**93.3**

4.10 SLAB View

Model Name: SLAB View	
Person of Contact:	
	Dr. Jesse L. Thé Lakes Environmental Consultants, Inc. 250 Keats Way, Unit 18 Waterloo, Ontario N2L 6J5 Canada Tel (519)746-6157 Fax (519)746-0793 E-mail jesse@lakes-environmental.com
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	***Score: 2.5***
	SLAB View (Lakes Environmental, 1997) is a graphical user interface for the SLAB dispersion model (Ermak, 1990). It provides an integrated environment where the user can easily set up the input, run the SLAB model, and graphically display the results. The software runs under Microsoft's various Windows environments. The reader is referred to the corresponding review table for more technical information on the SLAB model. *SLAB View* has a database that includes properties for about 200 chemicals, including hydrogen sulfide (sour gas). The database can be updated to include new chemicals. The current version of the software provides some additional technical features for SLAB. For example, *SLAB View* can calculate the initial liquid mass fraction and the equivalent source area for a two-phase release. With the generic version of SLAB, the user needs to perform his own calculations. Similar to SLAB, *SLAB View* does not calculate the source strength. (According to the developer, a future version of the software will include a source term module.)
A2. Grid Options for Eulerian and Trajectory Models	***Score: n/a***
	See discussions for the generic SLAB model.
A3. Quality of Physical Processes Simulated	***Score: n/a***
	See discussions for the generic SLAB model.

A4. Sparse Data Treatment		***Score: n/a***
	See discussions for the generic SLAB model.	
A5. Overwater Dispersion		***Score: n/a***
	See discussions for the generic SLAB model.	
A6. Model Evaluation History		***Score: n/a***
	See discussions for the generic SLAB model.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 3***
	SLAB View comes with a comprehensive user's guide (Lakes Environmental, 1997) that describes (1) a tutorial, (2) setup and input options, and (3) output options. The user's guide is well written and the page layout is of high-quality. Many screen samples are included to illustrate various features of the program. A copy of the user's manual for the generic SLAB model (Ermak, 1990) is also included.	
B2. Model Options		***Score: n/a***
	See discussions for the generic SLAB model.	
B3. Data Preparation Time		***Score: 3***
	See discussions for the generic SLAB model. The data preparation time is even less with *SLAB View*, mainly because the chemical properties are now available through a chemical database.	
B4. Ease of Data Acquisition		***Score: n/a***
	See discussions for the generic SLAB model.	
B5. Model Interface to Preprocessors / GUI		***Score: 3***
	SLAB View provides an intuitive menu-driven environment where the user can easily prepare and analyze a SLAB model run. The program runs under various Microsoft Windows environments. The *Input Options* menu of *SLAB View* allows the user to specify all the necessary information to make a SLAB model run. Depending on the release type, the *Input Options* menu knows what input parameters are not required. For example, for an evaporating pool release, the user does not need to specify the source height, which defaults to zero, and the source mass, which is relevant only for an instantaneous release. Input parameters such as the initial liquid	

	mass fraction and the equivalent source area can be internally calculated by *SLAB View* if necessary. The user is required to hand calculate these parameters when running SLAB and other GUI programs for SLAB. Like the original SLAB model, *SLAB View* also supports multiple meteorological conditions for the same release scenario in one model run. *SLAB View* has a state-of-the-art help system. The user can access conventional on-line help via the "help" button on various menu screens, where the help information is mostly derived from Section 3 of the user's manual for the original SLAB model (Ermak, 1990). In addition, concise help information is automatically displayed whenever the user clicks on a certain input field. *SLAB View* accepts a base map in many formats, including DXF (Drawing Interchange Format from Autodesk), BMP (Windows bitmap), DLG (Digital Line Graphs from USGS), LU/LC (Land Use/Land Cover data from USGS), and ArcView 5 (from ESRI). *SLAB View* can overlay concentration contours on the base map to provide a perspective of the potential impacts resulting from an accidental release of toxic chemicals. The user can import an existing SLAB input file to *SLAB View*. This feature is useful for an experienced user who prefers to run the generic SLAB model in batch mode to efficiently make many model simulations, and then use *SLAB View* as a tool to graphically display the results. *SLAB View* allows the user to specify a wind direction (not required by the SLAB model) so that the cloud footprint can be properly aligned on the base map. The angle denotes the direction *towards* which the wind is blowing, e.g., 45° means that the wind is blowing towards the northeast (southwesterly). This is different from the convention used in meteorology where the angle denotes the direction *from* which the wind is blowing, e.g., 45° means that the wind is blowing from the northeast (northeasterly).	
B6. Run-Time Diagnostics		***Score: 1.5***
	See also discussions for the generic SLAB model. *SLAB View* does not trap run-time errors that occur within the SLAB code. However, the software does conduct a comprehensive quality check on the user inputs to eliminate potential run-time errors. Whenever a run-time error occurs, *SLAB View* simply prompts the user to check input parameters for validity.	
B7. Post-Run Diagnostics		***Score: 3***
	After a SLAB run is completed, *SLAB View* generates high-quality plots to display modeling results. The plots include (1) time-averaged plume footprint, (2) instantaneous puff contours at certain output times internally determined by SLAB, and (3) centerline concentration versus downwind distance. The user can customize the plots (e.g., change axis scale, tick marks, colors, shading, and labels) to further enhance the appearance.	

	The program does not give the user direct access to the output listing file generated by the generic SLAB model.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: n/a***
	See discussions for the generic SLAB model.	
C2. UNIX / PC Portability		***Score: 1***
	The *SLAB View* software runs only on IBM-compatible personal computers.	
C3. Run Time		***Score: n/a***
	See discussions for the generic SLAB model.	
C4. Code Flexibility and Readability		***Score: n/a***
	Not applicable, since the source code is not available.	
D. Cost (Non-Ranking)		
	Government agencies can obtain the software and technical support free of charge. For commercial users, the cost of the software is $1,750, which also covers first year's technical support. Technical support for each additional year is $400.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	SLAB's source code is available to the public via EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/). The *SLAB View* software is available from the model developer in diskettes. Only executable code is included in the package. The source code is proprietary.	
F. Language for Model and GUI (Non-Ranking)		
	The generic version of the SLAB model is written in FORTRAN 77. The *SLAB View* software is written in Borland's Delphi and C++.	

Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)	**7**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes	**84.6**

4.11 SLAB for Windows

Model Name: SLAB for Windows	
Person of Contact:	
	Dick Perry BEE-Line Software P.O. Box 7348 Asheville, NC 28802 Tel (704)258-1895 (the 704 area code is to be changed to 828 in a few months from 3/98) Fax (704)258-1821 E-mail dperry@beeline-software.com
A. Science and Credibility (Ranking)	
A1. Technical and General Descriptions	***Score: 2.5***
	The *SLAB for Windows* software (Bowman Environmental, 1997) is a graphical user interface (GUI) program for the public-domain SLAB model (Ermak, 1990). The software runs under Microsoft's various Windows environments, including 3.1, 95, and NT. The reader is referred to the corresponding review table for more technical information on the SLAB model. The *SLAB for Windows* software provides value-added features such as: • a menu-driven environment in which the user can prepare the inputs and analyze the results for a SLAB application, • a chemical database that includes properties for nearly 400 chemicals, including hydrogen sulfide (sour gas) • an on-line help system, and • presenting modeling results in various graphical forms, including centerline concentration vs. downwind distance and concentration contours. The user can enter new chemicals to the chemical database if necessary. The current version of the software does not provide any additional technical features for SLAB. For example, it is still the user's responsibility to estimate the initial liquid mass fraction for a two-phase release, and to perform source term calculations to determine the source strength. A new version including a source term module is under development.
A2. Grid Options for Eulerian and Trajectory Models	***Score: n/a***
	See discussions for the generic SLAB model.

A3. Quality of Physical Processes Simulated		***Score: n/a***
	See discussions for the generic SLAB model.	
A4. Sparse Data Treatment		***Score: n/a***
	See discussions for the generic SLAB model.	
A5. Overwater Dispersion		***Score: n/a***
	See discussions for the generic SLAB model.	
A6. Model Evaluation History		***Score: n/a***
	See discussions for the generic SLAB model.	
B. Ease of Use (from User's Perspective) (Ranking)		
B1. User's Guide		***Score: 2***
	SLAB for Windows has a brief 12-page user's guide providing instructions on the use of the software. Since (1) the input requirements for the SLAB model are simple, (2) the program design of *SLAB for Windows* is quite logical and intuitive, and (3) much technical information has already been included in the on-line help system, the user's guide, although brief, is adequate.	
B2. Model Options		***Score: n/a***
	See discussions for the generic SLAB model.	
B3. Data Preparation Time		***Score: 3***
	See discussions for the generic SLAB model. The data preparation time for *SLAB for Windows* is further reduced mainly due to the fact that the user now has instant access to properties for nearly 400 chemicals.	
B4. Ease of Data Acquisition		***Score: n/a***
	See discussions for the generic SLAB model.	
B5. Model Interface to Preprocessors / GUI		***Score: 2.5***
	The *SLAB for Windows* software provides an easy-to-use, intuitive graphical user interface to the SLAB dispersion model. The integration of a comprehensive chemical database is especially helpful in helping the user prepare the required input data for SLAB. The *Manual Data Entry* screen of the software allows the user to specify all SLAB input parameters in a nicely-designed menu-driven environment.	

	Information on any data entry is provided via an on-line help system. The text included in the help system is mostly derived from Section 3 of the user's manual for the original SLAB model (Ermak, 1990), with other useful tips such as references to related EPA documents, and recommended data values for regulatory applications. Depending on the release type, the software knows whether a data entry is mandatory or optional. For example, for an evaporating pool release, the software does not require the user to specify the release height, since it must be zero; and the software does not require the user to specify the source mass, since it will be the product of the source emission rate and the duration specified by the user. After the user completes the *Manual Data Entry* screen and clicks the *Run SLAB Model* button to perform dispersion calculations, the software will first display and verify all data entries that have been specified by the user. The SLAB model will not run if there is any missing data. The input file prepared by *SLAB for Windows* is ASCII. However, the file structure is not the same as that for the generic version of SLAB. The original SLAB model supports multiple meteorological conditions for the same source configuration in a single model run. For example, the user can investigate the fate of pollutants from the same release under stable/light wind and neutral/moderate wind conditions in one model run. However, *SLAB for Windows* does not support such feature. *SLAB for Windows* does not support the import of a base map over which plume contours can be plotted.	
B6. Run-Time Diagnostics		***Score: 2***
	See also discussions for the generic SLAB model. The *SLAB for Windows* software also traps numerical errors of SLAB and provides suggestions to the problems. (Note that numerical errors rarely occur.)	
B7. Post-Run Diagnostics		***Score: 2***
	After a SLAB model run is completed, the user can view the distribution of centerline concentration as a function of downwind distance (or the c-x plot). The same plot also displays markers for the fenceline and toxic endpoint, by which the user can estimate potential impacts due to the release. Concentration contour plots are also available, provided that the user has purchased and installed a separate SURFER plotting package developed by Golden Software. The SURFER software is automatically launched by *SLAB for Windows* via a macro script (BAS) file. Since the macro script file is quite short (less than 10 lines) and simple, the contour plot thus created has a	

	relatively primitive appearance. For example, contours are not properly labeled; contour intervals are internally decided by SURFER, which might not always be satisfactory; and there are no titles on plot axes. It would be nice if the contour for the toxic endpoint of interest is also plotted to indicate so-called toxic area. Of course, the user can adjust the appearance of the contour plots within SURFER if necessary. The user can also save the regular output listing generated by the SLAB model to a file.	
C. Computation Requirements (Ranking)		
C1. Multiple Sources		***Score: n/a***
	See discussions for the generic SLAB model.	
C2. UNIX / PC Portability		***Score: 1***
	The *SLAB for Windows* software runs only on IBM-compatible personal computers.	
C3. Run Time		***Score: n/a***
	See discussions for the generic SLAB model.	
C4. Code Flexibility and Readability		***Score: n/a***
	Not applicable, since the source code is not available.	
D. Cost (Non-Ranking)		
	The cost is $950 for the software and technical support for the first year, with no difference between government agencies and commercial companies. Software service contact for each additional year can be purchased at about 20% of the software list price.	
E. Availability / Restrictions / Terms (Non-Ranking)		
	SLAB's source code is available to the public via EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/). The *SLAB for Windows* software is available from the model developer in diskettes. Only executable code is included in the package. The source code is proprietary.	

F. Language for Model and GUI (Non-Ranking)		
	The generic version of the SLAB model is written in FORTRAN 77. The *SLAB for Windows* software is written in Microsoft's Visual Basic.	
Total Number of Applicable Ranking Attributes (Out of the 17 Considered Above)		**7**
Normalized Composite Score (0 to 100) Based on Applicable Ranking Attributes		**74.4**

4.12 SUMMARY AND RECOMMENDATIONS

In this section, we reviewed seven toxic release models: AFTOX, ARCHIE, CANARY, DEGADIS, HGSYSTEM, SLAB, and TSCREEN; and three graphical user interface (GUI) programs: BREEZE HAZ SUITE, SLAB View, and SLAB for Windows. BREEZE HAS SUITE provides a GUI to DEGADIS, SLAB, and AFTOX, but only the GUI to DEGADIS was reviewed here. As suggested by their names, SLAB View and SLAB for Windows provide a GUI to SLAB. The scores for all models are summarized in Table 4-1. Section 1 describes the evaluation methodology and criteria.

AFTOX, ARCHIE, DEGADIS, HGSYSTEM, SLAB, and TSCREEN are in the public domain. However, the source code for ARCHIE is not available. Modifications to the HGSYSTEM code require prior permission from the model developers, Shell Research in U.K. CANARY, BREEZE HAZ SUITE, SLAB View, and SLAB for Windows are proprietary; their source codes are not available. The public-domain models are available for free, or with a nominal fee (a few hundred dollars) for the printing cost of the user's guides. BREEZE HAZ SUITE and SLAB View, although proprietary, are available for free to government agencies such as the MMS. The prices for SLAB for Windows and CANARY are $950 and $5,000, respectively. All models are mainly designed to run on the PC platform.

All proprietary models are actively supported and maintained by their developers. In addition to the GUI programs, the developers for BREEZE HAZ SUITE, SLAB View, and SLAB for Windows also support the dispersion codes, i.e., AFTOX, DEGADIS, and SLAB, which they did not develop. (We emphasize that AFTOX, DEGADIS, and SLAB have not been updated in ten years.) HGSYSTEM is still maintained and updated by Shell Research in U.K. However, a formal technical support policy is not in place. ARCHIE is essentially an "orphan" model with no support or update.

The models reviewed here estimate the consequences of accidental releases of hazardous air pollutants. All models except AFTOX and ARCHIE treat denser-than-air area-source releases, and approach Gaussian (neutrally buoyant) dispersion when the plume is sufficiently diluted. However, there are basically only three types of heavy-gas dispersion algorithms. HGSYSTEM's dispersion algorithm is also found in DEGADIS, and the DEGADIS+ module in BREEZE HAZ SUITE. SLAB's dispersion algorithm is also found in CANARY, SLAB View, and SLAB for Windows. TSCREEN's dispersion algorithm is based on the nomograms in Britter and McQuaid (1989). Previous model evaluation studies (e.g., Hanna et al., 1993) showed that all algorithms are comparable. However, the HGSYSTEM algorithm tends to predict a cloud height that is too shallow. This affects mainly on the cloud width rather than the cloud centerline concentration. TSCREEN does not predict the cloud width information.

Most models also treat releases that are initially dominated by momentum effects (e.g., due to pressurization). The AEROPLUME module in HGSYSTEM can handle a jet release with arbitrary orientation. Other models deal with either a horizontal or a vertical jet release. We liked SLAB's formulation where the same set of government equations is used to describe the complete release from the near-source region to the far field. Other models such as HGSYSTEM and DEGADIS use distinctly different modules to handle different dispersion regimes, e.g., airborne and ground-based. Thus, "kinks" sometimes exist in, for example, plots of centerline concentration with downwind distance.

Unlike a routine release, the source term of an accidental release is usually unknown. Therefore, the presence of a source-term module will greatly add to a model's usefulness. Out of the models reviewed,

ARCHIE, CANARY, HGSYSTEM, TSCREEN, and the EXPERT module in BREEZE HAZ SUITE can calculate source terms. This is the reason why these models scored relatively higher in the "Technical and General Descriptions" and "Quality of Physical Processes Simulated" categories. There are varying degrees of sophistication in estimating the source term. For example, ARCHIE and EXPERT use simple empirical equations to estimate a constant source term. HGSYSTEM, on the hand, could provide a complete description of the time evolution of the evaporation rate, pool size, pool temperature, pool composition, and cloud composition for an evaporating pool release (diked or undiked).

HGSYSTEM and DEGADIS allow the user to explicitly specify a time-varying release rate. This is useful in investigating the effectiveness of possible mitigation measures. CANARY could *internally* estimate and use a time-varying release rate.

All models allow the user to specify arbitrary meteorological conditions, except for TSCREEN. This is because TSCREEN is mainly used for screening purpose.

The vapor cloud will ignite or explode for flammable gases. ARCHIE and CANARY are the only two models that provide explicit estimates of fire and explosion hazards. The fire hazards are usually in terms of a radiant heat dose that will potentially cause second-degree burns. The explosion hazards are usually in terms of overpressure that will cause property damage or bodily injury. DEGADIS and HGSYSTEM use numerical integration to estimate the plume mass that is within the upper and lower flammability limits of the chemical, but do not proceed to calculate the potential impacts.

All models simulate one source at a time with a time-invariant meteorological condition. For planning purposes, a hypothetical meteorological condition, such as low-wind stable, is usually used. Therefore, the evaluation criteria of "Ease of Data Acquisition" and "Sparse Data Treatment" are not relevant, unlike the Eulerian photochemical models reviewed in Section 2.

All models assume that dispersion occurs over land with a uniform surface roughness, except for the HEGADAS module of HGSYSTEM that allows spatially varying surface roughness. None of the model was developed with overwater applications in mind, since most accidental releases occur over land. Therefore, the evaluation criteria of "Overwater Dispersion" does not apply. If these models are to be run over water, one suggestion is to use an adjusted stability class depending on the climatology of the difference between the air and sea surface temperatures. For example, the marine boundary layer over the eastern Gulf of Mexico is slightly convective most of the year because the sea surface temperature is higher than the air temperature (Hsu, 1997). Thus, a stability class "C" probably should be used for the models even the stability class determined by land-based methods shows otherwise.

The typical spatial scale treated by the models is on the order of a few kilometers. Applying these models to a distance beyond, for example, 10 km, is not recommended. This is mainly because by the time the toxic plume travels that far, the meteorological conditions may have already changed.

The user's guides for the models range from less than 20 pages (such as CANARY and SLAB for Windows) to many hundred pages (such as HGSYSTEM). The difference is mainly in the technical discussions of the models. All user's guides, long and short, provide adequate instructions on the use of the models.

The generic version of SLAB does not have any user interface program. However, the program is very easy to use, where the user needs to prepare only one short input control file. AFTOX, HGSYSTEM and

the generic version of DEGADIS have text-based user interfaces, where the user is basically prompted by a series of questions in order to completely specify a simulation. The latter two models can also be run in batch mode. ARCHIE, CANARY, and TSCREEN have slightly more advanced text-based user interfaces with rudimentary menus and some on-line help.

AFTOX, CANARY, DEGADIS, HGSYSTEM, and TSCREEN have built-in chemical database. The number of chemicals included are ~80, ~300, 7, 30, and 7, respectively. Hydrogen sulfide (sour gas), one of the chemicals that is of interest to the MMS, is included in the database for AFTOX and CANARY. ARCHIE and SLAB do not have a built-in chemical database. However, the user's manual for SLAB (Ermak, 1990) contains properties for 14 chemicals, including hydrogen sulfide. The chemical database for TSCREEN is not efficiently implemented, since only one property can be retrieved at a time.

BREEZE HAZ SUITE, SLAB View, and SLAB for Windows have full-fledged graphical user interfaces (GUIs) that run under Microsoft's Windows environments (3.1, 95, and NT). All GUI designs are intuitive and logical. A chemical database that includes properties for several hundred chemicals is always available, including hydrogen sulfide (sour gas). This is very helpful in reducing data preparation time. Some GUIs add additional values to the original dispersion code such as source-term estimations (for BREEZE HAZ SUITE) and auxiliary calculations that would normally be done by hand (for SLAB View).

All GUIs have graphic capabilities. However, the quality varies greatly, especially in contour plots. We liked the graphical design for BREEZE HAZ SUITE and SLAB View. The two GUIs also accept base maps over which plume contours can be drawn. The finished graphical products are informative. CANARY also has some graphical display capabilities. However, the applications are still DOS-based and support only the outmoded HP LaserJet II printer.

The run time for all models is quite fast, typically within a few minutes on a Pentium PC. The only exception is with transient releases, where it might take up to 15 minutes to finish a model run.

The FORTRAN source codes for DEGADIS, HGSYSTEM, SLAB, and TSCREEN are comparable in terms of flexibility and readability. The QuickBASIC code for AFTOX is more difficult to follow. Source codes for other models are not available for review.

Without considering various GUIs for the time being, we recommend that the MMS acquire the HGSYSTEM, SLAB, and CANARY models based on the above analyses. The three models have percent (normalized) scores of 87.9, 86.7, and 81.8, respectively (see Table 4-1). HGSYSTEM is the most sophisticated model that supports a wide range of releases. However, the model is also the most difficult to use. SLAB is elegantly designed, easy to use, and also with many powerful features. CANARY, despite of a skeleton user's guide, has a source term module. The reason why we did not recommend DEGADIS, also a good model, was because the code is technically comparable to the HEGADAS module in HGSYSTEM, and HGSYSTEM has many more other modules. ARCHIE also received relatively good rating with its practical approach, versatility, and a good user's guide. However, the model is not under any maintenance or support, and the source code is not available even though it is a public-domain model. AFTOX is not recommended due to its limited capabilities. TSCREEN is not recommended mainly because (1) the user does not have the option of specifying arbitrary meteorological conditions, (2) we identified some errors in program logic, and (3) the inefficient design of the user interface.

As to the graphical user interface (GUI) programs, we recommend the MMS acquire the BREEZE HAZ SUITE and SLAB View software. BREEZE HAZ SUITE nicely integrates different dispersion codes such

as SLAB, DEGADIS, and AFTOX into a common environment with standardized menus, commands, and databases. The software also includes a source-term module. SLAB View has many value-added features. Its software design is superb and its user's guide is well written. We did not recommend SLAB for Windows mainly because it does not include as many additional features as the other packages do. Its user's guide is also not on a par with others.

Table 4-1. Ratings for the (a) Science and Credibility, (b) Ease of Use, and (c) Computational Requirements Categories for Seven Toxic Release Models and Three Graphical User Interface Programs (GUI). Note That the Ratings for (a) and (b) Have a Weight That is Twice Larger Than That for the Ratings for (c). Each Individual Rating Can be Between 1 and 3, and is not Adjusted According to the Weight in the Table. See Section 1 for a Description of Evaluation Methodology and Criteria.

	AFTOX	ARCHIE	CANARY	DEGADIS	HGSYSTEM	SLAB	TSCREEN	BREEZE HAZ	SLAB VIEW	SLAB for WINDOWS
Tech & Gen	1.5	2.5	3	2.5	3	2.5	2	3	2.5	2.5
Grid Options	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Qual of Phys	2	2.5	3	3	3	3	1.5	3	n/a	n/a
Sparse Data	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Overwater	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Model Eval	3	1.5	3	3	3	3	3	n/a	n/a	n/a
S & C Score	13	13	18	17	18	17	13	12	5	5
User Guide	3	3	2	3	3	3	3	3	3	2
Options	2	3	2.5	2	3	2.5	1.5	n/a	n/a	n/a
Data Prep	2	3	3	3	2	3	2.5	3	3	3
Data Acq	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
GUI	2	2.5	2	2	2	n/a	1.5	3	3	2.5
Run Diag	2	2.5	2	2	3	2	2	2.5	1.5	2
Post Diag	2	2	3	2	2.5	2	2	3	3	2
Ease Score	26	32	29	28	31	25	25	29	27	23
Mult Source	1	1	1	1	1	1	1	n/a	n/a	n/a
UNIX/PC	1	1	3	2	2.5	3	1	1	1	1
Run Time	2	3	2	3	2.5	3	3	n/a	n/a	n/a
Code flex	1	n/a	n/a	3	3	3	2.5	n/a	n/a	n/a
Comp Score	5	5	6	9	9	10	7.5	1	1	1
Overall Score	44	50	53	54	58	52	45.5	42	33	29
Percent Score	66.7	79.4	84.1	81.8	87.9	86.7	68.9	93.3	84.6	74.4

5. OFFSHORE AND COASTAL DISPERSION (OCD) MODEL

The Offshore and Coastal Dispersion (OCD) model (Hanna et al., 1985; DiCristofaro and Hanna, 1989) is mainly used to simulate the effects of offshore emissions from point, area, or line sources on the air quality of coastal regions. The model includes special algorithms that account for overwater plume transport and dispersion, and the changes that take place as the plume crosses the shoreline. The model also includes parameterizations for the development of the thermal internal boundary layer (TIBL), plume fumigation, overwater surface boundary layer, plume dispersion over complex terrain, and platform downwash. The model was specifically evaluated with field experiments conducted in coastal areas, such as Ventura, Pismo Beach, and Carpinteria in California, and Cameron in Louisiana (DiCristofaro and Hanna, 1989). OCD has been used by the MMS for general review of offshore operator's plan, and is considered a "guideline" model by the EPA (USEPA, 1986a).

In a recent project funded by the MMS, many enhancements were added to OCD, including (1) a graphical user interface (GUI) program, (2) a new self-documenting control file, (3) a shoreline data processor, (4) more supported meteorological data formats, (5) the removal of hardwired array limits, and (6) more error messages (Chang and Hahn, 1997). All these enhancements were to make the model more user-friendly. Nonetheless, technical components of the model were not changed.

The OCD model and its GUI program are written in FORTRAN 77 and Visual Basic, respectively. The OCD model, the GUI program, and the user's guide (WordPerfect files) can be freely downloaded from EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/).

Besides the "programming" enhancements mentioned above, the code has not been significantly changed since early 1990s. In the following, we will briefly review various technical aspects of OCD in light of recent literature and advances in the areas of overwater and coastal dispersion, and provide recommendations when appropriate.

Overwater mixing height

OCD requires overwater meteorological data in order to characterize the overwater boundary layer. One of the mandatory variables is the overwater mixing height, which is not routinely measured. If the data are missing, OCD assigns a constant 500 m to the overwater mixing height. Although 500 m is representative of the climatology for the Gulf of Mexico; however, a constant overwater mixing height probably will not produce an adequate dynamic range of predicted concentrations. Hutzell and Chang (1998) proposed a new algorithm to calculate the overwater mixing height. The algorithm uses surface observations already required by OCD, and assumes that the mixed layer can be determined by the lifting condensation level (LCL), the convective mixing height, or the mechanical mixing height, depending on the stability regime. The algorithm requires observations of relative humidity. The variable is included in overwater meteorology used by OCD and is frequently set to a default value because sea buoys do not measure relative humidity until recent years. This algorithm then can produce incorrect values of the LCL if relative humidity is missing. The algorithm suggested by Hutzell and Chang (1998) also includes the formula proposed by Hsu (1997) to parameterize the height of the marine convective boundary layer. These new mixing height formulas should be further evaluated and tested. They should also be implemented in OCD to test whether they significantly improve the model performance when compared against field measurements. If the results are satisfactory, then the new formulas should be permanently implemented in OCD.

Parameterizations of the Marine Boundary Layer

The marine boundary layer can be properly described by the Monin-Obukhov similarity theory (e.g., Hsu, 1988; Arya, 1988). Some of the important parameters for the similarity theory include the friction velocity (u_*), the scaling virtual potential temperature (θ_{v*}), the Monin-Obukhov length (L), and the roughness length (z_0). Ideally, the above variables should be calculated with direct measurements of turbulent fluxes or with vertical profiles of wind speed, humidity, and temperature. (Note that z_0 is in fact an integration constant and cannot be directly measured.) However, these measurements are not routinely available, especially over water because of logistic problems. Therefore, the bulk transfer approach is often used to calculate u_*, θ_{v*}, L and z_0; where only the sea surface temperature, and the atmospheric wind speed, temperature, and humidity measured at one level are required; and where the drag coefficient (C_u) and the bulk transfer coefficient for heat (C_T) are used. A good review of various bulk transfer methods as of the mid 1980s is given by Blanc (1985), where he found that large variations (50~100%) in calculated wind stresses and heat fluxes often exist among different schemes.

The current OCD model uses an iterative algorithm (in subroutine PROFILE) to calculate u_*, θ_{v*}, L and z_0. The algorithm assumes that (1) C_u for neutral conditions ($C_u = 0.001\times(0.75+0.067u_{10})$, where u_{10} is the 10 m wind speed) can be used (Garratt, 1977); (2) C_T for neutral conditions (C_T=0.0013, independent of wind speed) can be used; and (3) z_0 is related to u_{10} as $z_0=2\times10^{-6}u_{10}^{2.5}$ (Hosker, 1974). There have been some new formulas suggested for calculating surface turbulent fluxes, and thus u_*, θ_{v*}, L, and z_0. For example, Hsu (1988) suggested more comprehensive expressions for C_u and C_T that depend on atmospheric stability. With wave height and length data becoming more available operationally, Hsu's (1988) formula for z_0 that depends on the wave information is also appealing when compared to the simpler Hosker (1974) formula. (However, the new formula would require more input data than does the original model) Clayson et al. (1996) proposed a new method to calculate turbulent fluxes that involves modeling the physical processes that drive the interfacial sublayers of the ocean and atmosphere. The method is based on the surface renewal theory, which assumes that transfer at the ocean-atmosphere interface is by molecular diffusion into Kolmogorov microscale (e.g., Panofsky and Dutton, 1984) eddies that are renewed intermittently after random contacts with the evaporating surface. The model explicitly incorporates an estimate of the time scale for Kolmogorov eddies, and also uses the sea surface temperature and the atmospheric wind speed, temperature, and humidity measured at a single level.

Implementation of the above new schemes should be straightforward, since the necessary code modifications are limited in subroutine PROFILE. The only exception is that additional data, e.g., wave height and length, might be required. According to past experience (e.g., Blanc, 1985), different schemes might yield wind stresses and heat fluxes, and thus u_* and L, that are quite different. This will have direct consequences in predicted concentrations. For example, in OCD the lateral and vertical turbulence intensities are proportional to u_*. If larger values of u_* are predicted, then predicted concentrations will be lower. Therefore, it is recommended that these potential new formulas be carefully evaluated before a decision is made regarding whether to implement them in OCD.

Use of overland meteorological data

OCD uses overwater observations of wind speed and direction in both overwater and overland areas. If on-site overwater meteorological observations are not available, then overland values are used. If overwater observations of wind speed and direction are available, then the only overland meteorological data used in the model are stability class, temperature, and optionally turbulence data. Wind speeds over water are generally higher than over land. The reason why no wind speed and direction variations between land and water are allowed is to prevent unrealistic mass convergence or divergence at the land/water interface. Although a spatially-varying wind field is not allowed within the framework of

straight-line Gaussian models, a distinction should still be made for cases when overland winds are more representative. One example would be when both sources and receptors are located over land, where the use of overwater wind speed might lead to less conservative results.

Vertical dispersion coefficient, σ_z

For Gaussian models, the vertical dispersion coefficient, σ_z, is relatively more uncertain than the lateral dispersion coefficient, σ_y. This is because field experiments usually provided adequate coverage in the horizontal direction only. Thus, σ_z is generally inferred from ground level concentration patterns. However, concentrations are also strongly influenced by other parameters such as plume rise, mixing height, and fumigation rate. Unfortunately, rigorous derivation of σ_z will be difficult, if not impossible, until high-quality vertical concentration data are taken at field or wind tunnel experiments. There is also another important issue. As long as σ_z is not based on direct field measurements, formulation for σ_z should be modified if algorithms for plume rise, mixing height, or fumigation rate are changed to ensure consistency.

Thermal internal boundary layer (TIBL)

Shoreline fumigation is a condition where high pollutant concentrations are observed in coastal areas. When an onshore flow reaches the land-water interface, mechanical and thermal effects lead to the development of a new internal boundary layer. If the land is much warmer than the water surface and the land surface is smooth enough, thermal effects dominate and a thermal internal boundary layer (TIBL) begins to develop. The simple empirical formula for the TIBL height implemented in OCD was based on a best-fit to the available data (DiCristofaro and Hanna, 1989). The growth of the TIBL height is a piece-wise linear function of the distance from the shoreline only. The more sophisticated theoretical equations evaluated by Stunder and Sethuraman (1985) and Sethuraman (1987) were not directly used. These models are not robust enough, i.e., they tend to produce unreasonably high or low values of the TIBL height when using one year or more of hourly meteorological data. Petersen et al. (1995) recently performed a series of wind tunnel experiments under different meteorological conditions to study in detail the growth of the TIBL height. Based on the wind tunnel experiments, Petersen (1997) then proposed a new formula for the TIBL height, which is subsequently included in the Advanced Shoreline Dispersion Model (ASDM; Grosch and Dunk, 1998). The new TIBL formula accounts for vertical profiles of temperature and wind speed, variations of the surface heat flux with inland distance, and a non-zero heat flux at the top of the TIBL. The new TIBL formula appears to be technically superior to the simple OCD formula. However, it has only been evaluated with a small number of tunnel experiments so far. Since the TIBL is an important factor in determining plume impacts on coastal areas, it is worthwhile to further evaluate the new TIBL height formulation with other coastal field data. Furthermore, it is also important to investigate whether the new formula is robust for operational applications, rather than just a selected number of special cases.

Multiple land/water transitions

For a complex shoreline, an offshore plume might move through a series of land masses and water bodies. The current version of the OCD model allows only one transition from water to land. In order to instruct the model to neglect insignificant water bodies or land masses, the user specifies a value for the minimum significant distance in the model control file. The minimum significant distance should be chosen with considerations of the estimated plume height and the slope of the TIBL (DiCristofaro and Hanna, 1989). If the distance along the plume path between two successive transitions is less than the minimum distance, then both transitions are ignored by the model. (This is done in the GEOM subroutine.) Once a controlling transition is defined, OCD then uses the virtual source approach (in polar coordinates, done in

the VIRT subroutine) to account for the transition between the marine and overland boundary layers. In theory, the above ad hoc procedure can be relaxed to account for multiple transitions between land and water. Mathematically, it means that the virtual source approach would be repeated for multiple transitions. However, caution must be exercised in order to ensure that such mathematical calculation is physically meaningful. As suggested by the way the original minimum distance is estimated, air mass transition does not occur instantly because the slope of the TIBL is not vertical. In the recent Kit Fox field experiments (Briggs et al., 1997) where one roughness element array is surrounded by another array with a different height, it is also found that the boundary layer wind profiles and concentration patterns measured in the outer array still exhibit characteristics of the inner array. Therefore, the "memory" of the boundary layer must be accounted for when dealing with multiple transitions of land and water. More analyses are necessary to study the physics of multiple transitions before they can be implemented in the OCD model.

Impacts on offshore areas due to coastal sources

OCD was initially designed to simulate the effects of offshore sources on coastal regions. As a result, the model has a sophisticated procedure to determine the timing for an offshore plume to enter the TIBL. At the transition, the model uses the virtual source technique to account for the change in dispersion regimes (from overwater to overland) in polar coordinates. OCD also properly handles the cases when sources and receptors are both overwater or overland. However, a close review of the code shows that OCD does not correctly calculate the impacts on offshore areas from coastal sources. For example, in subroutine CALC, due to an insufficiency in the program logic, when a land-based plume travels to overwater areas, the change in dispersion regime is not triggered and the code continues to perform dispersion calculations as if the plume were still overland. The OCD code should be carefully reviewed and modified to ensure that the land-to-water as well as water-to-land pathways are correctly treated.

Shoreline database

OCD requires the shoreline geometry information to determine the change in plume dispersion as the plume crosses the land-sea interface. A processor called MAKEGEO was developed to generate the shoreline information from existing databases. This greatly speeds up and simplifies the data preparation procedures. Furthermore, unlike the traditional approach where data were manually prepared, the user can now always reproduce the results. Currently, MAKEGEO includes databases for only the U.S. coasts of Pacific, Atlantic, Gulf of Mexico, and Alaska. It would be ideal if the databases can be expanded to cover other geographical areas such as Canada and Mexico. This can further increase the popularity of the model.

Documentation

After the GUI program was developed in 1996, a new OCD user's guide (Chang and Hahn, 1997) was also rewritten with current Windows-based word processing software (i.e., WordPerfect). However, other topics in the original user's guide (DiCristofaro and Hanna, 1989) such as technical descriptions and model evaluation with field experiments were not converted and "modernized" at the same time. They are still prepared by an outmoded, DOS-based word processing application, Chi-Write, which is no longer widely-available. As a result, the only distribution medium is through hard copy. Moreover, some of the technical discussions are no longer up-to-date because of the new features (such as the preparation of the shoreline data) added to the enhanced OCD code. In order to be consistent, preserve valuable information, and simplify future distribution, we recommend that the remaining materials (about 100 pages) in the 1989 OCD user's guide be retyped and combined with the 1997 user's guide to become an integrated document. The new document should also include more figures that further illustrate various

modeling concepts, such as how the model accounts for the land/water/TIBL transitions and the virtual source in polar coordinates.

Suggestions for the OCD model in many technical areas were provided above. Most of these suggestions can be easily implemented in the code because of OCD's modular design. However, like any other model improvement/development projects, we emphasize the importance of comprehensive evaluation. Some of the issues that should be considered include:

- Are the new algorithms physically meaningful even though they can be implemented computationally?
- How will the new algorithms affect predicted concentrations? Because of the interaction among different processes, a parameter might not always have a monotonic effect on predicted concentrations.
- Are we getting the right answers for the right reasons? Sometimes, because of cancellation of errors, a model will still yield reasonable answers despite of errors.
- Are the new algorithms robust enough, so that they always run successfully with, for example, one year of data that include all kinds of combinations of meteorological variables?
- Do the new algorithms require data that are not always routinely available?

6. SUMMARY

The Minerals Management Service (MMS) uses different types of air dispersion models to perform tasks such as environmental impact studies and regulatory analyses in order to regulate the activities of offshore operators. The MMS would like to expand the current suite of air quality models used. In order to ensure that MMS' model selections are scientifically credible and can withstand possible critiques, a critical review of the following four types of air quality models is necessary:

- Regional-scale dispersion models for applications where phenomena such as advection, deposition, and potential chemical transformations of pollutants are important on a spatial scale up to 1000 km. Eulerian photochemical grid models might be best for this purpose.
- Lagrangian trajectory (puff) models for instantaneous and short-duration emissions, or for releases when spatially-varying meteorological fields are important.
- Toxic release models for analysis of consequences of accidental releases of hazardous pollutants.
- Steady-state Gaussian models for general review of offshore operator's plan when the source-receptor distance is less than 50 km or so.

Based on MMS' needs, we considered the following six major model evaluation categories, where some of the categories were further divided into a number of subcategories or attributes (see Section 1 for details):

A. Science and Credibility
   A1. Technical and general descriptions
   A2. Grid options for Eulerian and trajectory models
   A3. Quality of physical processes simulated
   A4. Sparse data treatment
   A5. Overwater dispersion
   A6. Model evaluation history
B. Ease of Use (From User's Perspective)
   B1. User's guide
   B2. Model Options
   B3. Data preparation time
   B4. Ease of data acquisition
   B5. Model interfaces to preprocessors / GUI
   B6. Run-time diagnostics
   B7. Post-run diagnostics
C. Computational Requirements
   C1. Multiple sources
   C2. UNIX / PC portability
   C3. Run time
   C4. Code flexibility and readability
D. Cost
E. Availability / Restrictions / Terms
F. Language for Model and GUI

Only Categories A, B, and C were used to rank the models, where a score between 1 to 3 was assigned to each attribute. 3 = good, very flexible or state-of-the-art; 2 = fair, less flexible, or somewhat out of date;

and 1 = poor or not flexible. Categories D, E, and F are for information only. To account for varying degree of importance, we further assigned a weight to the score for each attribute. The attributes for Categories A and B have a weight of 2, and the attributes for Category C have a weight of 1. We then designed a normalized model score (0 to 100%) that is based on the summation of weighted scores over all applicable attributes divided by the summation of weighted highest possible scores over all applicable attributes. This normalized score is then used to produce the final model ranking.

The current review is not intended to be comprehensive. Instead, four to seven "representative" models in each model category (except for steady-state Gaussian models, see below) were chosen for review, and the top two to three in each category are then recommended. The omission of a model does not mean in any way that the model is inferior or less desirable. For steady-state Gaussian models, we limited our review to the technical components in the Offshore and Coastal Dispersion (OCD) model, which has been a regulatory model used by the MMS.

The evaluation mainly consisted of reviews of the user's guide, technical documentation, peer-reviewed journal articles, conference proceedings, web pages, and the source code for each model. Model developers and users were interviewed if necessary. This study is not a formal performance evaluation, where the model results are compared against field data.

The following models were chosen for evaluation:

Regional-scale dispersion models (see Section 2):

- CALGRID ←
- CAMx ←
- SAQM
- UAM-IV
- UAM-V ←

Lagrangian trajectory models (see Section 3):

- CALPUFF ←
- HYSPLIT_4 ←
- INPUFF
- MESOPUFF II
- SLAM

Toxic release models (see Section 4):

- AFTOX
- ARCHIE
- CANARY ←
- DEGADIS
- HGSYSTEM ←
- SLAB ←
- TSCREEN
- BREEZE HAZ SUITE (GUI only) ←
- SLAB View (GUI only) ←
- SLAB for Windows (GUI only)

The models marked by arrows are our recommendations based on the evaluation criteria and methodology described in Section 1 and above. These models were recommended mainly because of their high

technical qualities, relevance to MMS' special needs (e.g., overwater dispersion, multiple sources, and environmental impact studies), and proven track records. The two graphical user interface (GUI) programs, BREEZE HAZ SUITE and SLAB View, were recommended because of their state-of-the-art design, ease of use, and value-added features such as source term calculations and graphical functions.

Section 5 gives our recommendations for the Offshore and Coastal Dispersion (OCD) model in technical areas such as the overwater mixing height, parameterizations of the marine boundary layer, the use of overland meteorological data, the vertical dispersion coefficient, the thermal internal boundary layer, multiple land and water transitions, and impacts on offshore areas due to coastal sources. Recommendations are also given in operational areas such as the shoreline database and the documentation. We caution that while it is relatively easy to upgrade the OCD code to incorporate new theories and algorithms because of OCD's modular design, any changes must be subject to careful evaluation. Some of the important issues to consider include (1) whether the new algorithms are physically meaningful; (2) how the new algorithms affect predicted concentrations; (3) potential cancellation of errors; (4) whether the new algorithms are robust enough so that they will always succeed when running with, for example, one year of data; and (5) whether the new algorithms require data that are always readily available.

REFERENCES

AIChE, 1996: *Guidelines for Use of Vapor Cloud Dispersion Models, Second Edition.* Authored by Steven R. Hanna, Peter J. Drivas, and Joseph C. Chang. Center for Chemical Process Safety, American Institute of Chemical Engineers, 345 East 47th Street, New York, NY 10017.

Arya, S.P.S., 1988: *Introduction to Micrometeorology.* Academic Press, 308pp.

Atchison, M.K., D. Dean, and S. Seely, 1996: Operational evaluation of forecast and diagnostic atmospheric models in a land/sea environment. Proceedings of the 11th Conference on Numerical Weather Prediction, Norfolk, VA. American Meteorology Society, Boston, MA. 361-362.

Atchison, M.K., D. Dean, and S. Seely, 1998: The use of prognostic model output as a data source for the Short-Range Layered Atmospheric Model. 10th Joint Conference of Air Pollution Meteorology with the Air and Waster Management Association, Phoenix, Arizona. American Meteorological Society, Boston, Massachusetts.

ATMES Report, 1992: Evaluation of long range atmospheric transport models using environmental radioactivity data from the Chernobyl accident, W. Klug, G. Graziani, G. Grippa, D. Pierce, and C. Tassone (Eds), Elsevier Science Publishers, Linton Rd., Essex, England.

Beals, G.A., 1971: *A Guide to Local Dispersion of Air Pollutants.* Air Weather Service Technical Report 214.

Blanc, T.V., 1985: Variation of bulk-derived surface flux, stability, and roughness results due to the use of different transfer coefficient schemes. *J. Phys. Oceanogr.*, **15**, 659-669.

Bowman Environmental, 1997: *SLAB for Windows Manual.* Bowman Environmental, Inc., P.O. Box 7348, Asheville, NC 28802.

Briggs, G.A., R.E. Britter, S.R. Hanna, J.A. Havens, S.B. King, A.G. Robins, W.H. Snyder, and K.W. Steinberg, 1997: Advances in dense gas dispersion modeling of accidental releases over rough surface during stable conditions. 22nd NATO/CCMS International Technical Meeting on Air Pollution Modeling and its Application, Clermont-Ferrand, France.

Briggs, G.A., 1975: *Plume Rise Predictions.* Lectures on Air Pollution and Environmental Impact Analyses, Workshop Proceedings, Boston, MA, 27 September - 3 October, 1975, 59-111, American Meteorological Society, Boston, MA.

Britter, R.E., and J. McQuaid, 1989: *Workbook on the Dispersion of Dense Gases.* U.K. Health and Safety Executive, Contract Research Report No. 17/1988.

CARB, 1996: *General Description of the SAQM Emissions Preprocessing Software (EPS) (Part 4 of SAQM Final Report).* California Air Resources Board, Sacramento, CA.

Carhart, R.A., A.J. Policastro, M. Wastag, and L. Coke, 1989: Evaluation of eight short-term long-range transport models using field data. *Atmos. Environ.*, **23**, 85-105.

Carter, W.P.L., 1990: A detailed mechanism for the gas-phase atmospheric reactions of organic compounds. *Atmos. Environ.*, **24A**, 481-518.

Carter, W.P.L., 1996: Condensed atmospheric photooxidation mechanisms for isoprene. *Atmos. Environ.*, **30**, 4275-4290.

Chang, J.C., and K.J. Hahn, 1997: *User's Guide for Offshore and Coastal Dispersion (OCD) Model, Version 5*, prepared for Minerals Management Service, Gulf of Mexico OCS Region, 1201 Elmwood Park Blvd., New Orleans, LA 70123-2394, by Earth Tech, 196 Baker Avenue, Concord, MA 01742.

Chang, J.S., R.A. Brost, I.S.A. Isaksen, S. Madronich, P. Middleton, W.R. Stockwell and C.J. Walcek. 1987: *A three-dimensional Eulerian acid deposition model, physical concepts and formulation. J. Geophys. Research*, **92**, 14,681-14,700.

Chang, J.S. and Y. Li, 1996: *SAQM Meteorological Processor User's Guide (Draft) (Part 3 of SAQM Final Report).* Atmospheric Sciences Research Center, State University of New York at Albany, Albany, NY.

Chang, J.S., Y. Li, M. Beauharnois, H.-C. Huang, C.-H. Lu and G. Wojcik, 1996*: SAQM Users Guide (Part 2 of Final Report).* Atmospheric Sciences Research Center, State University of New York at Albany, Albany, NY.

Chang, J.S., S. Jin, Y. Li, M. Beauharnois, C.-H. Lu, H.-C. Huang, S. Tanrikulu and J. DaMassa. 1997. *The SARMAP Air Quality Model.* Atmospheric Sciences Research Center, State University of New York at Albany, Albany, NY.

Clayson, C.A., C.W. Fairall, and J.A. Curry, 1996: Evaluation of turbulent fluxes at the ocean surface using surface renewal theory. *J. Geophys. Research*, **101**, 28503-28513.

Computer Sciences Corporation, 1991a: *Gridded Model Information Support System (GMISS) User's Guide. Volume II: UAM Subsystem.* EPA-450/91-009. Available from NTIS: (703) 487-4650 as PB91-206268LEU.

Computer Sciences Corporation, 1991b: *Gridded Model Information Support System (GMISS) User's Guide. Volume III: Model Concentration Data Retrieval Subsystem.* EPA-450/91-032. Available from NTIS: (703) 487-4650.

DiCristofaro, D.C., and S.R. Hanna, 1989: *OCD: The Offshore and Coastal Dispersion Model, VolumeI: User's Guide.* Prepared for Minerals Management Service, 381 Elden Street, Herndon, VA 22070-4817, by Earth Tech, 196 Baker Avenue, Concord, MA 01742.

Douglas, S.G., G.E. Mansell, T.C. Myers, M.M. Jimenez and D.L. Perry, 1995: *Application of UAM-V to the Northeast as Part of Phase I of the Modeling Ozone Cooperative (MOCA).* Final Report SYSAPP-95/049 prepared by Systems Applications International for the MOCA Technical Committee, Edison Electric Institute, Washington, D.C.

Douglas, S.G., R.C. Kessler and E.L. Carr, 1990: *User's Guide for the Urban Airshed Model. Volume*

III: User's Manual for the Diagnostic Wind Model. EPA-450/4-90-007C. Available from NTIS: (703) 487-4650 as PB91-131243.

Draxler, R.R., and G.D. Hess, 1997: *Description of the HYSPLIT_4 Modeling System.* NOAA Technical Memorandum ERL ARL-224, Air Resources Laboratory, Silver Spring, MD, 24 pp.

Draxler, R.R., 1992: *Hybrid Single-Particle Lagrangian Integrated Trajectories (HY-SPLIT): Version 3.0 – User's Guide and Model Description.* NOAA Technical Memorandum ERL ARL-224, Air Resources Laboratory, Silver Spring, MD.

Draxler, R.R., R. Dietz, R.J. Lagomarsino, and G. Start, 1991: Across North America Tracer Experiment ANATEX), Sampling and analysis. *Atmos. Environ.*, **25A**, 2815-2836.

Emery, C.A., M.P. Ligocki, P.D. Guthrie, R.D. Scheffe and D. Axelrad, 1996: *Development of an air quality modeling system to investigate long-range transport and surface deposition of toxics and PM10.* Proceedings of the Ninth Joint Conference on Applications of Air Pollution Meteorology. American Meteorology Society, Boston, MA. 136-140.

ENSCO, 1997a: *Short-Range Layered Atmospheric Model (SLAM) User's Manual.* ENSCO, Inc., Applied Research and Systems Division, 445 Pineda Court, Melbourne, FL 32940. 44 pp, in HTML (hyper-text mark-up language) format.

ENSCO, 1997b: *Short-Range Layered Atmospheric Model (SLAM) Technical Description.* ENSCO, Inc., Applied Research and Systems Division, 445 Pineda Court, Melbourne, FL 32940. 26 pp, in HTML (hyper-text mark-up language) format.

ENVIRON International Corporation, 1997: *User's Guide to the Comprehensive Air Quality Model with Extensions (CAMx): Version 1.10.* ENVIRON International Corporation, Novato, CA.

Ermak, D.L., 1990: *User's Manual for SLAB: An Atmospheric Dispersion Model for Denser-Than-Air Releases.* UCRL-MA-105607, Lawrence Livermore National Laboratory, Livermore, CA.

Evans, R.J., M.K. Atchison, D. Dean, and S. Seely, 1998: Effects of topographical and gridded data density on mesoscale model performance. Proceedings of the 12th Conference on Numerical Weather Prediction, Phoenix, AZ. American Meteorology Society, Boston, MA. 219-222.

FEMA, 1989: *Handbook of Chemical Hazard Analysis Procedures.* Prepared for the Federal Emergency Management Agency (FEMA), the U.S. Department of Transportation (DOT), and the U.S. Environmental Protection Agency (EPA). Availabe from FEMA, Publications Office, 500 C Street, S.W., Washington, D.C., 20472.

Ferber G.J., J.L. Heffter, R.R. Draxler, R.J. Lagomarsino, F.L. Thomas, R.N. Dietz, and C.M. Benkovitz, 1986: *Cross-Appalachian tracer experiment (CAPTEX-83), Final Report.* NOAA Tech. Memo ERL ARL-142, Air Resources Laboratory, Silver Spring, MD, 60 pp.

Fleischer, M.T., 1980: *SPILLS, An Evaporation/Air Dispersion Model for Chemical Spills on Land.* Shell Development Center, Westhollow Research Center, P.O. Box 1380, Houston, TX, 77001.

Garratt, J.R., 1995: *The Atmospheric Boundary Layer.* Cambridge Atmospheric and Space Science

Series, Cambridge University Press, Cambridge, England.

Garratt, J.R., 1977: Review of drag coefficients over oceans and continents. *Mon. Wea. Rev.*, **105**, 915-929.

Gassman, F., P. Gaglione, S.E. Gryning, H. Hasenjager, E. Lyck, H. Richner, B. Neininger, S. Vogt, and P. Thomas, 1986: *Experimental Investigation of Atmospheric Dispersion Over Complex Terrain in a Prealpine Region (Experiment SIESTA).* EIR-Bericht, Nr. 604, 133 pp.

Gery, M.W., G.Z. Whitten, J.P. Killus and M.C. Dodge, 1989: A photochemical kinetics mechanism for urban and regional scale computer modeling. *J. Geophys. Res.*, **94**, 12925-12956.

Godowitch, J.M., 1989: *Evaluation and Sensitivity Analyses Results of the MESOPUFF II Model with CAPTEX Measurements.* EPA-600/3-89-056. U.S. Environmental Protection Agency, Research Triangle Park, NC.

Golder, D., 1972: Relations between stability parameters in the surface layer. *Boundary Layer Meteorology*, **3**, 46-68.

Grell, G.A., J. Dudhia and D.R. Stauffer, 1995*: A Description of the Fifth-Generation Penn State/NCAR Mesoscale Model (MM5).* NCAR Technical Note NCAR/TN-398 + STR, National Center for Atmospheric Research, Boulder, CO.

Grosch, T.G., and R. Dunk, 1998: The development of an advanced Shoreline Dispersion Model. Paper 98-TAB.08P, 91st Annual Meeting of the Air and Waste Management Association, San Diego, California.

Guo, Z., N.K. Lolk and S.G. Douglas, 1996*: User's Guide to Objective Analysis Software for Preparation of Cloud and Precipitation Input Files for the UAM-V Modeling System.* SYSAPP-96/057. Systems Applications International. San Rafael, CA.

Haagenson, P.L., J. Dudhia, D.R. Stauffer and G.A. Grell, 1994*: The Penn State/NCAR Mesoscale Model (MM5) Source Code Documentation.* NCAR Technical Note NCAR/TN-392 + STR, National Center for Atmospheric Research, Boulder, CO.

Hanna, S.R., and M.E. Fernau, 1997*: Photochemical Model Evaluations in the Northeastern United States.* Final Report prepared by Earth Tech, Inc. for the American Petroleum Institute, Washington, D.C.

Hanna, S.R., J.C. Chang, and J.X. Zhang, 1996a: *Technical Documentation of HGSYSTEM/UF_6 Model.* Prepared by Earth Tech, 196 Baker Avenue, Concord, MA 01742, for Lockheed Martin Energy Systems, Inc., Oak Ridge, TN 37831. Document available from the Office of Scientific and Technical Information, P.O. Box 62, Oak Ridge, TN 37831, Tel (423)576-8401.

Hanna, S.R., G.E. Moore and M.E. Fernau, 1996b: Evaluation of photochemical grid models (UAM-IV, UAM-V, and the ROM/UAM-IV couple) using data from the Lake Michigan Ozone Study (LMOS). *Atmos. Environ.*, **30**, 3265-3279.

Hanna, S.R., J.C. Chang, and D.G. Strimaitis, 1993: Hazardous gas model evaluation with field

observations. *Atmos. Environ.*, **27A**, 2265-2285.

Hanna, S.R., L.L. Schulman, R.J. Paine, J.E. Pleim, and M. Baer, 1985: Development and evaluation of the Offshore and Coastal Dispersion model. *J. Air Poll. Control Assoc.*, **35**, 1039-1047.

Hao, W., 1996: Private communications, the New York State Department of Environmental Conservation, Albany, NY.

Harley, R.A., A.G. Russell, G.J. McRae, G.R. Cass and J.H. Seinfeld, 1993: Photochemical modeling of the Southern California Air Quality Study. *Environ. Sci. Technol.*, **27**, 378-388.

Havens, J.A., and T.O. Spicer, 1985: *Development of an Atmospheric Dispersion Model for Heavier-Than-Air Gas Mixtures.* Final report to the U.S. Coast Guard, CG-D-23-85. USCG HQ, Washington, DC.

Hess, G. D., G.A. Mills and R.R. Draxler, 1997: Comparison of HYSPLIT_4 model simulations of the ETEX data, using meteorological input data of differing spatial and temporal resolution. ETEX symposium on Long-Range Atmospheric Transport, Model Verification and Emergency Response, 13-16 May, Vienna, Austria.

Hoot, T.G., R.N. Meroney, and J.A. Peterka, 1973: *Wind Tunnel Tests of Negatively Buoyant Plumes.* EPA/650/3-74-003. U.S. Environmental Protection Agency, Research Triangle Park, NC.

Hosker, R.P., 1974: A comparison of estimation procedures for overwater plume dispersion. *Proceedings of the Symposium on Atmospheric Diffusion and Air Pollution*, American Meteorological Society, 281-288.

Hsu, S.A., 1997: Estimating overwater convective boundary layer height from routine meteorological measurements for diffusion applications at sea. *J. of App. Meteorol.*, **36**, 1245-1248.

Hsu, S.A., 1988: *Coastal Meteorology.* Academic Press, 260pp.

Hutzell, W.T., and J.C. Chang, 1998: An algorithm for the overwater mixing height to the Offshore Coastal and Dispersion Model. 10th Joint Conference of Air Pollution Meteorology with the Air and Waster Management Association, Phoenix, Arizona. American Meteorological Society, Boston, Massachusetts.

Irwin, J., 1997: A comparison of CALPUFF modeling results with 1977 Inel field data results. 22nd NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application. Clermont-Ferrand, France, June 2-6, 1997.

Jiang, W., M. Hedley and D.L. Singleton, 1998: Comparison of the MC2/CALGRID and SAIMM/UAM-V photochemical modeling systems in the lower Fraser Valley, British Columbia. *Atmos. Environ.*, **32**, 2969-2980.

Johnson, W.B., et al., 1987: *The Shoreline Environment Atmospheric Dispersion Experiment (SEADEX), Vol I – Experimental Design and Measurement Systems, Vol II – Meteorological and Gas Tracer Data, and Vol III – Ground-Based and Airborne Lidar Data (NUREG/CR-4950).* Nuclear Regulatory Commission, Washington, DC.

Kahler, J.P., R.G. Curry, and R.A. Kandler, 1980: *Calculating Toxic Corridors.* AWS-TR-80-003.

Kunkel, B. A., 1988: *User's Guide for the Air Force Toxic Chemical Dispersion Model (AFTOX).* AFGL-TR-88-0009. Air Force Geophysics Laboratory, Hanscom AFB, MA 01731.

Kumar, N. and F.W. Lurmann, 1997a: *Peer Review of Environ's Ozone Source Apportionment Technology and the CAMx Air Quality Models.* STI-996203-1732-RFR. Sonoma Technology, Inc., Santa Rosa, CA. Available at www.camx.com.

Kumar, N. and F.W. Lurmann, 1997b: *Comparison of CAMx and UAM-V Model Performance for Two Ozone Episodes in the Eastern United States.* STI-996203-1733-FR. Sonoma Technology, Inc., Santa Rosa, CA. Available at www.camx.com.

Kumar, N., A.G. Russell, T.W. Tesche and D.E. McNally, 1994: Evaluation of CALGRID using two different ozone episodes and comparison to UAM results. *Atmos. Environ.*, **28**, 2823-2845.

Lakes Environmental, 1997: *User's Guide for SLAB View.* Lakes Environmental Consultants, Inc., 250 Keats Way, Unit 18, Waterloo, Ontario, N2L 6J5, Canada.

Ligocki, M.P. and G.Z, Whitten, 1992: Modeling air toxics with the Urban Airshed Model. Paper 92-84.12 in the proceedings of the 85th Annual Meeting of the Air and Waste Management Association, Kansas City.

Lu, R. and R.P. Turco, 1996: Ozone distributions over the Los Angeles Basin: Three-dimensional simulations with the SMOG model. *Atmos. Environ.*, **30**, 4155-4176.

Lurmann, F.W., A.S. Wexler, S.N. Pandis, S. Musarra, N. Kumar and J.H. Seinfeld, 1997: Modeling urban and regional aerosols -- II. Application to California's South Coast Air Basin. *Atmos. Environ.*, **31**, 2695-2715.

Mitchell, A.E., Jr., 1982: A comparison of short-term dispersion estimates resulting from various atmospheric stability classification methods. *Atmospheric Environment*, **16**, 765-773.

Morris, R.E., T.C. Myers, G.E. Mansell, C.A. Emery and M.A. Yocke, 1994: *Photochemical Modeling of the Lake Michigan Region for the 1991 Lake Michigan Ozone Study (LMOS) Episodes Using the Nested-Grid Urban Airshed Model.* Final Report SYSAPP94-93/174, Systems Applications International, San Rafael, CA.

Morris, R.E. and T.C. Myers, 1990: *User's Guide for the Urban Airshed Model. Volume I: User's Manual for UAM (CB-IV).* EPA-450/4-90-007A. Available from NTIS: (703) 487-4650 as PB91-131227.

Morris, R.E. T.C. Myers, E.L. Carr, M.C. Causley and S.G. Douglas, 1990: *User's Guide for the Urban Airshed Model. Volume II: User's Manual for the UAM (CB-IV) Modeling System.* EPA-450/4-90-007B. Available from NTIS: (703) 487-4650 as PB91-131235.

Mudan, K.S., 1983: Gravity spreading and turbulent dispersion of pressurized releases containing liquid aerosols, IUTAM Symposium, September 1-3, The Hague, The Netherlands.

Myers, T.C., P.D. Guthrie and S.-Y.Wu, 1996: The Implementation of a Plume-in-Grid Module in the SARMAP Air Quality Model (SAQM). SYSAPP-96/06. Prepared for the San Joaquin Valleywide Air Pollution Study Agency, Sacramento, CA.

Ooms, G., A.P. Mahieu, and F. Zelis, 1974: The plume path of vent gases heavier than air, First International Symposium on Loss Prevention and Safety Promotion in the Process Industries, (C.H. Buschman, Editor), Elsevier Press.

Panofsky, H.A., and J.A. Dutton, 1984: *Atmospheric Turbulence, Models and Methods for Engineering Applications*. John Wiley & Sons, 397pp.

Petersen, R.L., 1997: Development and evaluation of an improved algorithm for estimating TIBL height. 10th Joint Conference of Air Pollution Meteorology with the Air and Waster Management Association, Phoenix, Arizona. American Meteorological Society, Boston, Massachusetts.

Petersen, R.L., M.A. Ratcliff, and B.C. Cochran, 1995: *Wind Tunnel Modeling of Shoreline Fumigation for the Werner Station – Interim Progress Report.* Cermak Peterka Petersen, Inc., Project 1013, sponsored by New Jersey Power and Light.

Petersen W.B., and L.G. Lavdas, 1986: *INPUFF 2.0 - A Multiple Source Gaussian Puff Dispersion Algorithm, User's Guide.* EPA/600/8-86/024. Atmospheric Sciences Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Petersen, W.B., 1982: *Estimating Concentrations Downwind from an Instantaneous Puff Release.* EPA/600/3-82-078. U.S. Environmental Protection Agency, Research Triangle Park, NC.

Pielke, R.A., W.R. Cotton, R.L. Walko, C.J. Tremback, W.A. Lyons, L.D. Grasso, M.E. Nicholls, M.D. Moran, D.A. Wesley, T.J. Lee and J.H. Copeland, 1992: A comprehensive meteorological modeling system – RAMS. *Meteorol. Atmos. Phys.*, **49**, 69-91.

Post, L., 1994a: *HGSYSTEM 3.0 Technical Reference Manual.* TNER.94.059, Shell Research Limited, Thornton Research Centre, P.O. Box 1, Chester, U.K., CH1 3SH.

Post, L., 1994b: *HGSYSTEM 3.0 User's Manual.* TNER.94.058, Shell Research Limited, Thornton Research Centre, P.O. Box 1, Chester, U.K., CH1 3SH.

Quest Consultants, 1997: *CANARY by Quest, User's Manual*, Quest Consultants, Inc., 908 26th Avenue, N.W., Suite 103, Norman, Oklahoma 73069.

Rao, K.S., 1982: *Analytical Solutions of a Gradient-Transfer Model for Plume Deposition and Sedimentation.* NOAA Technical Memorandum ERL ARL-109, 75pp; EPA-600/3-82-079, U.S. Environmental Protection Agency, Research Triangle Park, NC 27711; available from NTIS as PB 82-215 153, Springfield, VA.

SAI, 1996a: *User's Guide to the Variable-Grid Urban Airshed Model (UAM-V).* SYSAPP-96-95/27r (revised edition), Systems Applications International, San Rafael, CA.

SAI, 1996b: *User's Guide: Preprocessors for Preparation of UAM-V Initial and Boudary Concentration Data Files.* SYAPP-96/086, Systems Applications International, San Rafael, CA.

SAI, 1996c: *User's Guide for the UAM/UAM-V Boundary Condition Extration Program (EXRACT BC).* SYSAPP-96/005, Systems Applications International, San Rafael, CA.

SAI, 1996d: *User's Guide: Postprocessing System for the Urban Airshed Model, Nested Grid Version (UAM-V).* SYSAPP-96/009r2, Systems Applications International, San Rafael, CA.

SAI, 1995a: *User's Guide to the Systems Application International Mesoscale Model (Version 3.1).* SYSAPP-95/070, Systems Applications International, San Rafael, CA.

SAI, 1995b: *User's Manual for Variable Grid UAM (UAM-V) Preprocessor and Utility Programs.* SYSAPP-95/033, Systems Applications International, San Rafael, CA.

SAI, 1995c: *User's Guide for the MM2UAMV Software.* SYSAPP-95/086, Systems Applications International, San Rafael, CA.

Scheffe, R.D. and R.E. Morris, 1993: A review of the development and application of the Urban Airshed Model. *Atmos. Environ.*, **27B**, 23-39.

Scire, J.S., D.G. Strimaitis, and R.J. Yamartino, 1998: *A User's Guide for the CALPUFF Dispersion Model (Version 5.0), Draft*, Earth Tech, 196 Baker Avenue, Concord, MA 01742.

Scire, J.S., E.M. Insley, R.J. Yamartino and M.E. Fernau, 1995a: *A User's Guide for the CALMET Meteorological Model.* Report No. 1406. Earth Tech, Inc., Concord, MA.

Scire, J.S., E.M. Insley, D.G. Strimaitis, J.C. Chang, and E. Chang, 1995b: *Testing of Meteorological and Dispersion Models for Use in Regional Air Quality Modeling.* Prepared for the CADMUS Group, Inc., Waltham, MA; by Earth Tech, 196 Baker Avenue, Concord, MA. Earth Tech Report No. A314-01.

Scire, J.S., R.J. Yamartino, G.R. Carmichael and Y.S. Chang, 1989: *CALGRID: A Mesoscale Photochemical Grid Model. Volume II: User's Guide.* Final Report A049-1, Sigma Research Corporation (now Earth Tech, Inc.), Concord, MA.

Scire, J.S., F.W. Lurmann, A. Bass, and S.R. Hanna, 1984a: *User's Guide to the MESOPUFF II Model and Related Processor Programs.* EPA-600/8-84-013, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Scire, J.S., F.W. Lurmann, A. Bass, and S.R. Hanna, 1984b: *Development of the MESOPUFF II Dispersion Model.* EPA-600/3-84-057, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Sethuraman, S., 1987: *Analysis and Evaluation of Statistical Coastal Fumigation Models*, Report EPA-450/4-87-002, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Spicer, T.O., and J.A. Havens, 1990: *DEGADIS (Dense Gas DISpersion) - Version 2.1.* EPA/SW/DK-90/034a, EPA/OAQPS, Research Triangle Park, NC. Report available from the National

Technical Information Service, Publication no. PB90-213893, Springfield, VA.

Spicer, T.O., 1990: *Implementation of DEGADIS v2.1 on a Personal Computer.* Prepared for the American Petroleum Institute, 1220 L Street, Northwest, Washington, DC 20005.

Stunder, M., and S. Sethuraman, 1985: A comparative evaluation of the coastal internal boundary-layer height equations. *Boundary Layer Meteorology*, **32**, 177-204.

Strimaitis, D.G., J.S. Scire, and J.C. Chang, 1998: Evaluation of the CALPUFF dispersion model with two power plant data sets. 10th Joint Conference of Air Pollution Meteorology with the Air and Waster Management Association, Phoenix, Arizona. American Meteorological Society, Boston, Massachusetts.

Tang, R.T., S.C. Gerry, J.S. Newsome, A.R. Van Meter, R.A. Wayland, J.M. Godowitch and K.L. Schere, 1990: *User's Guide for the Urban Airshed* Model. Volume V: Description and Operation of the ROM-UAM Interface Program System. EPA-450/4-90-007E. Available from NTIS: (703) 487-4650 as PB91-131268.

Touma, J.S., W.M. Cox, H. Thistle, and J.G. Zapert, 1995: Performance evaluation of dense gase dispersion models. *J. Applied. Meteorol.*, **34**, 603-615.

Trinity Consultants, 1997: *BREEZE HAZ User's Guide for Windows, User's Guide for DEGADIS+, SLAB, AFTOX, INPUFF, EXPERT, and SUITE.* Trinity Consultants, Inc., P.O. Box 14205, Research Triangle Park, NC 27709-4205.

U.S. EPA, 1995a: *Interagency Workgroup on Air Quality Modeling (IWAQM): Assessment of Phase I Recommendations Regarding the Use of MESOPUFF II.* EPA-454/R-95-006. Available from EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/). U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. EPA, 1995b: *User's Guide for the Industrial Source Complex (ISC3) Dispersion Models, Volume II – Description of Model Algorithms.* EPA-454/B-95-003b. Available from EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/). U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. EPA, 1994a: *A Revised User's Guide to MESOPUFF II (V5.1).* EPA-454/B-94-025. Available from EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/). U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. EPA, 1994b: *User's Guide to TSCREEN, A Model for Screening Toxic Air Pollutant Concentrations (Revised).* EPA-454/B-94-023. Available from EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/). U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. EPA, 1993a: *User's Guide for the Urban Airshed Model. Volume VIII: User's Manual for the Quality Assurance System.* EPA-454/B-93-004. Available from NTIS: (703) 487-4650

U.S. EPA, 1993b: *Interagency Workgroup on Air Quality Modeling (IWAQM), Phase I Report: Interim Recommendation for Modeling Long Range Transport and Impacts on Regional Visibility.* EPA-

454/R-93-015. Available from EPA's SCRAM bulletin board (http://www.epa.gov/ttn/scram/). U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. EPA, 1992a: *User's Guide for the Urban Airshed Model. Volume IV: User's Manual for the Emissions Preprocessor System 2.0.* EPA-450/4-90-007D(R). U.S. Environmental Protection Agency, Research Triangle Park, NC. Available from NTIS: (703) 487-4650 as PB93-122380.

U.S. EPA, 1992b: *User's Guide for the Urban Airshed Model. Volume VI: User's Manual for the Postprocessing System.* EPA-450/4-90-007F. U.S. Environmental Protection Agency, Research Triangle Park, NC. Available from NTIS: (703) 487-4650 as PB92-145382/AS.

U.S. EPA, 1992c: *User's Guide for the Urban Airshed Model. Volume VII: User's Manual for the Performance Evaluation System.* EPA-450/4-90-007G. U.S. Environmental Protection Agency, Research Triangle Park, NC. Available from NTIS: (703) 487-4650 as PB92-224849/AS.

U.S. EPA, 1992d: *Workbook of Screening Techniques for Assessing Impacts of Toxic Air Pollutants (Revised).* EPA-454/R-92-024. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. EPA, 1989: *User's Guide for RVD 2.0 – A Relief Valve Discharge Screening Model.* EPA-450/4-88-024. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. EPA, 1988: *Screening Procedures for Estimating the Air Quality Impact of Stationary Sources.* EPA-450/4-88-010. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. EPA, 1986a: *Guideline on Air Quality Models (Revised).* EPA-450/2-78-027R. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. EPA, 1986b: E*valuation of Short-Term Long-Range Transport Models, Volumes I and II.*. EPA-450/4-86-016a and b. U.S. Environmental Protection Agency, Research Triangle Park, NC.

Wexler, A.S., F.W. Lurmann and J.H. Seinfeld, 1994: Modeling urban and regional aerosols: I. Model development. *Atmos. Environ.*, **28**, 531-546.

Wilkinson, J.G. and R.A. Emigh, 1995: *The Emissions Modeling System (EMS-95) User's Guide.* Prepared by Alpine Geophysics, Boulder, CO for the Texas Natural Resource Conservation Commission, Austin, TX.

Wilkinson, J.G., C.F. Loomis, D.E. McNally, R.A. Emigh and T.W. Tesche, 1994: *Technical Formulation Document: SARMAP/LMOS Emissions Modeling System (EMS-95).* AG-90/TS26 and AG-90/TS27. Prepared by Alpine Geophysics, Pittsburgh, PA for the Lake Michigan Air Directors Consortium, Des Plaines, IL and the Valley Air Pollution Study Agency, Sacremento, CA.

Witlox, H.W.M., 1988: *User's Guide for the HEGADAS Heavy Gas Dispersion Program.* Shell Research Limited, Thornton Research Centre, P.O. Box 1, Chester, U.K., CH1 3SH. Report available from the National Technical Information Service, Publication no. PB89-164560, Springfield, VA

Yamartino, R.J, 1993: Nonnegative, conserved scalar transport using grid-cell-centered, spectrally

constrained Blackman cubics for applications on a variable thickness mesh. *Mon. Weather Review*, **121**, 753-763.

Yamartino, R.J., J.S. Scire, G.R. Carmichael and Y.S. Chang, 1992: The CALGRID mesoscale photochemical grid model -- I. Model formulation. *Atmos. Environ.*, **26A**, 1493-1512.

Yarwood, G., G. Wilson, R.E. Morris and M.A. Yocke, 1997: *User's Guide to the Ozone Tool: Ozone Source Apportionment Technology for UAM-IV*. ENVIRON International. Novato, CA.

The Department of the Interior Mission

As the Nation's principal conservation agency, the Department of the Interior has responsibility for most of our nationally owned public lands and natural resources. This includes fostering sound use of our land and water resources; protecting our fish, wildlife, and biological diversity; preserving the environmental and cultural values of our national parks and historical places; and providing for the enjoyment of life through outdoor recreation. The Department assesses our energy and mineral resources and works to ensure that their development is in the best interests of all our people by encouraging stewardship and citizen participation in their care. The Department also has a major responsibility for American Indian reservation communities and for people who live in island territories under U.S. administration.

The Minerals Management Service Mission

As a bureau of the Department of the Interior, the Minerals Management Service's (MMS) primary responsibilities are to manage the mineral resources located on the Nation's Outer Continental Shelf (OCS), collect revenue from the Federal OCS and onshore Federal and Indian lands, and distribute those revenues.

Moreover, in working to meet its responsibilities, the **Offshore Minerals Management Program** administers the OCS competitive leasing program and oversees the safe and environmentally sound exploration and production of our Nation's offshore natural gas, oil and other mineral resources. The MMS **Royalty Management Program** meets its responsibilities by ensuring the efficient, timely and accurate collection and disbursement of revenue from mineral leasing and production due to Indian tribes and allottees, States and the U.S. Treasury.

The MMS strives to fulfill its responsibilities through the general guiding principles of: (1) being responsive to the public's concerns and interests by maintaining a dialogue with all potentially affected parties and (2) carrying out its programs with an emphasis on working to enhance the quality of life for all Americans by lending MMS assistance and expertise to economic development and environmental protection.