Review of Models Used for Determining Consequences of UF₆ Release

Model Evaluation Report

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ABSTRACT

Three uranium hexafluoride- (UF_6 -) specific models -- HGSYSTEM/ UF_6 , Science Application International Corporation, and RTM-96; three dense-gas models -- DEGADIS, SLAB, and the Chlorine Institute methodology; and one toxic chemical model -- AFTOX -- are evaluated on their capabilities to simulate the chemical reactions, thermodynamics, and atmospheric dispersion of UF_6 released from accidents at nuclear fuel-cycle facilities, to support Integrated Safety Analysis, Emergency Response Planning, and Post-Accident Analysis. These models are also evaluated for user-friendliness and for quality assurance and quality control features, to ensure the validity and credibility of the results. Model performance evaluations are conducted for the three UF_6 -specific models, using field data on releases of UF_6 and other heavy gases. Predictions from the

HGSYSTEM/ UF_6 and SAIC models are within an order of magnitude of the field data, but the SAIC model overpredicts beyond an order of magnitude for a few UF_6 -specific data points. The RTM-96 model provides overpredictions within a factor of 3 for all data points beyond 400 m from the source. For one data set, however, the RTM-96 model severely underpredicts the observations within 200 m of the source. Outputs of the models are most sensitive to the meteorological parameters at large distances from the source and to certain source-specific and meteorological parameters at distances close to the source. Specific recommendations are being made to improve the applicability and usefulness of the three models and to choose a specific model to support the intended analyses. Guidance is also provided on the choice of input parameters for initial dilution, building wake effects, and distance to completion of UF_6 reaction with water.

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EXECUTIVE SUMMARY

Accidental releases of uranium hexafluoride (UF_6) continue to present a potentially significant hazard at nuclear fuel-cycle facilities licensed by the Nuclear Regulatory Commission (NRC). Understanding the possible distribution of hazardous materials (uranyl fluoride [UO_2F_2] and hydrogen fluoride [HF]) in the environment resulting from an accidental release of uranium hexafluoride (UF_6) is important for understanding the adequacy of safety measures to prevent such accidents and to mitigate their effects. Such an analysis of consequences is viewed as an essential part of an Integrated Safety Analysis (ISA). Also, Emergency Planning (EP) for responding to such accidents is improved by advance analysis of the likely paths of the released cloud or plume of these hazardous materials. In the event of an accident involving the release of UF_6 from a facility, a Post-Accident Analysis (PAA) is also performed by NRC, to evaluate both the severity of the accident and its potential health impacts on the local population.

For each of these analyses--ISA, PAA, EP, mathematical models determine the concentrations of uranium and HF in air, to support the assessment of health impacts on exposed individuals. A number of mathematical models are currently available that simulate the release and transport of contaminants in air. Of these, seven models have been selected as being suitable to support the ISA, PAA, and EP. Three of these models--HGSYSTEM/ UF_6 , SAIC, and RTM-96 directly include UF_6 -specific capabilities; three others--DEGADIS, SLAB, and the Chlorine Institute

methodology, were developed for dense gases in general; and the last model--AFTOX--was developed to handle the dispersion of toxic chemicals.

The objective of this study is to evaluate the seven models regarding their capabilities in modeling the important processes involved in the release and transport of UF_6 and its reaction products in the atmosphere; their applicabilities to ISA, PAA, and EP; and their user interface and Quality Assurance and Quality Control features. Accordingly, the model evaluation process is divided into three specific tasks: (1) evaluation of model components; (2) evaluation of model applicability; and (3) evaluation of model's user interface and Quality Assurance and Quality Control features. Source term, chemistry and thermodynamics of UF_6 , and atmospheric dispersion are the primary model components evaluated. Under the model applicability task, the ability of each model to address site-specific considerations at a nuclear fuel-cycle facility and the requirements of ISA, EP, and PAA are evaluated. User friendliness, correctness and clarity of model documentation, verification and validation information, and ease of use are some of the user interface and Quality Assurance and Quality Control features of the models that are evaluated.

A number of criteria questions and weighted maximum scores have been developed for each of the three tasks, and each model has been evaluated and scored. Scores are combined to rank models under each task and for their overall capabilities. The HGSYSTEM/ UF_6 and SAIC models are determined to possess the most process-level capabilities for modeling the dispersion of UF_6 and its reaction products in the

atmosphere. The RTM-96 model is determined to provide a screening-level methodology for a quick, bounding assessment of the health impacts from a nuclear fuel-cycle facility. However, documentation for the RTM-96 model does not provide any justification to support the claim made therein that the model provides consistently conservative estimates of the health impacts. The other four models do not possess adequate UF₆-specific process-level capabilities. None of the seven models can independently evaluate and report source terms for all potential accident scenarios identified as part of this study (Nair, *et al.*, 1997). As a result of the initial model scores from this study and based on the results of reviews of dense gas models in general (Touma, *et al.*, 1995; Hanna, *et al.*, 1993) and the reviews of the potential models for UF₆ conducted in the past (Sykes & Lewellen, 1992), this study restricts detailed performance assessments to the HGSYSTEM/UF₆, SAIC, and RTM-96 models.

The DEGADIS, SLAB, and AFTOX models and the Chlorine Institute methodology are not recommended for use in consequence analysis of UF₆ releases at fuel-cycle facilities because they do not address UF₆-specific chemistry, thermodynamics, and dispersion.

Model performance is assessed using direct comparison of model predictions with field measurements; these comparisons are made graphically and statistically. For models containing multiple modules, performance of each individual module has been assessed. Field measurements of concentrations are available for UF₆, ammonia (NH₃), HF, and a mixture of Freon-12 and nitrogen (N₂), from

a number of experimental and accidental releases of these heavy gases, along with meteorological and other data on the nature of the release. Field data for UF₆ are available from: (1) three experimental releases made at Bordeaux in France between 1986 and 1989; (2) an accidental release at Gore, Oklahoma; and (3) an accidental release at the Comurhex Plant in France. Field data for the other heavy gases are available from (1) Goldfish trials conducted at the Nevada Test Site (HF); (2) Desert Tortoise releases at the Nevada Test Site (NH₃); and (3) Thorney Island releases (mixtures of Freon-12 and N₂) in the United Kingdom.

For model performance tests conducted with heavy gases other than UF₆, predictions of contaminant concentrations from the HGSYSTEM/UF₆ model are within a factor of 2 of the field measurements. For four of the seven data sets that were tested, the SAIC model provides predictions of contaminant concentrations, within a factor of 2. For the other data sets, most predictions from the SAIC model fall within an order of magnitude of the measured concentrations; however, the predictions of average concentrations underestimates the observations. The RTM-96 model is developed specifically for UF₆. Therefore, it has not been tested with data from other heavy gases.

For the Bordeaux UF₆ experiments, predictions of total uranium concentrations from the HGSYSTEM/UF₆ model are within an order of magnitude of the measurements, with most values falling within a factor of 2. Predictions made from the SAPLUME module of the SAIC model overestimate the measured concentrations; however, the

predictions are within an order of magnitude of the observations. Predictions from the SACRUNCH module of the SAIC model are within a factor of 5 for distances greater than 10 meters (m). At 10 m, the module overpredicts by 3 orders of magnitude. The RTM-96 model severely underestimates the measurements at near-source distances of less than 200 m (a number of predictions are over an order of magnitude below observations), and overestimates them at longer distances, with most predictions within a factor of 3 of the observations.

For the Gore, Oklahoma, release, modeling the source as a continuous release yields better predictions from the HGSYSTEM/UF₆ model at distances greater than 1400 m from the source than modeling the source as a combined puff and continuous release. At 160 m from the source, the only location between the source and 1400 m where a measured value was available, modeling the source as a combined release yields better predictions. However, most of predictions with both approaches are within a factor of 2 of the observations. Modeling the source as a continuous release yields underestimates of the measurements from the SAIC model at distances greater than 1400 m from the source and an overestimate at 160 m from the source. Modeling the source as a combined release yields overestimates from the SAIC model at all distances. Overpredictions from the SAIC model are above a factor of 2 and within two orders of magnitude, and the underpredictions are within an order of magnitude. Of the three models, the RTM-96 model provides the most accurate predictions (within a factor of 3) at all distances with a bias toward overestimation.

For the Comurhex release, predictions from both HGSYSTEM/UF₆ and RTM-96 models provide good agreements with predictions of HF concentrations (within a factor of 2) at two locations reported by Doumenc, *et al.* (1978). The SAIC model underestimates the concentrations at both locations by more than a factor of 2. The RTM-96 model provides consistently conservative estimates at distances greater than 400 m (0.25 miles) from the source. At these distances, the results support the claim made in the model documentation that the RTM-96 model represents a conservative, screening-level model.

Detailed sensitivity analyses are conducted on all modules of the HGSYSTEM/UF₆ and SAIC and RTM-96 models. Sensitivity of the output concentrations of total uranium to each input parameter has been determined for each module at two locations, one close to the source and one far away from the source. At greater distances from the source, the output concentration of total uranium is most sensitive to meteorological parameters such as atmospheric stability, wind speed, and surface roughness length for all models. At closer distances, the output concentrations of total uranium for all models are most sensitive to certain source-specific parameters such as source height or source size and also to meteorological parameters such as atmospheric stability, wind speed, and surface roughness length.

Modeling approaches presented in this study can be used to conceptualize and model releases of UF₆ from fuel-cycle facilities, using the three models. Based on the performance of the three models and depending on the performance requirements

at a fuel-cycle facility, specific recommendations are made for the choice of a specific model to support ISA, EP, and PAA. A number of recommendations are made for the HGSYSTEM/UF₆, SAIC, and RTM-96 models, which can improve their applicability and usefulness to ISA, EP, and PAA.

During the course of model testing, it becomes apparent that the modeler requires considerable judgment to set up the input file for every new application. This judgment affects the accuracy of the model in predicting the consequences of a UF₆ release. To alleviate some of the difficulties in preparing the input files, a discussion of initial dilution, building wake effects, and distance to completion of UF₆ reaction with water is provided in Appendix A.

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1 INTRODUCTION

1.1 Background and Objective

The accidental release of uranium hexafluoride (UF_6) represents a potentially significant hazard at nuclear fuel-cycle facilities licensed by the Nuclear Regulatory Commission (NRC). Understanding the possible distribution of the hazardous materials (uranyl fluoride [UO_2F_2] and hydrogen fluoride [HF]) in the environment, resulting from an accidental release of UF_6 , is important for understanding whether safety measures are adequate to prevent such accidents and to mitigate their effects. Such an analysis of consequences is viewed as an essential part of an Integrated Safety Analysis (ISA). Also, emergency planning (EP) for responding to such accidents benefits from advance analysis of the likely paths of the released cloud or plume of these hazardous materials.

Consequence evaluation for UF_6 releases is currently being conducted by using analytical models that take into account both dense gas behavior and the chemistry and thermodynamics of UF_6 in the atmosphere.

NRC has identified three areas, within the licensing process, that could use analytical models to the consequences of UF_6 release: (1) ISA; (2) emergency planning (EP); and (3) post-accident analysis (PAA). ISA is a systematic effort to identify process upsets, or conditions at a facility, that could lead to releases. Analytical models are necessary to predict the concentration of

the relevant chemical species after a potential release. For EP, a model capable of predicting the concentrations of UF_6 and its reaction products in the vicinity of the facility is useful for the analysis of potential accident scenarios. For a PAA, analytical models are useful in estimating potential human health impacts, to help health officials respond to any immediate or long-term health concerns that could result from exposure to the chemicals released during an accident.

NRC contracted with *SENES* Oak Ridge, Inc., to assess the effectiveness and applicability of various analytical models that are currently available for evaluating the consequences of a UF_6 release. The objective of the present assessment is to help NRC judge the acceptability of such models for use in three areas of NRC regulatory responsibility: (1) analysis of potential accidents identified in the ISA process; (2) analysis of potential accidents for use in EP; and (3) PAA. It should be noted that the purposes for which the models are being evaluated do not include their uses during emergency response.

1.2 Evaluation Process and Criteria

At the onset of the project, a complete evaluation process was established for review and assessment of models that could be used to estimate impacts from accidental releases of UF_6 . The process consisted of the evaluation of three essential elements: (1) model components, (2) model applicability, and (3) user interface and Quality Assurance

(QA) and Quality Control (QC).

Primary elements of model component evaluation included source term, dispersion, and model performance. UF₆-specific chemistry and thermodynamics were also recognized as key modeling components. Because UF₆-specific chemistry and thermodynamics directly influence the estimation of the source term, plume development, and dispersion characteristics, chemistry and thermodynamics were evaluated within the categories of source term and dispersion components. The evaluation of model applicability included consideration of each model's usefulness for ISA, EP, PAA, and certain site-specific factors. The user friendliness, documentation, and QA and QC protocols of models were evaluated under the user interface and QA and QC evaluation criterion. Nair, *et al.* (1997) provide detailed descriptions of the entire evaluation process.

To facilitate an objective evaluation of the models, a set of evaluation criteria and a scoring methodology were developed as guidelines for each element of the evaluation (Nair, *et al.*, 1997). Reviews of the UF₆ models presented in this document strictly follow these guidelines. Throughout this document, the term "model" is used to represent all aspects of a model: mathematical formulation, theoretical basis, documentation, user's manual, algorithms, codes, etc.

1.3 Selection of Models

At the beginning of the project, a number of models were identified as potentially useful for supporting integrated safety analysis, emergency planning, and post-accident analysis at fuel-cycle facilities. They included but were not limited to the following: CHARM; SAFER; PLUME; SAIC (containing SAPLUME, SACRUNCH, and SADENZ modules); VAPACT; CYLIND; the RTM-93 (replaced by RTM-96) model; and the straight-line Gaussian Plume Model. It was decided, in light of the various reviews of dense gas models in general (Touma, *et al.*, 1995; Hanna, *et al.*, 1993) and the reviews of potential models for UF₆ conducted in the past (Sykes and Lewellen, 1992), that the number of models to be reviewed in this study should be limited to a few that are judged to be robust by the previous reviews.

Hanna, *et al.* (1993) evaluated 15 hazardous gas models using data from eight field experiments. The models included seven publicly available models (AFTOX, DEGADIS, HEGADAS, HGSYSTEM, INPUFF, OB/DG, and SLAB); six proprietary models (AIRTOX, CHARM, FOCUS, GASTAR, PHAST, and TRACE); and two "benchmark" analytical models (the Gaussian Plume Model and the analytical approximations to the Britter and McQuaid Workbook nomograms). The most consistent predictions of plume centerline concentrations were obtained from the Britter and McQuaid,

CHARM, Gaussian Plume, HEGADAS, HGSYSTEM, PHAST, and SLAB models.

Touma, *et al.* (1995) evaluated seven dense gas dispersion models using data from three field experiments. The models included two public-domain models (DEGADIS and SLAB) and five proprietary models (AIRTOX, CHARM, FOCUS, SAFEMODE, and TRACE). The evaluation used field data from the Desert Tortoise experiments (releases of pressurized ammonia); the Burro tests (liquefied natural gas spill); and the Goldfish experiments (anhydrous HF spills). When model results were compared across the three datasets, all models provided predictions within a factor of two of the measured concentrations of various species in air.

Sykes and Lewellen (1992) considered five models for the evaluation of their effectiveness in modeling UF_6 releases: PLM89A, TRIAD, HGSYSTEM, ADAM, and SLAB. The first two models were developed specifically to handle UF_6 releases. Sykes and Lewellen concluded that none of the candidate models met all the requirements for a safety analysis model. The necessary modifications and enhancements to make each model useful for safety analysis were outlined. Based on the recommendations of Sykes and Lewellen (1992), the HGSYSTEM model was modified to include UF_6 -specific physical and chemical mechanisms, release scenarios, and user interfaces.

After discussions with NRC, the focus of this project was directed to public-

domain models that could be easily procured and accessed by users at the fuel-cycle facilities. Five detailed models and two screening-level models were selected for this review. The detailed models were DEGADIS (Spicer and Havens, 1989); SLAB (Ermak, 1990); HGSYSTEM/ UF_6 (Hanna, *et al.*, 1994a, 1994b; Post, 1994); SAIC (Kaiser, 1993); and AFTOX (Krunkel, 1991). The screening-level models were RTM-96 (NRC's Response Technical Manual; US NRC, 1996) and the Chlorine Institute methodology (Chlorine Institute, 1991). The RTM-96 model is a revised version of the RTM-93 model (US NRC, 1993). Other dense gas models, such as ALOHA (USEPA, 1995), that provide capabilities similar to DEGADIS and SLAB, and are based on one or more of these models, but that do not possess the capabilities to handle the chemistry and thermodynamics of UF_6 , were not selected for this review.

Specific information about several of the models should be noted. The HGSYSTEM/ UF_6 model consists of eight modules, each of which is applicable to specific release and dispersion characteristics. Similarly, the SAIC model consists of three independent modules, SACRUNCH, SADENZ, and SAPLUME, each with its own well-defined capabilities. The HGSYSTEM/ UF_6 and SAIC models contain UF_6 -specific chemistry, thermodynamics, and plume development algorithms. Primary modules in the HGSYSTEM/ UF_6 and SAIC models and the links among the various modules are presented in Figure 1.1. The RTM-96 model represents a

screening-level, hand-calculation procedure, which was developed to predict conservative estimates of health impacts from the releases of UF_6 into the atmosphere. The RTM-96 model addresses UF_6 -specific chemistry in a limited manner. It does not include algorithms that simulate UF_6 -specific thermodynamics, or atmospheric dispersion of gases, vapors, and aerosols of liquid droplets, or solid particles, or a plume consisting of various mixtures of the above airborne materials, with

densities greater than that of air. It uses a passive plume characterization defined by Gaussian plume models to perform the dispersion calculations. The DEGADIS and SLAB models and the Chlorine Institute methodology are dense gas models. The Chlorine Institute methodology uses a graphical procedure involving isopleths to identify areas of concern for different release scenarios involving chlorine. The AFTOX model uses a Gaussian plume approach for the dispersion calculations.

HGSYSTEM/UF₆ Modules:

DATAPROP	generates physical properties
SPILL	transient liquid release from a pressurized vessel
LPOOL	evaporating multi-compound liquid pool model
HFSPILL	SPILL version specifically for hydrogen fluoride (HF)
AEROPLUME	high-momentum jet model
HEGABOX	dispersion of instantaneous heavy gas releases
HFPLUME	AEROPLUME version specifically for hydrogen fluoride (HF)
HEGADAS	heavy gas dispersion (steady-state and transient version)
PGPLUME	passive Guassian dispersion

SAIC Modules:

SACRUNCH	steady-state continuous ground-based release
SADENZ	instantaneous (puff) ground-based release
SAPLUME	Continuous stack and jet releases from valves or pipework

Figure 1.1 Primary modules in the HGSYSTEM/UF₆ and SAIC models and the links among them.

2 MODEL COMPONENT EVALUATION

Source term and dispersion are the primary model components that will be discussed in this section. The chemistry and thermodynamics of UF_6 and the interactions of UF_6 and its products of reaction with atmospheric moisture directly influence the source term and dispersion components. Therefore, these influences are handled as part of the evaluation of source term and dispersion. The evaluations are based on the descriptions of the components in the individual model documentation. For each evaluation criterion identified in Nair, *et al.* (1997), a complete analysis was conducted to determine the adequacy of the model to satisfy the theoretical and practical considerations embedded in the criterion. Actual testing of model algorithms using model simulations was not performed to support the qualitative evaluations; independent testing of model components using simulations is presented and discussed in Section 3.

2.1 Source Term Evaluation

None of the evaluated models has the capability to explicitly calculate the source terms, based on process-level knowledge of the parameters that lead to a release, for any of the four major categories of accidents presented in Section 3.1 of Nair, *et al.* (1997) and in Section 2.1.1 of this document. The user must perform certain source-term calculations before conducting a complete simulation. A complete calculation of the source term would require the estimation of the following terms by the model: rate and duration of UF_6 release; temperature of release; fractions released in various phases;

and type of release (jet, pool, stack, etc.). Three models have been specifically developed for UF_6 : HGSYSTEM/ UF_6 , SAIC, and RTM-96. Therefore, capabilities of these models with respect to UF_6 will be discussed in greater detail than the capabilities of other evaluated dense gas models.

The HGSYSTEM/ UF_6 model does provide the capability for internal calculation of the source term from the rupture of a liquid-filled tank. However, for a rupture occurring from a heated tank that is filled with a mixture of solid and liquid, the model cannot perform the calculations for a jet release even if the pressure and temperature are known. Moreover, it does not provide default recommendations for a set of pressure and temperature conditions that can be used for a conservative upper estimate of a release. When a jet release from a liquid-filled tank is modeled, the knowledge of pressure and temperature allows the model to independently estimate the release rate. However, because the model does not estimate the duration of release, the user must provide this quantity once the release rate is estimated by the model. For releases from a pool of liquid or a depressurized tank with a large diameter rupture, the HGSYSTEM/ UF_6 model requires the user to specify the emission rate instead of calculating it internally. This may be appropriate for a post-accident scenario when some knowledge of the accident exists. However, for emergency response planning or for an integrated safety analysis, the release rate should be calculated by the model. Alternatively, release rates for a range of potential release scenarios can be calculated in advance and made available to the modeler using the methods provided in

Appendix B of the updated Accident Analysis Handbook (US NRC, 1997).

The SAIC model requires the user to specify the release rates for all types of releases. It has no internal algorithm to calculate the release rate. This may be adequate for a post-accident analysis when all of the necessary input information may be available directly or derived from measured data. For integrated safety analysis and emergency planning, however, the user must perform the release calculations outside of the model. A further complication with the SAIC model is that it requires the user to specify an initial plume configuration for which the plume size, distance from the source, amount of air entrained, and fractions of various chemicals and phases present must be calculated by the user before running the code. Again, release rates for a range of potential release scenarios can be calculated in advance and made available to the modeler using the methods provided in Appendix B of the updated Accident Analysis Handbook (US NRC, 1997).

The RTM-96 model does not incorporate any of the characteristics of a release except the quantity and duration of release, both provided by the user. It performs the same set of calculations, regardless of the type of release, to provide a "bounding estimate" of impacts to the affected population.

In summary, none of the models considered for evaluation in this study was designed to calculate the complete source term from the initial conditions of a UF_6 release for the four categories of accidents (Nair, *et al.*, 1997; Section 2.1.1 of this document).

In Section 3, the model tests conducted using field/experimental data are discussed. The difficulties encountered in the preparation of source term information for each of the above models will be described within Section 3.

The evaluations presented in this section were conducted with the understanding that none of the models can explicitly calculate source terms from a knowledge of release/accident characteristics. These evaluations have been conducted in accordance with the protocols presented in Nair, *et al.* (1997). Some of the evaluation criteria and rationales for awarding scores were modified to account for the fact that the models do not independently calculate the source terms. Scores awarded to each model and the rationale for the scores are discussed below. The scoring criteria and maximum score for each criterion are included in Table 2.1.

2.1.1 Criteria Evaluation

Criterion 1. *How many accident categories can the model's source term algorithm handle?*

Four categories of accidents have been identified by Nair, *et al.* (1997): (A) failure of valve/pigtail, resulting in release of liquid UF_6 ; (B) failure of valve/pigtail, resulting in release of UF_6 vapor; (C) rupture of cylinder filled with liquid UF_6 ; and (D) rupture of cylinder filled with solid UF_6 . The thermodynamic properties of UF_6 dictate that when liquid UF_6 is released from a pressurized cylinder, valve, or pigtail, under ambient atmospheric conditions, immediate flashing results in the formation of solid and

vapor phases. Therefore, a dispersion model that accepts a ground-level release with an input of (1) the total UF_6 release rate, (2) the fractions released in vapor and solid phases, and (3) the release temperature and pressure, would be able to handle all four categories of UF_6 releases. Models that directly accept the above quantities as input for the source term were assigned a maximum score of 8 points out of 10, with 2 points deducted for not having the built-in capabilities to calculate these specified quantities.

Thus, the SAIC, RTM-96, and DEGADIS models were awarded 8 points each. The AFTOX and SLAB models were awarded 7 points because they could not handle solid-phase releases, although they could handle liquid-phase releases. The Chlorine Institute methodology received only 5 points because it could not handle solid-phase releases; it performs internal calculations specifically only for the releases of chlorine in liquid and vapor forms; and its thermodynamics are not relevant for UF_6 .

If the release is from a cylinder filled with liquid UF_6 , the user can specify the initial pressure and temperature in the HGSYSTEM/ UF_6 model to obtain the release or source term. The model will automatically estimate the quantities of UF_6 generated in solid and vapor phases when flashing occurs. If the release is specified as a mixture, the user must provide all information regarding the release characteristics. Similarly, when UF_6 is released from a ground spill, the rate of release must be specified by the user. There is no internal mechanism within the HGSYSTEM/ UF_6 model to calculate the source term (quantities such as rate and duration of UF_6 emission) from an initial

mass of UF_6 in the pool. The HGSYSTEM/ UF_6 model was awarded 8.5 points because it provides the capabilities of estimating the source term from the rupture of a liquid-filled cylinder when the temperature and pressure within the cylinder are specified along with the size of the rupture.

Criterion 2. *Does the source term module handle puff as well as continuous releases?*

The HGSYSTEM/ UF_6 model can handle releases in the form of instantaneous puffs, elevated two-phase continuous momentum jets, and continuous releases of heavy vapors from the ground level. The SAIC model can handle ground-level, continuous, and puff releases of heavy vapors and releases of buoyant or heavy plumes from stacks, relief valves, and broken pipework. The DEGADIS, SLAB, and AFTOX models and the Chlorine Institute methodology can also all handle both instantaneous and continuous releases. Each of these models was awarded the full 15 points. The RTM-96 model, on the other hand, does not distinguish between the two types of releases and uses just the total quantity of UF_6 released as the input, with the objective of providing a bounding estimate without regard to the rate or height of release. This model was awarded 10 points.

Criterion 3. *Do the release or source term cases listed in the model reflect past accidents and/or possible future accidents that may occur?*

Of the models tested, only the HGSYSTEM/ UF_6 , SAIC, and RTM-96 models contain modules that were specifically developed for UF_6 . All three,

however, lack mechanisms to convert the dynamics of an accident into a source term; in other words, the user must convert an accident into a release rate and the fractions in vapor and solid phases. Therefore, if a release were to occur from the rupture of a liquid-filled tank, the user must perform an external calculation of the amounts that flash to vapor and solid phases, based on the prevailing conditions during the accident. (Only the HGSYSTEM/UF₆ model calculates these fractions and the release rate, when the pressure, temperature, and diameter of the rupture are specified.) Both the HGSYSTEM/UF₆ and SAIC models provide the capability of modeling the changes brought about by prevailing release and ambient conditions within a very short time interval after the initial release. Therefore, accurate specification of the initial release fractions may not be as critical as the specification of the total amount of UF₆ released, diameter of rupture, pressure, temperature, etc. It would be worthwhile to conduct a sensitivity analysis to evaluate the effect of changing the initial specifications of UF₆ fractions in the various phases on the predicted concentrations of UF₆ and its products of reaction with the atmospheric water vapor.

Both the HGSYSTEM/UF₆ and SAIC models were developed on the basis of information gathered from past accidents involving releases of dense gases, and both are capable of handling various types of releases (e.g., instantaneous puff, continuous) typically associated with accidents involving the releases of UF₆ and other dense gases. Each was awarded the full 15 points.

The RTM-96 model assumes that a specified fraction of the initial UF₆ released becomes airborne and estimates an upper-bound impact to an exposed individual. Again, this situation seems to preclude the need for specific knowledge of the accident, but this theory should be tested to ensure that the model actually provides an upper-bound estimate of the impact. Because of its uniform treatment of all accidents, the RTM-96 model was awarded 10 points. Each of the other models was awarded 10 points, because they were all based on accidents involving dense gas releases other than UF₆ and do not contain the required algorithms to handle the phase changes, reactions, and heat exchanges associated with the release of UF₆.

Criterion 4. *Does the source term algorithm contain mechanisms to translate an internal leak source into an external source?*

None of the evaluated models had this capability. Each model was awarded 5 points out of a maximum of 15 for being able to handle a vent release from the top of a building/facility.

Criterion 5. *Does the source term algorithm contain mechanisms to analyze failure modes, and does it quantify the release amount within an appropriate phase?*

As discussed earlier, none of the models contains the capabilities to analyze the release mode and quantify the release amount associated within the appropriate individual phases. All models could handle two-phase releases of dense gases, though not in appropriate phases. The

HGSYSTEM/UF₆ and SAIC models, as mentioned earlier, are not capable of handling all three phases at release. However, because of embedded thermodynamics (as explained in the evaluation of Criterion 3), they are superior to the other models as they can handle UF₆-specific phase changes at the time of release. They were awarded 25 points each out of 30. The RTM-96 model was also awarded 25 points because its treatment of phases is based on the thermodynamics of UF₆. The other models were awarded 20 points each because they could all handle two-phase releases, but were not specifically designed to handle the thermodynamics and phase changes necessary to describe UF₆ interaction with the ambient atmosphere.

Criterion 6. *Does the source term contain UF₆ reaction relationships with air, and does it quantify final products (HF, UO₂F₂, heat, etc.)?*

Once the release is specified, the thermodynamics and mass and energy balance modules in the HGSYSTEM/UF₆ model contain mechanisms to handle chemistry of UF₆ with atmospheric moisture, phase changes of UF₆, generation of heat, production of HF and UO₂F₂, entrainment of air, etc., in the near-source region. The model was awarded the full 25 points.

The SAIC model requires that some calculations be performed by the user before the definition of the initial plume characteristics. However, once the initial plume characteristics are specified, it will conduct the remaining calculations as well as the HGSYSTEM/UF₆ model. The sensitivity of the SAIC model to the

accurate definition of the initial plume is not clearly presented in the document description. The model was awarded 20 points.

The RTM-96 model accounts for all the changes in a bounding fashion and provides estimates of impacts from HF and total uranium, the primary toxicants of concern. Because of this simplistic treatment, the model was awarded only 15 points. All other models, which have no UF₆-specific capabilities, were awarded 10 points each, because they can be used with UF₆ as the primary contaminant, and, for the case when the reaction of UF₆ with atmospheric moisture is complete, the results can be used to estimate the concentrations of reaction products. Section 3.2.1 provides a complete discussion of the calculation of the concentrations of reaction products from UF₆ concentration.

2.1.2 Results of the Source Term Evaluation

Table 2.1 summarizes the scores awarded to each model for each criterion. Table 2.2 presents the evaluation summary of the source term component. The HGSYSTEM/UF₆ and SAIC models are seen to be clearly superior to all other models, primarily because of their UF₆-specific capabilities. The RTM-96 model also scores well as a screening-level model, for the same reason.

2.2 Dispersion Evaluation

Specific evaluation criteria for the dispersion component were identified in Nair, *et al.* (1997). The influences of the chemistry and thermodynamics of UF₆ and its products of

reaction on the dispersion of the plume containing these species are addressed as part of the evaluation of the dispersion component. Table 2.3 presents the criteria that were evaluated and the maximum score for each criterion.

2.2.1 Criteria Evaluation

Criterion 1. *Ability to deal with transient releases.*

Most of the reported accidents involving UF_6 have typically lasted from a few minutes to, at the most, 45 minutes. Releases that last for a few seconds can be treated as instantaneous, and those that last longer can be treated as continuous. Typically, a continuous source is treated as a short-term transient if it lasts for only a few minutes and as steady-state if it lasts longer. For a short time after release, the source term characteristics could be strongly dependent on the elapsed time since the occurrence of the accident. The characterization of the source and the ability to handle such time-dependent, short-term releases within the dispersion modules are critical to the accurate estimation of health impacts on the public. Simulation of transient, short-term releases by steady-state dispersion models could result in severe overestimation of persistent contaminant concentrations at receptor locations. In this evaluation, the capabilities of a model to handle all three types of releases (instantaneous, continuous/short-term or transient, and continuous/steady-state) were evaluated.

The HGSYSTEM/ UF_6 model has been designed to handle all three types of releases.

The HGSYSTEM/ UF_6 model was awarded the full 25 points.

The SAIC model consists of three separate modules: SACRUNCH, SAPLUME, and SADENZ. SACRUNCH and SAPLUME provide the capability for handling continuous releases. SADENZ provides the capabilities to handle instantaneous puff releases. However, none of the modules seems to provide the capability to handle short-term releases. It should be noted that the SAIC model does allow input of the duration of release. However, this parameter is used to incorporate the effects of cloud meander and averaging times and to calculate the duration of exposure for a receptor for estimating health impacts. The SAIC model was awarded 20 points.

The RTM-96 model was formulated for use as a screening-level model, to estimate an upper-bound value. It is not designed to handle instantaneous or short-term releases. It handles dispersion using a steady-state Gaussian plume approach, with a constant rate of release for all types of releases. The RTM-96 model was awarded 17.5 points.

The DEGADIS, SLAB, and AFTOX models and the Chlorine Institute methodology provide the capabilities for handling all three types of releases. However, they do not provide the capabilities to handle UF_6 reactions and thermodynamics. These models were accordingly awarded 15 points each.

Criterion 2. *Ability to deal with dynamics of a buoyant plume.*

Of particular interest here is the question of whether a model provides the capability to

handle positively, negatively, and neutrally buoyant plumes as dictated by the prevailing thermodynamics, chemical reactions, and atmospheric stability during different stages of the plume development and transport. Transitions from an initial negatively buoyant plume to a positively buoyant plume to a final stage of neutral buoyancy must all be adequately addressed by the model.

Both the HGSYSTEM/UF₆ and SAIC models provide the capabilities to address all three phases of plume development with specific attention to UF₆ and its reaction products, including heat. Both models were awarded the full 25 points each.

The RTM-96 model only can handle a passive plume, and the dynamics of a buoyant plume are completely neglected in its formulation. As a result, the RTM-96 model was awarded 0 points.

The DEGADIS and SLAB models and the Chlorine Institute methodology do not have the capabilities to include UF₆-specific reactions and thermodynamics and are strictly dense gas models. Therefore, they provide limited capabilities to handle all three phases of a plume life. The DEGADIS and SLAB models were awarded 15 points each. The Chlorine Institute methodology was awarded 10 points because it represents only a graphical procedure.

The AFTOX model is a Gaussian puff/plume model with no capabilities to handle UF₆-specific reactions and thermodynamics. Because it is more sophisticated than the RTM-96 model in its treatment of Gaussian plumes, it was awarded 5 points.

Criterion 3. *Representation of the dynamics of a transient release.*

None of the models uses transient meteorological information to completely address the dynamics of a transient release from the point of release. However, a majority of accidents are of short duration, typically less than 15 minutes. Therefore, incorporation of changes in meteorological parameters in this short timeframe is not critical. Another objective of this criterion is to ensure that an instantaneous puff release, a short-term release, and a continuous release are each treated using appropriate dispersion algorithms. The evaluation of this criterion is closely linked to Criterion 1 in this section. Additional evaluation features include the presence of algorithms for air entrainment into the plume, the incorporation of UF₆-specific reactions and thermodynamics, the plume lift-off, and the removal processes.

The HGSYSTEM/UF₆ and SAIC are capable of handling most of the features specific to the release and dispersion of UF₆. However, the SAIC model does not provide an option to model a short-term release lasting for only a few minutes, unlike the HGSYSTEM/UF₆ model. Since short-term release was already covered under Criterion 1, both were awarded the maximum 15 points.

The RTM-96 model does not handle transient dynamics at all. It was awarded 0 points.

The DEGADIS and SLAB models do not contain UF₆-specific transient features dealing with chemistry and thermodynamics, and they do not handle plume lift-off from

the ground. These models were awarded 7.5 points each because they do possess other transient capabilities such as treatment of various types of releases, air entrainment, gravity slumping, etc.

The AFTOX model handles transient releases for a neutrally buoyant plume quite well. However, it cannot handle UF_6 -specific chemistry and thermodynamics, air entrainment, gravity slumping, plume lift-off, etc. It was awarded 5 points.

The Chlorine Institute methodology handles dense gas features in a similar manner to the DEGADIS and SLAB models. However, in addition to the limitations identified in those models, the Chlorine Institute methodology is restricted to a graphical, screening-level approach. It was awarded 2.5 points.

Criterion 4. *Representation of turbulent dispersion.*

The HGSYSTEM/ UF_6 model uses lateral and vertical standard deviations as functions of downwind distance and stability class, based on the numerical formulations of the Pasquill-Gifford standard deviations (Hanna, *et al.*, 1982) by Turner and Busse (1973), and Stern, *et al.* (1984). The model does not provide for any correlations between the lateral standard deviations and the surface roughness. It allows for an increasing vertical standard deviation with increasing surface roughness. In addition, the effects of concentration averaging times are included for both lateral and vertical standard deviations. The HGSYSTEM/ UF_6 model does not account for the effect of urban heating in its treatment of dispersion coefficients. Vertical wind profiles are handled on the basis of curves depicting

Pasquill-Gifford-Turner turbulence types as functions of Monin-Obukhov length and surface roughness length, as presented in Hanna and Chang (1993). For the dense gas portion of the model, entrainment, vertical wind shear, horizontal drag, horizontal and vertical impacts from the plume impinging the ground, buoyancy and gravity slumping, heat exchange with the ground, and heats of reactions are all addressed within the mass, momentum, and energy balance equations for the development and transport of the plume within the atmospheric boundary layer. The HGSYSTEM/ UF_6 model presents an overall robust treatment of atmospheric turbulence. The model was awarded 12 points out of 15.

The SAIC model handles the dispersion for a far-field, neutrally buoyant plume in a manner similar to the HGSYSTEM/ UF_6 model. It also provides the capability to handle the effects of urban heating on dispersion coefficients. Its treatment of the dynamics of dense gas dispersion, however, is not as robust as that of the HGSYSTEM/ UF_6 model. Processes such as plume impingement on the ground, vertical wind shear, and horizontal drag are not addressed in the mass, momentum, and energy balance equations. On the other hand, major processes such as air entrainment and gravity slumping are handled by the model. The model was awarded 10 points.

The RTM-96 model is based on a simple Gaussian plume modeling approach for conservative, screening-level estimates. The model was awarded 5 points for its very limited treatment of turbulent dynamics. The DEGADIS and SLAB models also account for the mass, momentum, and energy balances by including air entrainment,

heat exchange with the ground, and some dynamics of phase change. However, neither model accounts for the UF_6 -specific chemistry and thermodynamics. Transitions from one type of plume to another cannot be easily handled. Treatment of passively buoyant plumes is comparable to that of the HGSYSTEM/ UF_6 and SAIC models. These models were awarded 7.5 points each.

The AFTOX model was formulated to handle contaminant dispersion using the Gaussian plume approach. Air entrainment, heat transfer, chemistry, and thermodynamics are not included as essential components of the model. The model was awarded only 5 points.

The Chlorine Institute methodology provides for the treatment of turbulence within the dense gas and neutrally buoyant plumes and for the treatments of energy and mass balance between chlorine, the ground, and the atmosphere. However, it is a graphical methodology used for screening and cannot handle UF_6 -specific dynamics. The model was accordingly awarded only 5 points.

Criterion 5. *Ability to consider building wake effects.*

The presence of a building in close proximity to or downwind from a release can substantially affect the initial plume dimensions and mixing and, therefore, concentrations at nearby receptors. Typically, large buildings exist at nuclear fuel processing plants, and the effects of their presence on the exposure of the nearby population must be taken into account when modeling the transport of UF_6 and the products of its reactions.

The HGSYSTEM/ UF_6 model accounts for three specific effects because of the presence of buildings: (1) plume confinement by canyons formed between adjacent buildings; (2) increased concentrations on building faces from releases from vents; and increased concentrations on the downwind face of a building (near-wake) because of releases from sources on the buildings. Of all the models being evaluated, the HGSYSTEM/ UF_6 model addresses the presence of buildings most effectively. Therefore, it was awarded the maximum 25 points.

The SAPLUME module in the SAIC model has a building wake model that can be accessed by the use of the "BUOYANCY" card. Other modules of the SAIC model do not address building effects. Therefore, the SAIC model was awarded 10 points.

The DEGADIS, SLAB, and AFTOX models and the Chlorine Institute methodology do not address the effects of the presence of buildings. They were each awarded 0 points.

The RTM-96 model accounts for building wake in the near-source domain, but it does not include other effects, as done by the HGSYSTEM/ UF_6 model. It is also a screening-level approach. Therefore, the model was awarded 10 points.

Criterion 6. *Ability to incorporate terrain effects.*

The primary emphasis here is the ability to account for the presence of major topographic features such as valleys and mountains that directly affect the local wind flow patterns. It should be noted that the

effect of surface roughness length on turbulence has already been addressed in Criterion 4. None of the models being evaluated accounts for the terrain effects. All models were awarded 0 points each out of 10 for this criterion.

Criterion 7. *Incorporation of plume chemistry.*

For modeling the development and dispersion of a plume from a UF_6 -release, six factors must be accounted for in a quantitative manner within the mass, momentum, and energy balance equations: (1) the phase changes of UF_6 ; (2) reactions of UF_6 with atmospheric water vapor; (3) formations of UO_2F_2 and HF ; (4) reactions of HF with water vapor, generation of heat from the hydrolysis of UF_6 ; (5) heat of sublimation of UF_6 ; (6) and entrainment of moisture-laden ambient air. Only two models, HGSYSTEM/ UF_6 and SAIC, directly account for these factors until the plume becomes neutrally buoyant, when it is assumed that all reactions have ceased. Both the HGSYSTEM/ UF_6 and SAIC models were awarded the full 25 points each. The RTM-96 model does not directly incorporate the reactions of UF_6 and HF with water vapor or the phase changes involving UF_6 . However, the model accounts for the proportions of the reactants and products in the final plume mixture at 50 percent relative humidity in the atmosphere; it then calculates concentrations within the plume using a Gaussian approach for passive plume dispersion to produce a conservative, screening-level estimate. The model was awarded 15 points.

None of the other models directly handles UF_6 -specific chemistry or thermodynamics.

The DEGADIS and SLAB models and the Chlorine Institute methodology do have provisions for any accommodation of heat generation and losses from phase changes (though not for UF_6) and for estimation of plume characteristics using mass, momentum, and energy balance equations. The DEGADIS and SLAB models were awarded 5 points each. The Chlorine Institute methodology was awarded only 2.5 points because it is a graphical approach. The AFTOX model had no provisions for handling chemistry or thermodynamics for any species and was awarded 0 points.

Criterion 8. *Representation of statistical fluctuations.*

Both mean and peak concentrations are important in assessing the potential health effects from a release of UF_6 . To evaluate the impacts to a maximally exposed individual, the peak concentration is the useful quantity; to evaluate the impacts to a typically exposed individual, the mean or average concentration is the useful quantity. The UF_6 dispersion models should, therefore, provide as output both the peak and average concentrations. When estimating the concentrations, the models should also incorporate the effects of time-averaging to account for plume meander.

The HGSYSTEM/ UF_6 model reports average (uniform) concentrations within a plume. It provides multiplying factors to account for building wake effects, time averaging, etc. However, this model does not directly provide maximum concentrations within the plume. The model documentation (Hanna, *et al.*, 1994) recommends multiplying the mean concentration by a factor of 1.3 to 1.4 to

determine the peak concentrations. For integrated safety analysis and emergency planning, these outputs may not provide upper-bound estimates unless other conservative assumptions are built in throughout the model to yield an upper-bound estimate of the mean. For a post-accident analysis, the HGSYSTEM/UF₆ model may provide a more reasonable estimate of the true but unknown plume concentration. For these reasons, the HGSYSTEM/UF₆ model was awarded 7.5 points out of 15 points.

The SAIC model reports the cloud centerline concentrations during the negative-buoyancy phase. At a given distance, it reports the mean cloud centerline concentration and the peak centerline concentration during the neutrally buoyant phase of the plume transport. It also provides a time-averaging algorithm to account for plume meander, but it does not provide the average plume concentration at a given distance. For integrated safety analysis and emergency response planning, these outputs are adequate. For a post-accident analysis, the model would probably overpredict the true concentrations. For these reasons, the SAIC model was awarded 12.5 points.

The RTM-96 model provides an upper-bound estimate of the impact without providing significant information on the mean or peak concentrations. It also does not provide an explicit value for the UF₆ concentration at any downwind location. Since it is purely a screening-level model, the RTM-96 model was awarded 2.5 points.

The DEGADIS, SLAB, and AFTOX models and the Chlorine Institute methodology were each awarded 2.5 points, primarily because

they did not provide estimates of predicted concentrations that specifically addressed UF₆-related issues.

Criterion 9. *Separate models for source term representation and atmospheric dispersion.*

The primary purpose of this criterion is to evaluate the modularity of the models. However, the three models that account for UF₆-specific source and dispersion modeling do not allow for a complete treatment of the source term. The question of modularity is still applicable within the dispersion analysis because of the presence of an initial phase in which the plume becomes dense and begins to interact with the ground, a second phase when the plume is dense and ground-based, and a final phase in which it becomes neutrally or positively buoyant. Treatment of each phase in a modular fashion permits a clear assessment of the different phases of the plume during transport and transition from one phase to the next.

The HGSYSTEM/UF₆ model provides an explicit module for each phase of the plume transport. But, the transition is only semi-automatic. Even though the user has to prepare only one input file for the whole analysis starting with the first module (for example, AEROPLUME), the user must modify the input to the next module (for example, PGPLUME) created as an output by the first module. The HGSYSTEM/UF₆ model was awarded 10 points out of 15 for modularity, noting that the modularity could have been combined with an automatic transition from one phase to the next. The SAIC model does not provide an explicit executable module for each phase of

the plume transport. It does provide for automatic transition from one phase to the next and is therefore more user-friendly. The decrease in explicit modularity is compensated for by a less cumbersome simulation. The model was awarded 12 points.

The RTM-96 model is a hand calculation in which each step is explicitly calculated. However, it is a screening-level approach with oversimplification of all dispersion processes. The model was awarded 7.5 points.

The DEGADIS model handles modularity in a similar manner to the SAIC model, but it does not have UF_6 -specific dynamics. Transition from one phase of the plume to another is based solely on the properties of chemicals it can handle. Therefore, the model was awarded 5 points.

Modularity of the SLAB model could not be clearly determined. However, it has the same limitations that DEGADIS has. It was awarded 4 points.

The AFTOX model seems modular, but because its applicability to UF_6 -release and transport is marginal, it was awarded only 2.5 points.

The Chlorine Institute methodology is a graphical technique for which modularity is not a relevant factor. It is also not directly applicable for a UF_6 release. It was awarded 2.5 points.

Criterion 10. *Representation of aerosol dynamics.*

This criterion deals with aerosol formation, transport, and depletion by the processes of deposition. Release of UF_6 into the atmosphere in liquid form results in an immediate flashing of UF_6 into vapor and solid forms. The fractions of solids formed and their subsequent conversions to the gaseous phase are controlled by the prevailing energy balances within the plume. Once the UF_6 reacts with atmospheric moisture, the resulting UO_2F_2 is also in the solid phase. Modeling the depletion of the solid-phase reactants and products from the gravity-slumping, ground-hugging, and passive plumes is important for the accurate prediction of downwind concentrations.

The HGSYSTEM/ UF_6 model provides detailed algorithms to account for the formation and the changing fraction of aerosols in the plume from the initial amount of UF_6 released, the conditions of release, and the prevailing conditions in the atmosphere and using the thermodynamics associated with the phase changes, chemical reactions, and atmospheric mixing. It also includes algorithms for the removal of large (typically UF_6) and small (typically UO_2F_2) aerosols. However, the depletion of aerosols does not affect the predicted downwind concentrations of UF_6 and its products of reaction because the model does not account for depletion in the mass of contaminants in the plume. It should be noted that the critical element of aerosol dynamics for the UF_6 problem is the formation of solid UF_6 with its sublimation and subsequent

reaction, because this affects the heat balance and buoyancy of the plume. The HGSYSTEM/UF₆ model was awarded 4 points out of a maximum of 5.

The SAIC model also provides detailed algorithms to account for the formation and changing fractions of aerosols in the plume. It provides dry deposition algorithms for the removal of gaseous species. However, the removal of aerosols does not seem to be addressed at all. Therefore, the SAIC model was awarded 4 points.

The RTM-96 model accounts for aerosol formation implicitly by assuming that a fraction of the initial release becomes airborne in the plume and the remaining UF₆ is not available for further transport. It does not account for any deposition. Because the RTM-96 model is a screening-level approach, it was awarded 3 points.

The DEGADIS, AFTOX, and SLAB models and the Chlorine Institute methodology do not address the thermodynamics for the formation of solid UF₆ or the reaction of UF₆ with the atmosphere. Consequently, their treatment of aerosol dynamics is not relevant to UF₆ releases. They were each awarded 0 points.

Criterion 11. *Interaction with fog.*

Interaction with fog results primarily in the rapid hydrolysis of UF₆, and removal, by wet deposition, of gases and particles, by the process of in-cloud scavenging. The HGSYSTEM/UF₆ model does account for the interaction with fog by accounting for in-cloud scavenging. It was awarded the full 5 points.

The SAIC, RTM-96, DEGADIS, SLAB, and AFTOX models and the Chlorine Institute methodology do not account for the interaction of UF₆ with fog. They were each awarded 0 points.

It should be noted that UF₆ interacts primarily with the water vapor and not the condensed water droplets in the fogwater. Specification of 100 percent relative humidity would then account conservatively for the interaction of UF₆ with atmospheric moisture in the HGSYSTEM/UF₆, SAIC, and RTM-96 models. Because this interaction has already been addressed in Criterion 7, it is not scored here.

Criterion 12. *Interaction with ground.*

The primary processes of importance in the interaction of a plume with the ground are the exchanges of heat and momentum between the two, gravity-spreading of an entraining plume during the gravity-slumping phase, and spreading of a ground-hugging plume. Other processes, such as wet and dry deposition, are addressed in other criteria for the evaluation of the dispersion component.

The HGSYSTEM/UF₆ model includes algorithms for both momentum and heat exchange between the plume and the ground. For the conservation of momentum, it addresses momentum exchange from plume impingement and drag exerted by the ground on the plume. It also provides algorithms to calculate the horizontal spreads of gravity-slumping and ground-hugging plumes. The heat exchange between the ground and plume is addressed in the governing energy balance equation. However, the functional form of

the heat transfer term is not presented anywhere in the documentation. The model was awarded the full 5 points for providing the above-mentioned capabilities.

The SAIC model addresses the heat exchange and spreading of a slumping plume. It does not directly address momentum exchange between the ground and the plume. Its formulation of algorithms to evaluate the plume dimensions and concentrations within the plume is considerably more simplified than the formulations of the HGSYSTEM/UF₆ model and addresses only processes of primary importance. To compare its capabilities with those of the HGSYSTEM/UF₆ model, detailed validation studies during each phase of the plume development subsequent to a plume release must be conducted. The model was awarded four points because of the reduced level of rigor and detail in its process formulations.

The DEGADIS and SLAB models and the Chlorine Institute methodology do not include UF₆-specific parameters affecting momentum and energy balances to assess the processes of gravity slumping and plume spreading. Therefore, even though mechanisms of heat and energy exchanges with ground may exist within the models, the ability of these secondary influences to yield meaningful results, in the absence of the primary influence of UF₆-specific thermodynamics (on the plume development), is highly questionable. The models were awarded 1 point each.

The RTM-96 and AFTOX models do not address any interactions between the plume and the ground surface. They were each awarded 0 points.

Criterion 13. *Removal (deposition) of UF₆ and reaction products to the ground.*

The primary emphasis of this criterion is to address the removal of UF₆ and its products of reaction from the plume, both for the estimation of the dry- and wet-deposition rates to assess the health impacts on humans from various indirect pathways and to assess the downwind contaminant concentrations by properly accounting for the depletion in the mass-balance equations. For UF₆, the removal processes may be more significant than previously thought; for example, removal of UF₆ from the plume during its initial descent and ground-hugging phases would result in less UF₆ being available for reaction and heat generation. This could affect the overall dynamics of the plume development and history. If the dry- and wet-deposition processes are not considered in the consequence analysis, estimates of both downwind concentrations and deposition rates of the reaction products of UF₆ with moisture at downwind locations could be severely overpredicted. Currently, there are no adequately validated models of dry or wet deposition during the initial stage of the release when UF₆ and its reaction products with moisture behave as a slumping/heavy vapor cloud or plume.

The HGSYSTEM/UF₆ model addresses the dry and wet deposition processes and gravity settling as a post-processing feature. These removal processes do not affect the estimate of mass balance; as a result, both deposition rates and concentrations in air could be overpredicted, and as discussed above, the plume development and history could also be affected. Since the severity of this treatment cannot be determined without model validation using field data, the

HGSYSTEM/UF₆ model was awarded 10 out of a maximum of 15 points for including the algorithms for the removal processes.

The SAIC model addresses only dry deposition process for gaseous species and for very small particles. It does not include gravitational settling of large particles or wet deposition by in-cloud and below-cloud scavenging. It does account for depletion in the mass balance. However, the treatments by both HGSYSTEM/UF₆ and SAIC models could each inaccurately model the plume development and history, and both could overestimate concentrations and deposition rates in the presence of significant removal processes. The SAIC model was awarded 5 points because it did not include algorithms for the estimation of dry- and wet-deposition processes of significance.

Each of the remaining models was awarded 0 points for not including wet- and dry-deposition processes at all.

Criterion 14. *Effects of accident mitigation measures.*

This criterion evaluates whether the activation of a particular mitigative system or control as a response to an accident results in a decrease in the potential health impacts. Since none of the models evaluated explicitly calculates the source term, the effects of mitigative measures on source term cannot be evaluated by these models. However, if the reduced source terms are calculated externally by accounting for each mitigative measure, all models can be used to estimate the resulting receptor-point atmospheric concentrations of UF₆ and its products of reaction with moisture. It should be noted that the statement of

Criterion 14 has been modified from the original statement in Nair, *et al.* (1997) to clearly convey the purpose of this evaluation criterion.

The HGSYSTEM/UF₆, SAIC, and RTM-96 models were each awarded 7.5 points out of 15 because they provide UF₆-specific capabilities. The DEGADIS and SLAB models were each awarded 5 points because they were not specifically designed for UF₆. The Chlorine Institute methodology was awarded 2.5 for being a graphical method, and the AFTOX model was awarded 0 points because of its inability to handle dense gas releases.

Criterion 15. *Possibility of plume separation.*

Gravitational settling or other removal processes may result in the removal of a part of the UF₆ from the original plume. The removed UF₆ can result in the origination of a separate plume. Alternatively, part of the plume containing primarily the lighter products of the reaction can become positively buoyant because of the associated thermal energy and can separate from the original plume. None of the evaluated models has the capability of treating plume separation. Each model was awarded 0 points out of 5.

Criterion 16. *Aerosol formation and the droplet size of reactive airborne aerosol.*

The initial flashing of liquid to vapor and solid phases has been partially addressed in Criterion 10. Criterion 16 focuses on the treatment of droplets of various sizes. Only the HGSYSTEM/UF₆ model recognizes the presence of large-sized aerosols of UF₆,

which undergo gravitational settling, and of smaller UO_2F_2 particles, which undergo dry deposition. However, as discussed earlier, the removal does not affect the mass balance or plume dynamics. The HGSYSTEM/ UF_6 model was awarded 4 points out of 5. All other models were awarded 0 points for not addressing size-specific aerosols.

Criterion 17. *Multiple sources and types of releases.*

For multiple releases occurring simultaneously, it would be advantageous to model all releases within a single simulation. Currently, none of the models being evaluated has this capability. However, each model can be run separately for each release,

and the results can be superimposed to obtain the combined effect of simultaneous releases from multiple sources. Therefore, all models were awarded 5 points out of 10.

2.2.2 Results of the Dispersion Evaluation

Table 2.3 summarizes the scores on dispersion evaluations awarded to all models for all criteria. Table 2.4 presents the evaluation summary for dispersion evaluations. The HGSYSTEM/ UF_6 and SAIC models are scored higher than the other models, primarily because of their UF_6 -specific capabilities. The RTM-96 model also scores marginally higher as a screening model for the same reason.

Table 2.1 Scores awarded to the models for the source term evaluation

Criteria	Maximum score	HGSYSTEM/ UF ₆	SAIC	RTM-96	DEGADIS	SLAB	AFTOX	CIM*
(1) How many accident categories can the model's source term algorithm handle?	10	8.5	8	8	8	7	7	5
(2) Does the source term module handle puff as well as continuous releases?	15	15	15	10	15	15	15	15
(3) Do the release or source term cases listed in the model reflect past accidents and/or possible future accidents that may occur?	15	15	15	10	10	10	10	10
(4) Does the source term algorithm contain mechanisms to translate an internal release to an external release?	15	5	5	5	5	5	5	5
(5) Does the source term algorithm contain mechanisms to analyze failure modes, and does it quantify the release amount within an appropriate phase?	30	25	25	25	20	20	20	20
(6) Does the source term contain UF ₆ reaction relationships with air, and does it quantify final products (HF, UO ₂ F ₂ , heat, etc.)?	25	25	20	15	10	10	10	10
Total score	110	93.5	88	73	68	67	67	65

* Chlorine Institute methodology.

Table 2.2 Summary of model scores for source term evaluation

Model name	Total score	Rank
HGSYSTEM/UF ₆	93.5	1
SAIC	88	2
RTM-96	73	3
DEGADIS	68	4
SLAB	67	5
AFTOX	67	5
Chlorine Institute methodology	65	7

Table 2.3 Scores awarded to models for atmospheric dispersion evaluation

Criteria*		Maximum score	HGSYSTEM/ UF ₆	SAIC	RTM-96	DEGADIS	SLAB	AFTOX	CIM**
(1)	Ability to deal with transient releases	25	25	20	17.5	15	15	15	15
(2)	Ability to deal with dynamics of a buoyant plume	25	25	25	0	15	15	5	10
(3)	Representation of the dynamics of a transient release	15	15	15	0	7.5	7.5	5	2.5
(4)	Representation of turbulent dispersion	15	12	10	5	7.5	7.5	5	5
(5)	Ability to consider building wake effects	25	25	10	10	0	0	0	0
(6)	Ability to incorporate terrain effects	10	0	0	0	0	0	0	0
(7)	Incorporation of plume chemistry	25	25	25	15	5	5	0	2.5
(8)	Representation of statistical fluctuations	15	7.5	12.5	2.5	2.5	2.5	2.5	2.5
(9)	Separate models for source term representation and atmospheric dispersion	15	10	12	7.5	5	4	2.5	2.5
(10)	Representation of aerosol dynamics	5	4	3	3	0	0	0	0
(11)	Interaction with fog	5	5	0	0	0	0	0	0
(12)	Interaction with ground	5	5	4	0	1	1	0	1
(13)	Removal (deposition) of UF ₆ and reaction products to the ground	15	10	5	0	0	0	0	0
(14)	Effects of accident mitigation measures	15	7.5	7.5	7.5	5	5	0	2.5
(15)	Possibility of plume separation	5	0	0	0	0	0	0	0
(16)	Aerosol formation and droplet size of reactive airborne aerosol	5	4	0	0	0	0	0	0
(17)	Multiple sources and types of releases	10	5	5	5	5	5	5	5
Total score		235	185	155	73	68.5	67.5	40	48.5

* Complete descriptions of the criteria are found in Section 3.2 of Nair, *et al.* (1997).

** Chlorine Institute methodology.

Table 2.4 Summary of model scores for dispersion evaluation

Model name	Total score	Rank
HGSYSTEM/UF ₆	185	1
SAIC	145	2
RTM-96	73	3
DEGADIS	68.5	4
SLAB	67.5	5
Chlorine Institute methodology	48.5	6
AFTOX	40	7

3 MODEL TESTING

To assess the performance of the selected models for real-life accidents involving releases of UF_6 into the atmosphere, it is essential to have UF_6 -specific data from previous accidents or from experiments carried out with the sole purpose of generating data for model testing. These data must include information such as release rate, temperature within the cylinder at the time of rupture, atmospheric stability, wind speed and direction, and time of day. Three UF_6 -specific data sets were identified that could be used for the model testing exercise in this study. The first data set, reported in Hanna, *et al.* (1994a), is from French experiments conducted in Bordeaux between 1986 and 1988. The second data set, reported in NRC (1986a; 1986b; 1986c), deals with the rupture of a 48Y cylinder filled with UF_6 in Gore, Oklahoma. The third data set, reported in Ducouret (1978), represents an accidental release of UF_6 from a 48Y cylinder at the Comurhex Plant in Pierrelotte, France.

In the absence of a larger number of data sets involving releases of UF_6 , it was decided to use four data sets of dense gas releases that have been used extensively in previous model-testing exercises (Touma, *et al.*, 1995; Hanna, *et al.*, 1993; Sykes and Lewellen, 1992). These data sets include the following: the "Goldfish" series of large-scale releases of anhydrous HF at the Department of Energy's Liquefied Gaseous Fuels Test Facility in Nevada; the "Desert Tortoise" series of large-scale releases of anhydrous ammonia (NH_3) at the Nevada Test Site; the continuous releases of heavy vapors of Freon-12 and nitrogen (N_2) at Thorney Island; and the instantaneous

releases of heavy vapors of Freon-12 and N_2 at Thorney Island. Summaries of these releases are provided in the documentation for the HGSYSTEM/ UF_6 (Hanna, *et al.*, 1994a) and SAIC (Kaiser, 1993) models. More specific information was obtained from the Modeler's Data Archive (MDA; Hanna, *et al.*, 1991); the data are also available from Dr. S. R. Hanna of the Earth Technology Corporation in Concord, Massachusetts, in electronic format.

In consultation with NRC and in light of the findings from other sections of this study that only the HGSYSTEM/ UF_6 , SAIC, and RTM-96 models were designed to handle UF_6 , it was decided to use only these three models for detailed testing. Model tests conducted with data on dense gases other than UF_6 are discussed first, followed by the discussions of tests conducted with UF_6 -specific data. Discussions of the sensitivity analysis conducted as part of this study are presented in Section 3.3.

3.1 Model Testing with Dense Gas Data

As presented in the previous section, four data sets representing releases of dense gases from Goldfish, Desert Tortoise, and Thorney Island were used to compare model predictions with observations. Simulations using the HGSYSTEM/ UF_6 model are discussed first, followed by those using the SAIC model. No simulations with dense gas data were conducted using the RTM-96 model because it was developed specifically, and only for, the release of UF_6 .

3.1.1 Simulations with the HGSYSTEM/UF₆ Model

Four separate tests were conducted using the HGSYSTEM/UF₆ model. Brief details of the tests and the specific modules from the HGSYSTEM/UF₆ model that were used are presented in Table 3.1.

The HGSYSTEM/UF₆ model reports average quantities over the plume cross-section. The predicted average concentrations were multiplied by a factor of 1.35 to obtain peak concentrations as recommended by Hanna, *et al.* (1994). Whenever the averaging times for the reported (observed) peak and average concentrations varied, the model was run twice. The first run used a shorter averaging time to obtain predicted average concentrations from which the peak concentrations could be estimated for comparison with the measured peak concentrations, and the second run used a longer averaging time to directly obtain the predicted average or mean concentrations for making comparisons with the measured average or mean concentrations.

(1) Goldfish

The Goldfish trials were conducted at the Frenchman Flat area of the Nevada Test Site. Pressurized HF was released from a spill pipe pointing downwind at a height of 1 m above the ground. Although six trials were conducted, only the first three are included in the MDA (Hanna, *et al.*, 1991) because the last three trials involved the study of water sprays.

Details of the Goldfish releases of HF are reported elsewhere (Hanna, *et al.*, 1994a;

Kaiser, 1993) and are not repeated here. The assumptions used to model the release of HF were as follows:

- Release consisted of 100 percent HF (*i.e.*, no air or water was mixed with the HF);
- A portion of liquid HF flashed on release and formed a turbulent jet;
- Unflashed liquid broke up into aerosol and remained in the jet cloud; and
- No liquid pooling occurred.

For simulations using the HGSYSTEM/UF₆ model, the releases were assumed to be continuous, at steady-state, and pressurized. Table 3.2 briefly presents the details of the runs conducted with the three Goldfish data sets. For Trial GF1, about 3460 kg of HF were released as a horizontal jet over a duration of 125 seconds (s) with an exit pressure of 6.8 atmospheres (atm), and a mass release rate of 27.7 kg s⁻¹. Average wind speed was 5.6 m s⁻¹ (measured at an elevation of 2 m), and atmospheric stability was neutral. For Trial GF2, about 3770 kg of HF were released as a horizontal jet over a duration of 360 s, with an exit pressure of 7.35 atm and a mass release rate of 10.5 kg s⁻¹. Average wind speed was 4.2 m s⁻¹ (measured at an elevation of 2 m), and atmospheric stability was neutral. For Trial GF3, about 3700 kg of HF were released as a horizontal jet over a duration of 360 s, with an exit pressure of 7.48 atm and a mass release rate of 10.3 kg s⁻¹. Average wind speed was 5.4 m s⁻¹ (measured at an elevation of 2 m), and atmospheric stability was neutral. Further details of the meteorology and source term at the time of the release are not presented here, and the reader is referred to Hanna, *et al.* (1994a);

Kaiser (1993); and the MDA (Hanna, *et al.*, 1991). For each of the three simulations, averaging times of 88.3 s and 66.6 s were used to obtain predictions for the average and peak concentrations, respectively. The data on averaging times were obtained from the MDA (Hanna, *et al.*, 1991).

(2) Desert Tortoise

Four trials with liquid NH_3 were conducted at the Nevada Test Site using the same release mechanism as used in the Goldfish experiments. Again, details of the Desert Tortoise releases of anhydrous NH_3 are provided elsewhere (Hanna, *et al.*, 1994a; Kaiser, 1993) and are not repeated here. The assumptions used to model the releases of NH_3 were as follows:

- Pressurized liquid NH_3 was released from a spill pipe 1 m above the ground;
- 18 percent of the liquid jet flashed into vapor phase;
- 82 percent of the liquid jet broke up into aerosols; and
- No pool of liquid was formed on the ground.

For simulations using the HGSYSTEM/UF₆ model, the releases were assumed to be continuous, at steady-state, and pressurized. For Trial DT1, the NH_3 was released as a horizontal jet over a duration of 126 s, with an exit pressure of 10 atm, and a mass release rate of 79.7 kg s⁻¹. Average wind speed was 7.4 m s⁻¹ (measured at an elevation of 2 m), and atmospheric stability was neutral. For Trial DT2, the NH_3 was released as a horizontal jet over a duration of 255 s, with an exit pressure of 11 atm and a mass release rate of about 112 kg s⁻¹.

Average wind speed was 5.8 m s⁻¹ (measured at an elevation of 2 m), and atmospheric stability was neutral. For Trial DT3, the NH_3 was released as a horizontal jet over a duration of 166 s, with an exit pressure of 11.2 atm, and a mass release rate of about 131 kg s⁻¹. Average wind speed was 7.4 m s⁻¹ (measured at an elevation of 2 m), and atmospheric stability was neutral. For Trial DT4, NH_3 was released as a horizontal jet over a duration of 381 s, with an exit pressure of 11.6 atm, and a mass release rate of 96.7 kg s⁻¹. Average wind speed was 4.5 m s⁻¹ (measured at an elevation of 2 m) in a stable (stability class E) atmosphere. Table 3.3 briefly presents the details of the simulations conducted using the four Desert Tortoise data sets.

(3) Thorney Island Continuous Releases

Three trials involving continuous releases were conducted in which approximately 2000 m³ of a mixture of Freon-12 and N_2 were released at a rate of 5 m³ s⁻¹ over a flat terrain. Data from only two of the trials were included in the MDA (Hanna, *et al.*, 1991) because of wind shifts during one of the trials (#46).

Detailed descriptions of the Thorney Island continuous releases are provided elsewhere (Hanna, *et al.*, 1994a; Kaiser, 1993) and are not repeated here. The assumptions used to model the releases of Freon-12 and N_2 were as follows:

- ground-level release;
- zero vertical momentum; and
- mole fractions of Freon-12 and N_2 of 0.32 and 0.68, respectively.

For simulations using the HGSYSTEM/UF₆ model, the releases were assumed to be continuous, at steady-state, and unpressurized. The HEGADAS module requires the input of pool length and half-width. Initial pool dimensions were 2.51 m × 1.25 m. The model runs did not indicate any sensitivity to the initial pool dimensions. For Trial TC45, about 4860 kg of Freon-12/N₂ mixture were released as an area source over a duration of 455 s at a release rate of 10.7 kg s⁻¹. Average wind speed was 2.3 m s⁻¹ (measured at an elevation of 10 m), and the atmosphere was stable (stability class E). For Trial TC47, about 4750 kg of Freon-12/N₂ mixture were released as an area source over a duration of 465 s at a release rate of 10.2 kg s⁻¹. Average wind speed was 1.5 m s⁻¹ (measured at an elevation of 10 m), and the atmosphere was stable (stability class F). Table 3.4 briefly presents the details of the runs conducted using the two data sets.

(4) Thorney Island Instantaneous Releases

Sixteen trials involving instantaneous releases were conducted in which approximately 2000 m³ of a mixture of Freon-12 and N₂ were released over a flat terrain. Nine of the 16 trials were included for evaluation in the MDA (Hanna, *et al.*, 1991). Detailed descriptions of the Thorney Island instantaneous releases are provided elsewhere (Hanna, *et al.*, 1994a; Kaiser, 1993) and are not repeated here. The assumptions used to model the releases of Freon-12 and N₂ are as follows:

- Mole fractions of Freon-12 and N₂ were altered to match the mixture composition for each trial;

- Initial pool-radius was 7 m; and
- No ambient air was entrained into the initial cloud.

Table 3.5 briefly presents the details of the model simulations.

3.1.2 HGSYSTEM/UF₆ Model Validation

Predictions from the HGSYSTEM/UF₆ model for the continuous releases from the three experiments (Goldfish, Desert Tortoise, and Thorney Island) are presented in Table 3.6 along with the measurements provided in the MDA (Hanna, *et al.*, 1991). Both mean and peak concentrations are presented in the table for the measured and predicted values. The ratios of predicted to observed concentrations (P/O ratios) are also presented. Results of the simulations for the Thorney Island instantaneous releases are presented in Table 3.7. Results of the continuous release simulations for Goldfish and Trial TC2 of Thorney Island indicate a tendency by the model to underpredict the mean and peak observed concentrations (P/O < 1). Results of the continuous release simulations for Desert Tortoise and Thorney Island for Trial TC1 indicate a tendency by the model to overpredict the mean and peak observed concentrations (P/O > 1). The P/O ratios for the Thorney Island instantaneous releases were not calculated. However, for these experiments, as shown in the following discussion, the tendency of the model to overpredict or underpredict can be demonstrated through other statistical tools.

In Figure 3.1, the predicted and observed mean concentrations are plotted against each other as a scatter diagram, using all of the available data from the Goldfish

experiments; the scatter diagram for the peak concentrations from the Goldfish experiments is presented in Figure 3.2. Figures 3.3 and 3.4 represent the scatter diagrams for the Desert Tortoise simulations for the mean and peak concentrations, respectively; Figures 3.5 and 3.6 represent the same set of scatter diagrams for the Thorney Island continuous releases; and finally, Figure 3.7 represents the scatter diagram for the Thorney Island instantaneous releases. Goldfish results show good agreement between predictions and observations though the tendency for underprediction by the HGSYSTEM/UF₆ model is evident. Desert Tortoise results indicate a model tendency to overpredict. Thorney Island results for the continuous releases indicate a reasonable match between predictions and observations (results from Trials TC1 and TC2 are combined in Figures 3.5 and 3.6). These generalized observations are valid for the comparisons of predicted and observed concentrations representing both mean and peak values. Thorney Island results for the instantaneous releases indicate that the HGSYSTEM/UF₆ model has a tendency to overpredict.

Using EPA's "Protocol for Determining the Best Performing Model" (USEPA, 1992b), a statistical analysis was conducted on the data from model predictions and observations to assess model performance. Table 3.8 presents the results of the analysis. Fractional bias is defined in this study as:

$$FB = 2 \left[\frac{P - O}{P + O} \right],$$

where P represents the predicted mean value of a statistic, O represents the observed

mean value of the same statistic, and FB represents the fractional bias of the same statistic.

Fractional bias has been selected as the basic measure of performance in this evaluation because it has two attractive features. First, the fractional bias is symmetric and bounded. Second, the FB is a dimensionless number, which is convenient for comparing the results from studies involving different concentration levels or even different pollutants. In the top half of Table 3.8, estimates of model bias are calculated and presented using all pairs of observed and predicted concentrations from each set of experiments. For example, all pairs of observed and predicted mean or average concentrations from all of the three experiments at Desert Tortoise are used to prepare the information under column DTA. The fractional bias of the mean or average of the concentrations shown in Table 3.8 is a good indicator of the tendency to underpredict (FB<0); overpredict (FB>0); or match closely (FB~0). As seen through P/O ratios and scatter diagrams, examinations of the fractional bias of the average of the concentrations show that the model predictions exhibit the following: (1) for Goldfish, a tendency to underpredict the mean concentration; (2) for Desert Tortoise, a tendency to overpredict; (3) for continuous releases from Thorney Island, tendencies to both under- and overpredict; and (4) for instantaneous releases from Thorney Island, a tendency to overpredict. These values also indicate that the predictions of peak concentrations for Goldfish experiments and mean concentrations for continuous release experiments at Thorney Island are relatively unbiased.

Figure 3.8 is a graphical illustration of model performance in which the fractional bias of the standard deviation (y axis) is plotted against the FB of the average (x axis) using predicted and measured values from all experiments. Models that plot close to the center of the graph (0,0) are relatively free from bias, whereas models that plot further away from the center tend to over- or underpredict. Values of the FB that are equal to -0.67 are equivalent to an underprediction by a factor of 2, whereas values that are equal to +0.67 are equivalent to an overprediction by a factor of 2. Extreme underpredictions are indicated by values of the fractional bias below -2.0 and extreme overpredictions are indicated by values of the fractional bias above +2.0. Figure 3.8 clearly shows that the FBs for the average and standard deviations from the HGSYSTEM/UF₆ model are contained within the ± 0.67 range, indicating that both overpredictions and underpredictions are within a factor of 2.

The geometric mean and standard deviations of the P/O ratios for all pairs of observations and predictions are also presented in Table 3.8 for each set of experiments. A geometric mean of 1.0 shows perfect agreement between predictions and observations; a value greater than 1.0 indicates a tendency to overpredict and a value less than 1.0 indicates a tendency to underpredict. The biases from the geometric mean of the P/O show similar characteristics as seen earlier from the fractional biases of the average.

Table 3.8 also presents a number of other indicators of the goodness of fit between the predictions and measurements. The first indicator describes the percentage of total predictions that were within a factor of 2 of

the observations. Of the total number of points for which both predictions and measurements were available from each site, 87.5 percent of the predicted peak concentrations from Goldfish and the predicted mean concentrations from Desert Tortoise were within a factor of 2 of the observations. When this information is combined with the information from the fractional bias analysis, it is clear that the predictions of peak concentrations at Goldfish were in better agreement with the observations than were the predictions of average concentrations at Desert Tortoise (fractional bias in the standard deviation for Desert Tortoise means concentration is higher than that for Goldfish peak concentrations). This is clearly borne out by the information on the next indicator -- the slope of the best-fit straight line passing through the origin when predicted concentrations are plotted against the observed concentrations -- that the slope for the predicted peak concentrations at Goldfish is 1.01 (Table 3.8).

3.1.3 Simulations with the SAIC Model

Four tests were conducted using the SAIC model, corresponding to the four tests conducted using the HGSYSTEM/UF₆ model as described in Section 3.1.1. The SACRUNCH module was used to simulate continuous releases, and the SADENZ module was used to simulate the instantaneous releases. It should be noted that the averaging time, applicable to the buoyant phase of the plume, is entered in the input-stream of the SAIC modules SACRUNCH and SAPLUME through the release duration parameter. This is discussed further in Section 3.2.1. Averaging times in the simulations conducted with the

SAIC model are consistent with those in the simulations conducted with the HGSYSTEM/UF₆ model, as presented in Section 3.1.1.

(1) Goldfish

Table 3.9 briefly presents the details of the runs conducted using the three Goldfish data sets reported in Hanna, *et al.* (1994a) and Kaiser (1993). Specific details about the field experiments have been presented in Section 3.1.1.

(2) Desert Tortoise

Table 3.10 briefly presents the details of the runs conducted using the four Desert Tortoise data sets for the Desert Tortoise experiments reported in Kaiser (1993). Specific details about the field experiments have been presented in Section 3.1.1.

(3) Thorney Island Continuous Releases

Table 3.11 briefly presents the details of the runs conducted using the two Thorney Island data sets reported in Kaiser (1993). Specific details about the field experiments have been presented in Section 3.1.1.

(4) Thorney Island Instantaneous Releases

Table 3.12 presents briefly the details of the Thorney Island simulations. Specific details about the field experiments have been presented in Section 3.1.1.

3.1.4 SAIC Model Validation

Results of the simulations with the SAIC model for the continuous releases are presented in Table 3.13. As in Section 3.1.2,

both mean and peak concentrations representing measurements and predictions are presented along with the P/O ratios. The mean concentrations for all experiments are consistently underpredicted by the SAIC model, as are peak concentrations from Thorney Island Trial TC1 and Goldfish Trials GF2 and GF3. On the other hand, the peak concentrations for Desert Tortoise, Goldfish Trial GF1, and Thorney Island Trial TC2 are overpredicted by the model. The maximum overprediction is represented by a factor of 2.7, and the maximum underprediction is represented by a factor of 10. In comparison with the P/O ratios of the HGSYSTEM/UF₆ model, the SAIC model shows an increased tendency to underpredict. Table 3.14 presents the results from the instantaneous simulations with the SAIC model conducted for Thorney Island. The P/O ratios for the instantaneous releases are not presented in the table as the same information can be obtained from the scatter diagrams discussed below.

Table 3.15 summarizes the statistics for the SAIC model using the Environmental Protection Agency's (EPA) "Protocol for Determining the Best Performing Model" (USEPA, 1992b). The fractional biases of the average for the mean and peak concentrations and the geometric means of the P/O ratios for all experiments (except peak Desert Tortoise and Thorney Island instantaneous concentrations) clearly show the tendency of the model to underpredict (FB<0).

Scatter diagrams for the SAIC simulations are presented in Figures 3.9 through 3.15. These diagrams verify the observations made before on the general tendency of the SAIC model to underpredict. Figure 3.16 presents

the fractional bias plot for the SAIC runs. When compared with the performance of the HGSYSTEM/UF₆ model, it is clearly seen that the bias toward underprediction is more significant in the SAIC model. However, the fractional biases do not cross the extreme values of ± 2.0 for any of the data sets and are within the ± 0.67 values for four of the seven data sets that were tested.

The percentages of paired data for which the predictions fall within a factor of 2 of the observations are generally lower than the percentages from the HGSYSTEM/UF₆ simulations (Tables 3.15 and 3.8). The slope of the best-fit line in Table 3.15 is seen to be generally less than 1 (except for peak concentrations for Desert Tortoise release and for Thorney Island instantaneous release), indicating underprediction. In summary, the above indicators imply that the predictions from the simulations of the HGSYSTEM/UF₆ model provide better agreement of predicted concentrations with the observed concentrations for the dense gases studied (fractional bias of the average within ± 0.67) than those from the simulations of the SAIC model.

3.2 Model Testing Using UF₆ Data

Data from experimental or accidental releases of UF₆ into the atmosphere are useful in understanding the behavior of UF₆ in the atmosphere and for testing dispersion models. Three data sets were considered in this study:

- (1) Data from a set of French experiments conducted between 1986 and 1989 at Bordeaux, as reported by Hanna, *et al.* (1994a).

- (2) Data from an accidental release at Comurhex plant in Pierrelotte, France, in 1977, as described by Ducouret (1978) and Doumenc, *et al.* (1978).
- (3) Data from the 4 January 1986 rupture of a UF₆ cylinder at the Sequoyah Fuel Facility in Gore, Oklahoma, as reported in NRC (1986a; 1986b; 1986c) and Kaiser (1993).

Two other accidents involving releases of large quantities of UF₆ were identified as potential sources of release and measurement data suitable for model testing. The first accident occurred in 1960 at Paducah, KY. It involved a release of about 2950 kg (6500 lbs) of UF₆ into the atmosphere from a heated steam chest.* The second accident occurred at the Portsmouth Gaseous Diffusion Plant in Portsmouth, OH, in 1978. About 9500 kg of UF₆ were released from a dropped metric (14-ton) UF₆ cylinder.

Direct measurements of the atmospheric concentrations of UF₆ or its reaction products were not made at the Paducah and Portsmouth facilities during or immediately after the accident.* Therefore, no air monitoring information at these facilities exists that can be used for model testing purposes. Furthermore, it was raining and snowing at 0°C during the accident at Portsmouth.* It is also not clear that the HGSYSTEM/UF₆ and SAIC models can address the thermodynamics and chemistry of UF₆ in the presence of both snow and rain.

Post-accident measurements of UF₆ and its reaction products were made in other media at Paducah, and Portsmouth facilities (e.g., in

* Lombardi, D., Lockheed Martin Energy Research Corporation, Oak Ridge, Tennessee, Personal Communications, S.K. Nair, SENES, September 26 and 30, 1996.

surface soils).^{*} However, reconstruction of atmospheric concentrations of UF₆, UO₂F₂, and HF from the time-integrated soil concentrations would involve multimedia fate and transport modeling, which is far beyond the scope of this study. Such fate and transport modeling would also introduce uncertainties in the calculated air concentrations, and the resulting information could become less useful for model testing. For all of these reasons, it is not feasible to perform the UF₆ release and dispersion calculations for these releases for the purposes of model testing.

Table 3.16 presents the modules from the HGSYSTEM/UF₆ and SAIC models that were used for the simulations conducted for UF₆ releases.

3.2.1 Model Outputs

Each model prints a different set of output concentrations in its output file for the UF₆-dispersion analysis. The HGSYSTEM/UF₆ modules for steady-state simulations print the concentrations of UF₆, UO₂F₂, HF, and total uranium in air at all downwind locations for which outputs are printed. The HGSYSTEM/UF₆ module for transient simulations, HEGADAS-T, provides the concentrations of UF₆, UO₂F₂, and HF in air at all downwind locations for which it provides outputs. Using the output concentrations of UF₆ and UO₂F₂, the total uranium concentrations can be easily estimated for a transient simulation.

The SAIC module SACRUNCH prints the mean and peak concentrations of UF₆ in air; the SADENZ module prints the mean concentrations of UF₆ in air; and the

SAPLUME module prints the mean concentrations of UF₆ at plume centerline elevation and at ground level. However, the output concentration of UF₆ represents the entire UF₆ inventory that was released from the source as if the UF₆ did not undergo any chemical reactions with the atmospheric moisture. In other words, the chemistry and thermodynamics of UF₆ reactions with atmospheric moisture are used by the SAIC model only to calculate the plume dispersion characteristics and concentrations of all species (UF₆, UO₂F₂, HF) in the plume at every point during the plume development, but the concentrations of the individual species are not printed out. Instead, the concentrations of UF₆, as if they do not undergo any reaction, are printed out. UF₆ undergoes the following chemical reaction with atmospheric moisture:

This reaction implies that for every mole of UF₆ (or uranium) that reacts, one mole of UO₂F₂ (or uranium) is formed so that the total number of moles of uranium remains conserved within the plume at any time after release. It should be noted that processes of deposition can result in removal of UO₂F₂ from the plume, which can reduce the total number of moles of uranium from the plume. However, the SAIC model does not account for depletion from deposition processes in its mass balance. Therefore, the total number of moles of uranium remain conserved within the plume in the SAIC model.

The UF₆ concentrations printed out by the SAIC model can, therefore, be used to estimate the total uranium concentration at any downwind distance by multiplying the printed UF₆ concentrations by the ratio of the molecular weight (MW) of uranium (238 g/g-mole) to the MW of UF₆ (352 g/g-mole).

^{*} Lombardi, D., Lockheed Martin Energy Research Corporation, Personal Communications, S.K. Nair, SENES, September 26 and 30, 1996.

However, the actual concentrations of UF_6 , UO_2F_2 , and HF cannot necessarily be calculated from the total uranium concentrations. A special case occurs when the reaction is complete or all of the UF_6 has been converted to UO_2F_2 and HF. For this special case, since one mole of UF_6 represents one mole of UO_2F_2 and four moles of HF, the UO_2F_2 concentration can be estimated by multiplying the output concentration of UF_6 by 0.875 ($= \text{MW of } \text{UO}_2\text{F}_2 / \text{MW of } \text{UF}_6$), and the HF concentration can be estimated by multiplying the output concentration of UF_6 by 0.2273 ($= 4 \times \text{MW of HF} / \text{MW of } \text{UF}_6$). For this special case, the UF_6 concentration in the air would be zero. This interpretation of the SAIC model output was discussed and confirmed with the model developer.*

The RTM-96 model estimates the total uranium intake by the inhalation pathway for a given release. It does not explicitly calculate the concentration of total uranium in the air. However, using the breathing rate, the total uranium concentration can be back-calculated for the RTM-96 model. The model also provides estimates of HF concentrations in the air. However, it is not appropriate to estimate the UF_6 and UO_2F_2 concentrations from the total uranium and HF concentrations because estimations of total uranium and HF concentrations in the RTM-96 model are not based on mass balance considerations.

In the documentation for the SACRUNCH module (Kaiser, 1993), it is stated that the plume passage time at a given point is used to predict the time-averaged concentration that is reported in the output. However, the SACRUNCH module is designed to model

continuous, steady-state releases. Estimation of the plume passage time (t_d) is not presented in the documentation. In the input stream, the release duration is assigned the same notation (t_d) that the plume passage time is assigned. Simulations conducted in this study indicated that the release duration is used by the SACRUNCH module to estimate the time-averaged concentration at a downwind concentration when the plume is in the buoyant phase; (*i.e.*, the release duration in the input stream is meant to represent the averaging time for the buoyant phase of the plume). This was confirmed with the developer of the SAIC model.* Therefore, all predictions with SACRUNCH and SAPLUME modules presented in this study correctly account for the averaging time, including the predictions for simulations conducted with heavy gases presented in Section 3.1.3.

3.2.2 Bordeaux Releases

A series of controlled UF_6 release tests were conducted at a French government test site near Bordeaux, France, between 1986 and 1989. UF_6 vapor was released from a 0.05 m-diameter pipe at a height of 3.15 m above ground over different time intervals. The first test lasted for 10 minutes and resulted in a release of 45.8 kg of UF_6 . The second test lasted for 30 minutes with 146.2 kg of UF_6 being released. The third test lasted for 15 minutes and 73.1 kg of UF_6 were released. Further details on release conditions and meteorology are presented in Hanna, *et al.* (1994a).

Table 3.17 presents the details of the simulations performed using the AEROPLUME and PGPLUME modules from the HGSYSTEM/ UF_6 model. For each

* Kaiser, G.D., Science Applications International Corporation (SAIC), Personal Communications, S.K. Nair, SENES, October 1 and 7, 1996.

* Kaiser, G.D., SAIC, Personal Communications, S.K. Nair, SENES, October 1 and 7, 1996.

simulation, the AEROPLUME module was used for estimating the near-field concentration (<10 m) when the plume is still heavier than air, followed by the PGPLUME module for far-field dispersion when the plume has become positively or neutrally buoyant (≥ 10 m). A sample averaging time of 3 minutes was indicated in the detailed description of the experimental releases provided by Bloom and Just (1993). Accordingly, an averaging time of 3 minutes was used to compare the model predictions with the observations.

Table 3.18 presents the details of the simulations performed using the SACRUNCH and SAPLUME modules from the SAIC model. Within the SACRUNCH module, the release is modeled as a ground-level source, and in SAPLUME modules it is modeled as an elevated source. Hand calculations were also performed for the three releases using the RTM-96 model. Simulations of the three French releases were also conducted by Hanna, *et al.* (1994a) using the HGSYSTEM/UF₆ model.

Results of the simulations using the HGSYSTEM/UF₆ model are presented in Tables 3.19 through 3.21, and those for the simulations using the SAIC model are presented in Table 3.22. In Table 3.19, the concentrations predicted by using two different averaging times (3 minutes and 10 minutes) are presented. As expected, the concentrations predicted by the simulation using the 10-minute averaging time are lower than those predicted by the simulation using the 3-minute averaging time. The P/O ratios are presented for the HGSYSTEM/UF₆ model in Tables 3.19 through 3.21 for the simulations of the three French releases conducted using the 3-minute averaging time. The P/O ratios from the HGSYSTEM/UF₆ model are consistently above 1. The

maximum value of P/O ratio was seen to be 6.8 for the release of 1986.

The scatter diagram from the simulations of the HGSYSTEM/UF₆ model, shown in Figure 3.17, also shows the tendency of the model to overpredict. The scatter diagram for the simulations conducted by Hanna, *et al.* (1994a) with the HGSYSTEM/UF₆ model are presented in Figure 3.18. At distances close to the source (≤ 30 m), results from Hanna, *et al.* (1994a) severely underpredict the observations (by as much as 5 orders of magnitude). At these distances, the predictions (at 1-m height) in this study were obtained from linear interpolation of model outputs at heights above and below the 1-m height. The linear interpolation is justified because of the close proximity to the source where the plume would still be well-mixed and not yet be Gaussian in the internal distribution of contaminants. Therefore, the different methods of interpolation used by the two modelers could partly account for the differences in the predicted values at distances close to the source.

Table 3.22 presents the results from the SAIC modules for all three experiments using both SACRUNCH and SAPLUME modules. Ignoring the results at 10 m, where the influence of the proximity to the source results in severe overpredictions, the SACRUNCH module shows a tendency to underpredict the observations from the third release and a tendency to overpredict the observations from the first release, and a mixed tendency for the second release (Figure 3.19).

Because the UF₆ was released at an elevation of 3.15 m, it was also decided to use the SAPLUME module within the SAIC model to simulate elevated releases, as stated

earlier. Comparisons of P/O ratios between the predictions of SACRUNCH and SAPLUME modules presented in Table 3.22 indicate that the SAPLUME module shows a consistent tendency to overpredict for all releases. It also shows a considerable improvement in predictions at 10 m.

Results from the RTM-96 model for the three French releases are presented in Table 3.23. Table 3.23 shows that the RTM-96 model provides conservative estimates of total uranium concentrations beyond 200 m (for the one data point) from the source. However, it severely underpredicts at closer distances. The predictions improve with distances up to 200 m, when the model begins to overpredict.

Statistical comparisons of predictions and observations for the Bordeaux releases are presented in Table 3.24 for the HGSYSTEM/UF₆ model simulations carried out in this study and by Hanna, *et al.* (1994a), for the SACRUNCH and SAPLUME modules of the SAIC model, and for the RTM-96 model simulations. Section 3.1.2 presents the details of the statistical tests. As seen in the P/O ratios from the HGSYSTEM/UF₆ simulations conducted in this study (Tables 3.19 to 3.21), the fractional bias of the average and the geometric mean of the P/O ratio also shows a tendency to overpredict (P/O > 0). Statistics from the results of the HGSYSTEM/UF₆ simulations conducted by Hanna, *et al.* (1994a) and the RTM-96 simulations indicate significant biases toward underprediction, primarily because of the severe underpredictions at shorter distances (associated with greater concentrations; see Figure 3.18 and Table 3.23).

Results of the fractional bias of the average from both SACRUNCH and SAPLUME modules show biases toward overprediction.

The geometric mean of the P/O ratio for the SACRUNCH module does not indicate the same tendency to overpredict. It should also be noted that the geometric standard deviations of the P/O ratios from the simulations of the SACRUNCH and SAPLUME modules are quite high, indicating a large scatter around the geometric mean of the P/O ratios.

The fractional bias plot for all model simulations is presented in graphical form in Figure 3.20. The plot confirms the results of Table 3.23. To summarize, the combination of AEROPLUME and GPLUME modules provides good agreement with observations when the results of this study are used. However, results of the study conducted by Hanna, *et al.* (1994a) indicate a tendency to underpredict by the same model, especially at closer distances. At farther distances, however, both studies provide good agreement with observations as seen in Figures 3.17 and 3.18. Both SACRUNCH and SAPLUME modules from the SAIC model indicate tendencies to overpredict total uranium concentrations. The SAPLUME module provides less overprediction than the SACRUNCH module at closer distances from the source, and the reverse is true at greater distances from the source. The RTM-96 model underpredicts at distances close to the source; the predictions get better with increasing distance until, at large distances from the source, it overpredicts.

3.2.3 Gore, Oklahoma, Release

Releases from the Sequoyah Fuels Conversion Facility near Gore, Oklahoma, have been documented in NRC (1986a; 1986b; 1986c). An independent evaluation of the UF₆ dispersion analysis is also provided in NRC (1986a; 1986b). The 48Y cylinder that ruptured contained about

13,380 kg (29,500 lbs) of UF_6 at the time of the accident. Of this amount, approximately 50 percent was assumed to be retained on site either through settling on the ground or on building surfaces or through capture in water that was sprayed to contain the release (NRC, 1986a). The rest was released to the air outside the building. The rupture in the tank was approximately $1.2 \text{ m} \times 0.61 \text{ m}$ in size, which allowed a pool of UF_6 to serve as a source. It was estimated that about 75 percent of the release occurred within the first 5 minutes of rupture, and the remaining UF_6 was released in the subsequent 40 minutes.

Kaiser (1993) performed UF_6 dispersion modeling using the SAIC module SADENZ based on his interpretation of the information presented in NRC (1986a; 1986b). In this study, the accident is modeled using three different approaches. First, the accident is modeled using the approach taken by Kaiser (1993) in an attempt to reproduce his result. Second, the accident is modeled as a continuous release at a constant rate of UF_6 emission lasting 45 minutes. Third, the release is modeled as a combination of an instantaneous puff and a continuous, steady-state source. Since the objective of the first approach was only to reproduce the simulation conducted by Kaiser (1993) using the SADENZ module from the SAIC model, other models were not tested with this approach. The second and third approaches were tested using all models.

3.2.3.1 Gore, Oklahoma, Simulation as Described in Appendix D of the SAIC Model Documentation (Kaiser, 1993)

Kaiser's simulation of the dispersion from UF_6 release at Gore, Oklahoma, was performed using the SADENZ module, and

the source was treated as an instantaneous puff release. Atmospheric conditions used in the SAIC modeling were as follows:

- D stability class;
- Wind-speed of 13.4 m s^{-1} ;
- Ambient temperature of 15°C ; and
- A relative humidity of 10 percent.

About 6820 kg of UF_6 were released into the puff-release outside the building. Using Figure 4.1.2.1 from NRC (1986b), Kaiser (1993) calculated that at about 1-km distance from the release, an individual could be exposed to a concentration of about $1.6 \times 10^{-5} \text{ kg m}^{-3}$ of UO_2F_2 for about 1 hour. Using the stoichiometry of the UF_6 reaction with atmospheric moisture, Kaiser (1993) converted the 1-hour exposure concentration of UO_2F_2 to the 1-hour exposure concentration of UF_6 , assuming that the UF_6 , after its release, had not reacted at all. He estimated the 1-hour exposure concentration of UF_6 as $1.8 \times 10^{-5} \text{ kg m}^{-3}$.

The modeling conducted by Kaiser (1993), using the SADENZ module, showed that an individual could have been exposed to a UF_6 concentration of $6.67 \times 10^{-5} \text{ kg m}^{-3}$ (if it were to remain in the unreacted UF_6 form) for up to 1 hour at distance of 781 m (see Section 3.2.1 for a full discussion of the interpretation of the output concentration of UF_6 from the SAIC model). It should be noted that at this distance the entire UF_6 would have been converted to UO_2F_2 and HF.

In this study, the same modeling assumptions described in Kaiser (1993) were used to reproduce the results of Kaiser.

Additional assumptions necessary to run SADENZ but not stated explicitly in Kaiser (1993) are as follows: initial UF_6 to air mixing ratio is 1:10; initial density of UF_6 -air

mixture is 4.60 kg m^{-3} ; fraction of the initially released UF_6 that is in the form of small solid airborne particles (before mixing with air) is 35 percent; and the release temperature is 56°C . At about 1 km (1090 m), the SADENZ model run in this study predicted an average concentration of $2.26 \times 10^{-3} \text{ kg m}^{-3}$ during the passage of vapor cloud. Time of cloud passage at a distance of 1090 m is 22.1 seconds (given by the model). So, an individual would have been exposed to a concentration of $1.39 \times 10^{-5} \text{ kg m}^{-3}$ ($= 22.1 \text{ s} / 3600 \text{ s} \times 2.26 \times 10^{-3} \text{ kg m}^{-3}$) of UF_6 (in the form of UO_2F_2 at a proportional UO_2F_2 concentration) for up to 1 hour. This matches closely with the concentration that Kaiser back-calculated at 1 km ($1.8 \times 10^{-5} \text{ kg m}^{-3}$) from NRC (1986b) and verifies Kaiser's results ($6.67 \times 10^{-5} \text{ kg m}^{-3}$ at 781 m) as presented in the documentation of the SAIC model (Kasier, 1993).

If the same scenario were to be simulated as a continuous release using the SACRUNCH module (for a constant release rate of $2.53 \text{ kg s}^{-1} = 6,820 \text{ kg} / 45 \text{ min}$), the predicted mean concentration of UF_6 at 1030 m is $4.55 \times 10^{-6} \text{ kg m}^{-3}$ and the predicted peak concentration is $1.33 \times 10^{-5} \text{ kg m}^{-3}$, which is also in the same order of magnitude as reported in Kaiser (1993).

Again, the reader is cautioned that the UF_6 concentration reported at any downwind distance as output by the SAIC model represents the UF_6 concentration as if UF_6 did not enter into any reaction and was simply dispersed in the atmosphere (see Section 3.2.1 for a complete discussion). The dispersion, however, does account for the thermodynamics and chemistry of the UF_6 reaction with atmospheric moisture.

3.2.3.2 Gore, Oklahoma - Continuous Release Assumption

The continuous, steady release approach was used primarily because it is the most straightforward way to define the release. For the Gore release, the release was modeled as a continuous release at a constant rate lasting for 45 minutes. Two factors should be kept in mind when using the Gore data for model testing: (1) much of the uranium was deposited on the ground close to the process building; and (2) the initial cloud characteristics were strongly influenced by building wake effects. Both factors impact the concentrations of UF_6 and its reaction products downwind of the process building.

Another important consideration with respect to model testing is that the air monitors at the Sequoyah Fuels Corporation facility were not directly downwind of the release (see Figure 3.21). At the time of the accident, on-site meteorological data (NRC, 1986a; 1986b) indicated that winds were flowing toward south-southeast, at an average speed of about 8 m s^{-1} with occasional gusts of up to about 13.8 m s^{-1} . The mean wind direction was about 338 degrees with a standard deviation of only about 6 degrees during the release period. Thus the assumption of a mean wind speed of 8 m s^{-1} from the north-northwest, made in NRC (1986a; 1986b), is appropriate. The atmospheric stability was determined to be of Pasquill category D. The ambient temperature was reported to be about 5°C , and the relative humidity was reported as approximately 40 percent.

The following atmospheric conditions were used in this study to model the Gore release using the SAIC module SACRUNCH, the HGSYSTEM/ UF_6 module HEGADAS-S, and the RTM-96 model:

- D stability;
- Wind speed of 8 m s^{-1} ;
- Ambient temperature of 9°C ; and
- A relative humidity of 40 percent.

A total of about 6820 kg of UF_6 was assumed to be released at a steady rate of 2.53 kg s^{-1} in 45 minutes. Table 3.25a compares the predictions of the HGSYSTEM/ UF_6 , SAIC, and RTM-96 models with the observations at two monitoring locations (A and I) as reported in Table 5.1.1 in NRC (1986a) and shown in Figure 3.21. Table 3.25b compares the predictions of the HGSYSTEM/ UF_6 model with the predictions of the ADPIC model at two locations (5, 17) as reported in Table 4.1.2.1 of NRC (1986a). It should be noted that the monitoring station at 1490 m was 210 m off the plume centerline. As presented in the footnote to Table 3.25a, the centerline concentrations representing the measured data were estimated from the off-centerline concentrations measured at the monitoring station, by assuming a Gaussian distribution of contaminants in the transverse direction.

Two scenarios were modeled using the HGSYSTEM/ UF_6 model. The first scenario simulated the release of UF_6 from a 1.22-m $\times$ 0.61-m pool (actual size of the rupture) at an average release rate of 2.53 kg/s over 45 minutes. As shown in Tables 3.25a and 3.25b, there is good agreement between the predictions of the HGSYSTEM/ UF_6 model and observations at all distances from the source except at 160 m. This disagreement could be because of the near-field influence of the buildings near the source.

A second scenario was designed to (crudely) simulate the influence of the building. It was assumed that the initial source was actually spread wider by the building, with an initial pool size of $150 \text{ m} \times 75 \text{ m}$. This

assumption accounts for the fact that there was a building located directly downstream of the source and a large puff formed between the building and the source. The initial dilution in a large volume can thus be accounted for in the steady-state model by increasing the initial pool size. The release was still modeled as a continuous release for 45 minutes at 2.53 kg s^{-1} . Comparisons of the HGSYSTEM/ UF_6 results with the observations (Tables 3.25a and 3.25b) show improved agreements with observations at the 160-m receptor and at the receptor location 17.

To obtain the total uranium concentrations from the UF_6 concentrations reported by the SAIC model, a conversion factor of 0.68 (see Section 3.2.1) was used. As seen from the predictions of the HGSYSTEM/ UF_6 model presented in the footnotes for Table 3.25a, all of the UF_6 has been converted to UO_2F_2 and HF at 1490 m; however, a good amount of UF_6 still remains unreacted at 160 m. Therefore, the total uranium concentrations predicted by the SAIC model at 160 m cannot be directly converted into UO_2F_2 and HF concentrations (see Section 3.2.1). However, at all other distances shown in Tables 3.25a and 3.25b, the total uranium concentrations from the SAIC model can be used along with reaction stoichiometry (Section 3.2.1) to obtain the model predictions for UO_2F_2 and HF concentrations. The SAIC model tends to underpredict the total uranium concentrations at 1490 m as well as the UO_2F_2 and HF predictions from the NRC modeling (NRC, 1986a) at 2310 m and 2820 m. At 160 m, the SAIC model tends to overpredict, probably because of the building effects not being accounted for.

The building effect was simulated using Scenario 2 with the HGSYSTEM/ UF_6 model only to show how the near-source

predictions can be improved. For this study, the third approach was developed as a more realistic way of modeling the Gore release. Therefore, the building effect simulation was not repeated with the SAIC model.

Predictions from the RTM-96 model are also presented in Tables 3.25a and 3.25b. Considering that the model represents a screening-level approach, it provides reasonable predictions of the total uranium and HF concentrations. Because no assumptions regarding release rate or type can be made for the RTM-96 model, only one set of calculations was completed for the RTM-96 model, assuming that 6820 kg of UF_6 were released in 45 minutes. The RTM-96 model provides conservative and the most accurate estimates (among the three models used here) of both UF_6 and HF concentrations at all distances.

Since only two data points with actual measurements from the Gore, Oklahoma, accident were available for the purposes of model testing, it was not feasible to conduct a statistical analysis to determine model bias and accuracy.

3.2.3.3 Gore, Oklahoma - Combined Puff and Continuous Release Assumption

In this analysis, the accident was treated as an instantaneous puff release combined with a steady-state release. Specifically, 5113.5 kg of UF_6 (75 percent of the total amount released) are released as a puff. In addition, the remaining (25 percent) UF_6 is released continuously for the entire duration of the accident (45 minutes) at a steady rate of 0.63 kg s^{-1} . In the opinion of the SENES team, this definition of the release scenario represents a more realistic interpretation of the Gore, Oklahoma, accident.

The HGSYSTEM/ UF_6 model provides the capability to model the puff-dispersion in a transient mode. Conducting the modeling in a transient mode allows the tracking of the UF_6 -cloud as a function of time. In other words, the transient module, HEGADAS-T, in the HGSYSTEM/ UF_6 model, provides, at any time after the release, the centerline, ground-level concentrations within the cloud at several points along the direction of cloud-movement (x-axis). This allows one to determine the cloud-arrival and cloud-passage times at a given receptor location.

The HEGABOX module of the HGSYSTEM/ UF_6 model, which handles an instantaneous, ground-level puff release, was used for the initial modeling of UF_6 release, reactions, and transport. Within the first 22 seconds, the HEGABOX module transitions to HEGADAS-T module; (*i.e.*, it generates input file for the simulation of the HEGADAS-T module). The HEGADAS-T module is then used to conduct the remaining simulation for each receptor. The HEGADAS-S module was used for the steady, continuous release.

The results of the puff-release modeling (from HEGADAS-T) are combined with the results of the continuous release modeling (from HEGADAS-S) at each receptor location to obtain the final concentrations of total uranium, UF_6 , UO_2F_2 , and HF.

Figure 3.22 shows the movement of the UF_6 -cloud over location A (160 m from the source) from 24 to 58 s (each vapor cloud in the figure is separated from the next by a 6-s interval) after release. At 24 s, the front of the puff has just reached the location and is quite small in dimension. Between 24 s and 58 s, the puff grows and moves downstream along the x-axis. At 60 s, the puff moves completely out of the 160-m location. At each time-step (modeling time step = 2 s)

between 24 s and 58 s, the HEGADAS-T module provides the concentrations of UF_6 , UO_2F_2 , and HF at 160-m in its output file. Concentration of total uranium as a function of time at 160-m is shown in Figure 3.23. Average concentration of total uranium for the puff release at 160-m is then calculated as an average over the period of cloud passage at that location. This calculation is carried out for each location of interest.

The average concentration is then scaled to appropriate cloud-passage time and added to the concentration from the continuous release. For example, at the 160-m receptor the average concentration of total uranium from Figure 3.23 is $2.46 \times 10^3 \text{ mg m}^{-3}$, and that from the continuous release (from HEGADAS-S) is 78.3 mg m^{-3} . The final 10-minute average UO_2F_2 concentration is then calculated as:

$$\begin{aligned} C_{\text{final}} &= (t_{\text{cloud}} \times C_{\text{cloud}} + t_{10} \times C_{10})/10 \\ &= (0.60 \text{ min} * 2.46 \times 10^3 \text{ mg/m}^3 + \\ &\quad 10 \text{ min} * 78.3 \text{ mg/m}^3)/10 \text{ min} \\ &= 226 \text{ mg/m}^3 \end{aligned}$$

As mentioned earlier, the time of cloud passage (t_{cloud}) is estimated graphically from Figure 3.23, and an averaging time of 10 minutes was used for the simulation of the continuous release. This procedure is repeated at each of the four desired locations where data for model comparison are available. Tables 3.26a and 3.26b present the results of the combined puff and continuous modeling approach using the HGSYSTEM/ UF_6 model. At 160 m, this approach results in a significant improvement in the predicted concentrations. The results at the other locations, however, show slightly more underprediction than before (when compared with Tables 3.25a and 3.25b).

The SADENZ module is a steady-state puff module within the SAIC model. However, it provides the average concentration within the puff at any downwind distance along with the time of puff passage across that point. Therefore, the combined approach implemented using the HGSYSTEM/ UF_6 model is repeated using the SADENZ and SACRUNCH modules of the SAIC model. Because the cloud passage time is explicitly printed out by the SADENZ module, no external calculation has to be carried out to estimate this variable, as must be done with the HEGADAS-T module. Calculations of the final concentrations of total uranium from SADENZ and SACRUNCH predictions are carried out in exactly the same manner as described for the HEGADAS-T and HEGADAS-S modules. Tables 3.27a and 3.27b present the results of the combined puff and continuous modeling using the SAIC model. At over 2000 m, all of UF_6 has reacted to form UO_2F_2 and HF (see footnotes in Tables 3.25a and 3.25b). Therefore, the predicted concentrations from the SAIC model can be used to estimate the UO_2F_2 and HF concentrations as explained in Section 3.2.1.

Because of the severe overprediction by the SADENZ module at 160 m, the prediction of total uranium concentration at this location has worsened in comparison with the prediction in Table 3.25a, using the second approach. At all points, the SAIC model tends to overpredict the observations when the combined puff and continuous release approach is used. With the continuous release approach, the model was consistently underpredicting. Again, since only two data points with actual measurements were available for the purposes of model testing from the Gore, Oklahoma, accident, it was not feasible to conduct a statistical analysis to determine model bias and accuracy.

To summarize, three different approaches were used to model the release of Gore, Oklahoma. The first approach was used to verify the simulation conducted by Kaiser (1993). Between the second and third approaches, the second approach using a continuous release of UF_6 , provided better matches with observations from the HGSYSTEM/ UF_6 model at all far-field locations; at 160 m, the third approach using a combined puff and continuous release of UF_6 , provided a better match. For the SAIC model, the third approach, provided a worse match at 160 m than the second approach; at farther distances, the third approach resulted in consistent overpredictions as opposed to consistent underpredictions using the second approach. Of the three models, the RTM-96 model provided the most accurate predictions (within a factor of 3) at all distances; with a bias toward overestimation.

3.2.4 Comurhex Plant Release

Ducouret (1978) provides the details of an accidental spill of UF_6 that occurred at the Comurhex Plant in France as a result of a handling error involving a 48Y cylinder. The cylinder contained 8830 kg of liquid UF_6 . About 7100 kg of liquid UF_6 spilled on the ground. Some aspects of Ducouret's description that are relevant to this study include the following.

- The duration of liquid flow from the cylinder leak was estimated to have lasted for 10-15 minutes.
- Application of water (from two large fire hoses) increased the fog and plume spreading.
- Application of carbon dioxide enabled the leak to be plugged,

- The area surrounding the 48Y container where the spill occurred did not exceed 1000 m^2 .
- Aggregate results recorded by the fixed monitoring stations throughout the passage of the toxic cloud, lasting less than 20 minutes, provide a fairly accurate idea of the quantities of hydrogen fluoride and uranium released from the building into the atmosphere. About 330 kg of uranium and 1600 kg of hydrogen fluoride were estimated to have been released.
- In the case of hydrogen fluoride, the 'workforce' limit (2.4 mg m^{-3}) was exceeded up to a distance of 1200 m from the source during the emission.
- In the case of uranium, contamination amounting to 10 mg m^{-3} was observed up to 600 m from the source of emission.

Ducouret (1978) provides no further useful data for model testing. However, a second paper by Doumenc, *et al.* (1978) describes the modeling of a 500-kg UF_6 release to the atmosphere and provides modeling results for HF that can be used for inter-model testing. The following meteorological conditions were assumed for modeling the

Comurhex release:

- Stability class D;
- Temperature of 26°C ;
- A relative humidity of 40 percent; and
- A wind speed of 9 m s^{-1} .

For the HGSYSTEM/ UF_6 and SAIC models, the source was treated as continuous with a constant emission rate of 0.833 kg s^{-1} for 10 minutes. This corresponds to 500 kg of UF_6 being released. The HEGADAS-S module from the HGSYSTEM/ UF_6 model and the SACRUNCH module from the SAIC model

were used. The predictions from the HGSYSTEM/UF₆ and SAIC models are presented in Table 3.28.

Based on the comparisons of model predictions at the two distances, the HF concentrations predicted using the HGSYSTEM/UF₆ model are in very good agreement with the two data points reported by Doumenc, *et al.* (1978); and the RTM-96 model provides a conservative estimate of the HF concentrations at 1200 m and very accurate prediction at 7840 m. Since all of the UF₆ has completely reacted at 1200 m, the predicted concentrations of UF₆ from the SAIC model can be used to estimate the HF concentration, as explained in Section 3.2.1. The SAIC model underpredicts the data points at both locations.

Again, because only two data points were available for the purposes of model testing from the Comurhex accident, it was not feasible to conduct a statistical analysis to determine model bias and accuracy.

3.2.5 P/O Ratios for All Simulations

P/O ratios were calculated for all simulations conducted in this study and presented in Sections 3.1.1 through 3.2.4. The P/O ratios for the mean values of all simulations conducted with the HGSYSTEM/UF₆ and SAIC models for all releases of heavy gases other than UF₆ are shown graphically in Figure 3.24; the corresponding ratios for the peak values are shown in Figure 3.25. The P/O ratios for all simulations conducted with the HGSYSTEM/UF₆, SAIC and RTM-96 for all UF₆ releases are shown graphically in Figure 3.26.

All predictions from the HGSYSTEM/UF₆ model fall within an order of magnitude of the observations. Most predictions from the

HGSYSTEM/UF₆ model are also seen to fall within a factor of 2 of the observations.

The SAIC model consistently underpredicts the mean concentrations for all heavy gases other than UF₆. However, its peak predictions for these gases are within an order of magnitude of the observations with a large number of predictions within a factor of 2 of the observations. Most predictions of UF₆ concentrations from the SAIC model fall within an order of magnitude of the observations. But it also overpredicts beyond an order of magnitude for a couple of observations. It should be noted that the data points at 10 m are omitted from Figure 3.26 for the Bordeaux simulations conducted using the SACRUNCH module for which the overprediction is by over 3 orders of magnitude.

The RTM-96 model provides predictions within a factor of 3 of the observations for most data points beyond 400 m (0.25 miles). For distances less than 400 m, the model provides extreme underpredictions (shown in Figure 3.26 as triangles) for Bordeaux data with predictions beyond an order of magnitude of the observations. It should be noted that at Gore, the model provides a P/O ratio of 2.6 at 160 m.

3.3 Sensitivity Analysis

The two primary objectives of conducting a sensitivity analysis are (1) to determine the parameters that most influence the predicted concentrations of UF₆ and their reaction products downwind of the source and (2) to determine the range of values that the predicted concentrations can take as a result of changing the values of input parameters in a realistic range. These objectives can be met by a full-scale uncertainty analysis conducted under a Monte Carlo framework.

However, the models being tested are not directly amenable to a full-scale uncertainty analysis in a Monte Carlo framework. Implementation of uncertainty analysis algorithms to complex models like HGSYSTEM/UF₆ and SAIC would require major effort and developmental work. Model development and modification being beyond the scope of this study, it was decided to conduct the sensitivity analysis by studying the effect of varying the value of a single input parameter in a specific range around its nominal value on the output concentration of total uranium, while maintaining the values of all other input parameters at their nominal values. Parameter values used in the deterministic analyses presented in Section 3.2 are treated as the nominal values.

3.3.1 Descriptions of the Sensitivity Analysis Simulations

Lists of key input parameters for each module of the HGSYSTEM/UF₆ and SAIC models are presented in Tables 3.29 and 3.30. The sensitivity analysis simulations were primarily carried out for UF₆ releases. Sensitivity simulations were conducted on all modules from the HGSYSTEM/UF₆ and SAIC models. Data sets from the 1986 Bordeaux and Gore releases were used to conduct sensitivity analyses for continuous releases. The Gore data set was used to conduct the sensitivity analyses on instantaneous puff releases. Corresponding sensitivity analyses were also conducted for the RTM-96 model.

For the 1986 Bordeaux release, sensitivity analyses were conducted on the AEROPLUME and PGPLUME modules from the HGSYSTEM/UF₆ model and on the SAPLUME module from the SAIC model. The experimental releases at Bordeaux consisted of releasing UF₆ from a

pipe as a jet; this allows the AEROPLUME and PGPLUME modules to be tested. The release occurred from a height of 3.15 m, which allows the SAPLUME module to be tested.

For the continuous release from a ruptured cylinder at Gore, Oklahoma, sensitivity analyses were conducted using the HEGADAS-S module from the HGSYSTEM/UF₆ model and the SACRUNCH module from the SAIC model. The continuous-release part of the combined puff and continuous-release modeling approach presented in Section 3.2.3.3 was used for the simulations.

Finally, for the puff part of the Gore, Oklahoma, release (see Section 3.2.3.3), sensitivity analyses were conducted using the HEGADAS-T module from the HGSYSTEM/UF₆ model and the SADENZ module from the SAIC model.

Sensitivity of the model predictions was tested for various input parameters. When an input parameter was used by different models, the same set of parameter values was used for the sensitivity analyses for all models. The input parameters that were varied in the sensitivity analyses are presented below, along with rationales for the choice of their parametric values.

Release Temperature

Rupture of the 48Y cylinder at Gore, Oklahoma, occurred primarily because of the heating of the cylinder, which resulted in the melting of UF₆, an increase in pressure and temperature within the cylinder, and finally, the rupture of cylinder (NRC, 1986c). The temperature in the cylinder at the time of the rupture was estimated to be about 361 - 366°K (NRC, 1986c). Accordingly, for the 1986 Bordeaux release, which occurred at

333°K, the maximum release temperature for the sensitivity analysis was set at 366.3°K; the corresponding maximum release temperature for the Gore release was set at 399.3°K, about 30°K higher than the temperature of actual release. The lowest temperature was set at the ambient level for the Bordeaux release and at 326.7°K (about 30°K below the actual release temperature) for the Gore release.

Source Height

The source height parameter is used for handling elevated releases in the HGSYSTEM/UF₆ and SAIC models. The 1986 Bordeaux release occurred at a source height of 3.15 m. Typical accidents involving releases of large quantities of UF₆ have occurred at elevations of less than a few meters from the ground level from a ruptured tank or valve. Therefore, this parameter was allowed to vary between 0.15 and 6.15 m. Note that this parameter is used only by the AEROPLUME and SAPLUME modules.

Atmospheric Stability

Atmospheric stability can change during the course of an accident, particularly if the accident occurs over several hours. Even for short-duration accidents, the stability can change during the accident, particularly if the accident were to happen early in the morning or late in the afternoon. Considering the fact that UF₆ accidents do not typically last for more than 30 to 40 minutes, it was decided to vary the stability class by one class in each direction about the measured stability class for each release.

Wind Speed

Primary uncertainty in this parameter arises from the actual location of a meteorological

monitoring station with respect to the location of the fuel-cycle facility; differences in topographic features between the monitoring station and the site; change in wind speeds during an accident, etc. Consequently, the resulting uncertainty in this parameter could vary from site to site. For this analysis, the wind speed was varied by $\pm 3 \text{ m s}^{-1}$ around the measured value at each site. When annual joint frequency distributions of wind speed, stability class, and wind direction are developed from measured short-term data, a variation of 3 m s^{-1} corresponds to changing from one wind-speed class to the next in the joint frequency distribution classification scheme used by the National Climatic Data Center at Asheville, North Carolina.

Relative Humidity

For the 1986 Bordeaux release, for which the relative humidity was measured at 100 percent, it was allowed to vary between 50 and 100 percent. For the Gore, Oklahoma, release, for which the relative humidity was measured at 40 percent, it was allowed to vary between 10 and 70 percent.

Surface Roughness Length (z_0)

The surface roughness length was varied between 0.01 to 1 m to represent a wide range of surface features anticipated near a fuel-cycle facility. A surface roughness length of 0.01 m represents a plowed field and a surface roughness length of 1 m represents a suburban area with medium, institutional buildings. Wheat fields, residential dwellings, and woodland forests are all encompassed within this range. Only urban areas and areas with smooth surfaces (e.g., areas with natural snow) are out of this range.

Source Size

The initial size of the source from a spill or from a ruptured tank is very important to accurately determine the volume of air that mixes with it, to calculate the reactions and thermodynamics within the air-UF₆ mixture, etc. The initial size of the puff is also important in the presence of a building directly downwind of the source when the puff can rapidly increase in size before being dispersed. Initial size of the puff can be obtained by observations at the site (for a post-accident analysis) or from the location of buildings or other obstructions (for an integrated safety analysis or emergency response planning).

For the Gore, Oklahoma, release, the sensitivity analysis was conducted using the scenario described in Section 3.2.3.3 involving the presence of the building in the downwind direction from the ruptured cylinder. For the HEGADAS-S and HEGADAS-T modules, the source was modeled as a pool with a dimension of 150 m × 75 m. Each dimension of the pool was varied by a factor of 2 about the nominal value for the sensitivity analyses. For the SACRUNCH module, the source plume had a radius of 75 m, and it was varied by a factor of 2 about this value; the same distribution was used for the radius of the source puff for the sensitivity analysis using the SADENZ module.

Momentum Flux

Momentum flux is used in the SAPLUME module in the SAIC model to estimate the plume rise associated with the source. This parameter is specified by the user from the UF₆ emission rate and the source diameter, as was done for the Bordeaux releases in this study. The momentum flux was allowed to

vary by a factor of 2 above and below the nominal value to study its effect on the predicted total uranium concentration.

Mixing Ratio

Entrainment is the process by which a contaminant cloud develops and spreads. In the SAIC model, the mixing ratio is defined as the ratio of the mass of the contaminant released to the mass of air entrained in the initial plume. In the SAIC model, the source is modeled as a plume or a puff a small distance downwind of the source where some entrainment of the ambient air has already occurred. It is provided as input by the user. The HGSYSTEM/UF₆ model internally calculates the amount of air entrained by the plume. Therefore, it does not use the initial mixing ratio as an input parameter. Different ranges of mixing ratios were used for the continuous (SAPLUME and SACRUNCH) and puff (SADENZ) modules of the SAIC model. For the SAPLUME module, a range of 1:1 to 1:10 was used; for the SACRUNCH module, a range of 1:5 to 1:20 was used; and for the SADENZ module, a range of 1:1 to 1:10 was used. For the simulations described for Bordeaux releases in Section 3.2.2, the SAPLUME module was run without any entrainment of air. For a continuous release, the SAIC documentation indicates mixing ratios between 1:5 and 1:11. Based on the modeling experience at SENES, a best fit of the measurements for continuous, ground-level releases was achieved at a mixing ratio of 1:10. For the instantaneous or puff release, the SAIC documentation provides a mixing ratio of 1:0.5 to 1:1. Based on the modeling experience at SENES, a best fit to the measurements was achieved at a mixing ratio of 1:2.

Initial Plume/Puff Velocity

Again, this parameter is used only by the SACRUNCH and SADENZ modules in the SAIC model. The source is defined within the SAIC model as a plume/puff a certain distance downstream of the actual source. Depending on the release characteristics of the source, the initial plume/puff could have varying initial velocity different from that of the ambient wind speed. The SAIC documentation suggests a value of 22 m s^{-1} in its examples. A lower limit of 11 m s^{-1} and upper limit of 30 m s^{-1} was chosen to study the effect of this parameter on the predicted total uranium concentrations.

Initial Distance of the Plume/Puff from the Source

This parameter is also used only by the SACRUNCH module in the SAIC model. It reflects the distance from the actual source where the initial source is defined by the user as a well-established plume in the SACRUNCH module. Consequently, this parameter and the initial plume velocity are interdependent. Again, because of the large uncertainty and arbitrariness in the choice of this parameter, a wide range of values (between 0 and 20 m) is used in the sensitivity analysis. The nominal value of 10 m was used from the examples provided in the SAIC documentation.

Initial Puff Density

For an instantaneous puff release, the density of the air and heavy gas mixture in an initial puff could vary depending on the amount of air entrained in the puff. The density would be bounded by the air density on the lower end and by the density of the heavy gas on the upper end. The nominal value of density used in Section 3.2.3.3 was

4.58 kg m^{-3} . The lowest density was set at 2.51 kg m^{-3} (approximately twice the density of air), and the highest density was set at the density of the pure vapor phase UF_6 at 12.9 kg m^{-3} .

Percent Solid Particles

The SAIC model uses this parameter to define the amount of UF_6 in mass percentage that is released as solid airborne particles. Nominal values for this parameter for Section 3 were chosen for each module from suggested values in the example input files in the SAIC models. Estimation of this parameter is part of the source term calculation, which is not conducted by the SAIC model. The parameter was varied around the nominal value in a large range: for the SAPLUME module, it was varied from 0 to 50 percent; for the SACRUNCH module, it was varied between 30 and 85 percent; and for the SADENZ module, it was varied between 15 and 60 percent.

Percent Droplets

The SAIC model uses this parameter in the SACRUNCH and SAPLUME modules to define the initial mass percentage of the released UF_6 that is in the form of liquid droplets. Again, estimation of this parameter is part of the source term calculation, which is not conducted by the SAIC model. Nominal values for this parameter for Section 3 were chosen for each module from suggested values in the example input files in the SAIC models. The parameter was varied around the nominal value in a large range: for the SAPLUME module, it was varied from 0 to 50 percent and for the SACRUNCH module, it was varied between 0 and 60 percent.

3.3.2 Results of the Sensitivity Analysis

Tables 3.31 to 3.37 and Figures 3.27 to 3.37 present the results of the sensitivity analyses conducted using the HGSYSTEM/UF₆, SAIC, and RTM-96 models. The three input parameters that most influence the predicted concentrations of total uranium are highlighted in the tables for all modules of the HGSYSTEM/UF₆ and SAIC models and for the RTM-96 model. The results from the HGSYSTEM/UF₆ modules are discussed first, followed by those from the SAIC modules and the RTM-96 model.

3.3.2.1 HGSYSTEM/UF₆ Modules

AEROPLUME and PGPLUME

The UF₆ release on April 10, 1986, at Bordeaux is modeled as a jet release using the AEROPLUME module. Initial dense phase quickly transforms to a buoyant phase and the buoyant phase is modeled by PGPLUME. Figure 3.27 shows the effect of varying the input parameters in the range shown in Table 3.31 on the total uranium concentration at 10 m. It is clear that at this close proximity to the source, the source height has the maximum effect on the predicted concentration at 1-m height, followed by atmospheric stability and wind speed. As the source height is lowered toward the receptor height, the receptor-point concentration increases, as expected. As the atmosphere becomes more stable (E-class), vertical mixing is reduced and output concentration increases. As wind speed increases, dilution increases and output concentration decreases. Similarly, as the surface roughness length increases, the atmospheric turbulence and mixing increase, and the output concentration is lowered. It is interesting to note that increasing and decreasing the release temperature both

reduce the output concentration. This is not easy to explain because the effect of release temperature has complex implications for the phase change of UF₆, its thermodynamics and the resulting mass and heat balance of the system, and the buoyancy and dispersion characteristics of the plume. However, the sensitivity of the output concentration to changes in temperature is very small. Similarly, relative humidity has very little influence on the final concentration of total uranium. The maximum change in the receptor-point concentration is slightly over an order of magnitude (a factor of 13.3).

Figure 3.28 shows the effect of varying the input parameters in the range shown in Table 3.31 on the total uranium concentration at 500 m. At this far-field receptor, the source height variation between 0.15 m and 6.15 m has very little influence. Stability and wind speed continue to be the dominant parameters along with surface roughness length, z_0 . The maximum change in the output concentration is less than 1 order of magnitude (a factor of 5.5).

HEGADAS-S

Table 3.32 and Figures 3.29 and 3.30 show the results of the sensitivity analysis conducted on the HEGADAS-S module, using data from Gore release. The Gore release was modeled as a continuous release, as presented in Section 3.2.3.3. Surface roughness length, stability, and wind speed show maximum influence on the output concentrations at both 160 m and 1490 m. Source size shows relatively minor influence on the output concentration. At 160 m, the surface roughness length has the maximum influence on the output concentration whereas at 1490 m, atmospheric stability has the most influence. The maximum change in the output concentration at 160 m

is less than 1 order of magnitude (a factor of 3.9). At 1490 m, the maximum change is just over an order of magnitude (a factor of 23.8).

HEGADAS-T

The results of the sensitivity analysis conducted on the transient HEGADAS-T module did not produce easy-to-discern outputs. Even when a single input variable is perturbed from its nominal value, the resulting changes during every time step of the model is not easy to track. Because of this, interpretation of the results of the analysis was not feasible, and the results of the analysis are not reported.

3.3.2.2 SAIC Modules

SAPLUME

Table 3.33 and Figures 3.31 and 3.32 present the results of the sensitivity analysis conducted using the April 10, 1986, release at Bordeaux. Source height, wind speed, and momentum flux exert the most influence on the output concentration of total uranium at 10 m. The output concentration is most sensitive to the source height. This was also the case with the HGSYSTEM/UF₆ model. Unlike the HGSYSTEM/UF₆ model, the stability has very little influence on the output concentration at this distance. Increasing momentum flux has the same effect as raising the source height, and the concentration decreases at this close distance. It is not clear, however, why the concentration at 10 m increases when the source height is increased from 3.15 m to 6.15 m. The maximum change in the receptor-point concentration is significantly lower than that of the HGSYSTEM/UF₆ model and is less than a factor of 2 (a factor of 1.5).

At 500 m, atmospheric stability, wind speed, and source height exert the most influence on the output concentration. Atmospheric stability has the maximum influence on the output concentration; the maximum changes are on the same orders of magnitude for the SAPLUME (a factor of 5.4) module and the HGSYSTEM/UF₆ model.

SACRUNCH

Sensitivity of the SACRUNCH module was studied using the Gore accident as modeled in Section 3.2.3.3 in the continuous release mode. Table 3.34 and Figures 3.33 and 3.34 provide the results of the sensitivity analysis. At 160 m, the module is most sensitive to percentage of solid UF₆ particles in the release, followed by relative humidity, surface roughness length, and wind speed. It should also be noted that the module terminated without solution when the relative humidity was increased for this simulation to a value of 70 percent. The behavior of the module with respect to relative humidity is not very clear and is probably dependent on the complex thermodynamics of reaction, plume mixing, etc. The maximum change in the output concentration is a factor of 8.8 at 160 m.

At 1490 m, stability, wind speed, and surface roughness length exert the most influence on the model results, as shown by the HEGADAS-S module. Atmospheric stability continues to be the most important parameter with respect to the output concentration at the far-field location. The maximum change in the output concentration was observed to be a factor of 7.2, significantly lower than that of the HEGADAS-S module.

SADENZ

Table 3.35 and Figures 3.35 and 3.36 show the results of the SADENZ simulations conducted using the Gore accident modeled as a puff, as explained in Section 3.2.3.3. At 160 m, initial mixing ratio, source size, and wind speed show the most influence on the output concentration. The maximum change in the output concentration as a result of variations in the mixing ratio is less than an order of magnitude (a factor of 5). At 1490 m, wind speed, stability, and source size exert the most influence on the output concentration. The maximum change in the output concentration as a result of variations in the wind speed is less than an order of magnitude (a factor of 4.8).

3.3.2.3 RTM-96 Model

Wind speed and stability were the only two user-specified parameters that were studied for their influence on the output concentrations of total uranium. The April 1986 release at Bordeaux and the Gore accident were used for the sensitivity analyses. The results of the sensitivity analysis for Bordeaux are presented in Table 3.36 and Figure 3.37. At 10 m, the model is not sensitive to the atmospheric stability primarily because it uses a constant dilution factor of 10^{-3} for all stability classes at any distance less than 400 m. The maximum change in the output concentration as a result of variations in the wind speed is less than an order of magnitude (a factor of 2.5). At 500 m, the model is more sensitive to wind speed than atmospheric stability. The maximum change in the output concentration as a result of variations in the wind speed is less than an order of magnitude (a factor of 2.5).

The results of the sensitivity analysis for Gore are presented in Table 3.37 and Figure

3.37. At the 160-m receptor, the model is not sensitive to the atmospheric stability primarily because it uses a constant dilution factor of 10^{-3} for all stability classes at any distance less than 400 m (0.25 miles). The maximum change in the receptor-point concentration as a result of variations in the wind speed is less than an order of magnitude (a factor of 2.2). At the 1490-m receptor, the model is more sensitive to atmospheric stability than to wind speed. The maximum change in the receptor-point concentration as a result of variations in the atmospheric stability is less than an order of magnitude (a factor of 5.4).

3.4 QA and QC on the Model Simulations

The following QA/QC procedures were followed by the SENES Team in conducting the simulations using the HGSYSTEM/UF₆, SAIC, and RTM-96 models.

- Model inputs were printed out and checked against input parameters taken from references cited earlier (in Sections 3.1 to 3.3) such as the Modelers Data Archive (MDA) (Hanna, *et al.*, 1991) for the Goldfish, Desert Tortoise, and Thorney Island releases. The RTM-96 runs were carried out in EXCEL spreadsheets (from Microsoft, Inc.), and the input values were checked against the references cited in Sections 3.1 to 3.3; model coefficients recommended for use by the RTM-96 model documentation (NRC, 1996) were used to check the values entered in the spreadsheets. Independent hand-calculations were also carried out to check the RTM-96 runs.

- Model outputs were printed out to show which model results at specific downwind distances were extracted for comparison with measured or observed data from the corresponding field experiments.
- Where errors were detected in the input data, the model input file was revised, and the model was rerun, to correct the results.
- All calculations have been checked and documented, and hard copies of the input and output files have been made. Handwritten comments were included in the documentation where further explanations of input parameters were required.

3.5 Conclusions

For model performance tests conducted with heavy gases other than UF_6 , predictions of contaminant concentrations from the HGSYSTEM/ UF_6 model were within a factor of 2 of the field measurements. For four of the seven data sets that were tested, the SAIC model provided predictions of contaminant concentrations within a factor of 2. For the other data sets, most predictions from the SAIC model fell within an order of magnitude of the measured concentrations; however, the predictions of average concentrations underestimated the observations. The RTM-96 model was developed specifically for UF_6 . Therefore, it was not tested with data from other heavy gases.

For the Bordeaux UF_6 experiments, predictions of total uranium concentrations

from the HGSYSTEM/ UF_6 model were within an order of magnitude of the measurements, with most values falling within a factor of 2. Predictions made from the SAPLUME module of the SAIC model overestimated the measured concentrations; however, the predictions were within an order of magnitude of the observations. Predictions from the SACRUNCH module of the SAIC code were within a factor of 5 for distances greater than 10 m. At 10 m, the module overpredicted by over 3 orders of magnitude. The RTM-96 model severely underestimated the measurements at near-source distances of less than 200 m (a number of predictions were over an order of magnitude below observations), and overestimated them at longer distances, with most predictions within an order of magnitude of observations. Documentation for the RTM-96 model does not provide any basis for using a fixed value of dilution factor (to account for atmospheric dispersion) for all distances of less than 400 m (0.25 miles) from the source. Therefore, it is not clear whether the model will consistently overestimate the total uranium concentrations at all sites under all conditions of release and meteorology.

Three different approaches were used to model the release of Gore, Oklahoma. In the first approach, the UF_6 concentration predicted by Kaiser (1993) in the documentation of the SAIC model was verified using the same set of release conditions and module as used by Kaiser. Modeling the source as a continuous release yielded better predictions from the HGSYSTEM/ UF_6 model at distances greater than 1400 m from the source than modeling the source as a combined puff and continuous release. At 160 m from the

source, modeling the source as a combined release yielded better predictions. However, most of predictions with both approaches were within a factor of 2 of the observations. Modeling the source as a continuous release yielded underestimates of the measurements from the SAIC model at distances greater than 1400 m from the source and an overestimate at 160 m from the source. Modeling the source as a combined release yielded overestimates from the SAIC model at all distances. Overpredictions from the SAIC model were above a factor of 2 and within 2 orders of magnitude, and the underpredictions were within an order of magnitude. Of the three models, the RTM-96 model provided the most accurate predictions (within a factor of 3) at all distances; with a bias towards overestimation.

For the Comurhex release, predictions from both HGSYSTEM/UF₆ and RTM-96 models provided good agreements with predictions of HF concentrations (within a factor of 2) at two locations reported in Doumenc, *et al.* (1978). The SAIC model underestimated the concentrations at both locations by over a factor of 2. The RTM-96 model provided consistently conservative estimates at distances greater than 400 m (0.25 miles) from the source. At these distances, the results support the claim made in the model documentation that the RTM-96 model represents a conservative, screening-level model.

Detailed single-parameter sensitivity analyses were conducted on all modules of the HGSYSTEM/UF₆ and SAIC models and on the RTM-96 model. Sensitivity of the output concentrations of total uranium to each input parameter was determined for

each module at two locations, one close to the source and one far away from the source. At large distances from the source, the output concentration of total uranium was most sensitive to meteorological parameters such as atmospheric stability, wind speed, and surface roughness length for all models. At closer distances, the output concentrations of total uranium for all models was most sensitive to certain source-specific parameters such as source height or source size and also to meteorological parameters such as atmospheric stability, wind speed, and surface roughness length.

For continuous releases, the maximum spread in the output concentrations of total uranium by the HGSYSTEM/UF₆ model was more than 1 order of magnitude (a factor of 23.8). The corresponding maximum spreads for the SAIC and RTM-96 models were less than an order of magnitude (a factor of 8.8 for the SAIC model and a factor of 5.4 for the RTM-96 model). For instantaneous puff release, the corresponding maximum spread from the SADENZ module was a factor of 5.

Depending both on the way a release scenario is modeled and the modeler, different sets of predictions can be obtained for the same location. For example, for the Bordeaux releases, the results of this study and the results from Hanna, *et al.* (1994a) differ considerably at near-source locations. For the Gore release, each approach provides a different set of predictions for the desired concentrations.

Modeling approaches presented in this study can be used to conceptualize and model releases of UF₆ from fuel-cycle facilities, using three models. Based on the performances of the three models discussed in this section and depending on the

performance requirements of a nuclear fuel-cycle facility, specific recommendations are made in Section 6.3 with respect to the choice of a model at a given facility to support an integrated safety analysis, an emergency response planning, and a post-accident analysis.

3.6 Notes on Model Testing

Some of the difficulties encountered while conducting the simulations with the three models are presented below.

- Whenever two modules are run in a sequential fashion using the HGSYSTEM/UF₆ model, one of the output files from the simulation of the first module serves as the input file for the simulation of the second module. This file has to be modified by the user before the second module can be run successfully. Though not a serious problem, it is not user-friendly, especially when performing several model runs in a sensitivity analysis.
- The SAIC model does not output concentrations of all constituents at different downwind distances from the source. For a UF₆ simulation, only UF₆ concentrations, as if it does not react at all, are provided as output. Because of lack of knowledge about the amount of UF₆ that has already reacted and converted to UO₂F₂, only the total uranium concentration can be derived from the reported UF₆ concentration. Even though the health impacts from HF exposure cannot be estimated except when UF₆ reaction is complete, the SAIC model can be used to predict the areas of HF and uranium exposures where regulatory limits described in NRC (1988) are exceeded. For a full description of the SAIC model outputs, the reader is referred to Section 3.2.1.
- The SAIC model requires the input of additional parameters along with the release rate of a contaminant at the point of release. It requires the modeler to conduct an external calculation to define the amount of air that has been entrained into the source plume (initial condition) and the fraction of the UF₆ or NH₃ or HF that has been converted into liquid-/solid-phase aerosols. For NH₃ and HF, these calculations can be conducted by other models [*e.g.*, TSCREEN (USEPA, 1992a)]. Certain values of mixing ratios also result in the termination of the model run, with no explanation of the error.
- Even though the assessment of the Gore, Oklahoma, release, using the HEGADAS-T module from the HGSYSTEM/UF₆ model, provided reasonable estimates of total uranium, UO₂F₂, and HF concentrations, the predictions from the module for the sensitivity analysis could not be easily explained.
- The SACRUNCH module requires the input of the duration of release. But it uses this parameter as averaging time. This error should be corrected to include averaging time as the input parameter. The duration of release is not important for the assessment of a continuous, steady-state release.

- During the course of model testing it became apparent that the modeler requires considerable judgment in the setting up of the input file for every new application. This judgment will affect the accuracy of the model's performance.

To alleviate some of the difficulties in preparing the input files, a discussion of initial dilution, building wake effects, and distance to completion of UF_6 reaction with water is provided in Appendix A.

Table 3.1 Field experiment, source type, and the HGSYSTEM/UF₆ module used for model testing

Field experiment	Source type	Applied HGSYSTEM/UF ₆ module
(1) Goldfish	HF aerosol, horizontal jet	HFPLUME/HEGADAS-S
(2) Desert Tortoise	NH ₃ aerosol, horizontal jet	DATAPROP/AEROPLUME/HEGADAS-S
(3) Thorney Island	Continuous area source of Freon-12 & N ₂	DATAPROP/HEGADAS-S
(4) Thorney Island	Instantaneous volume source of Freon-12 & N ₂	DATAPROP/HEGABOX/HEGADAS-T

Table 3.2 **Details of the simulations conducted with the HGSYSTEM/UF₆ model, using Goldfish data**

Run name	Trial ID	Comments
GF1A	GF1	Error with input release rate of 27.7 kg s ⁻¹ (model calculated a maximum of 21.0 kg s ⁻¹). Increased pressure and diameter so that model would accept mass flow rate of 27.7 kg s ⁻¹ . FINAL RUN*.
GF2A	GF2	Error with input release rate of 10.5 kg s ⁻¹ (model calculated a maximum of 7.7 kg s ⁻¹). Increased pressure and diameter so that model would accept mass flow rate of 10.5 kg s ⁻¹ . FINAL RUN*.
GF3A	GF3	Error with input release rate of 10.3 kg s ⁻¹ (model calculated a maximum of 7.8 kg s ⁻¹). Increased pressure and diameter so that model would accept mass flow rate of 10.3 kg s ⁻¹ . FINAL RUN*.

* Averaging time of 88.3 s was used to estimate the mean concentrations, and averaging time of 66.6 s was used to estimate peak concentrations.

Table 3.3 Details of the simulations conducted with the HGSYSTEM/UF₆ model, using Desert Tortoise data

Run name	Trial ID	Comments
DT1	DT1	Overprediction at 100 m.
DT1A	DT1	Re-run DT1 without RELEASE block in AEROPPLUME. Made no difference. Therefore used DT1 as FINAL RUN. For the estimation of mean concentrations, an averaging time of 80 s was used; for the estimation of peak concentrations, an averaging time of 1 s was used.
DT2	DT2	Averaging time of 160 s was used for the estimation of mean concentrations. FINAL RUN.
DT2A	DT2	Rerun DT2 with an averaging time of 1 s to estimate peak concentrations. FINAL RUN.
DT3	DT3	Averaging time of 120 s was used to estimate mean concentrations. FINAL RUN.
DT3A	DT3	Rerun DT3 with an averaging time 1 s to estimate peak concentrations. FINAL RUN.
DT4	DT4	Averaging time of 120 s was used to estimate mean concentrations. FINAL RUN.
DT4A	DT4	Rerun DT4 with an averaging time 1 s to estimate peak concentrations. FINAL RUN.

Table 3.4 Details of the simulations conducted with the HGSYSTEM/UF₆ model, using Thorney Island data for continuous releases

Run name	Trial ID	Comments*
TC1	TC45	FINAL RUN
TC2	TC47	Overprediction of results. Since model testing with the SACRUNCH module, as presented in the documentation for the SAIC model (Kaiser, 1993), described diluting the flow rate because of travel of release gas upwind and then downwind, tried rerunning with reduced mass flow rate.
TC2A	TC47	Rerun TC2 with mass flow rate divided by 4. Results underpredicted close in and overpredicted further out. FINAL RUN. It should be noted that another reasonable adjustment on another input variable could also have been made to achieve a closer agreement between prediction and observation.

* Averaging time of 30 s was used for the estimation of both mean and peak concentrations.

Table 3.5 Details of the simulations conducted with the HGSYSTEM/UF₆ model, using Thorney Island data for instantaneous releases

Run name	Trial ID	Comments*
TI6	TI6	Overprediction at 71, 141, and 283 m. Underprediction at 424 m using the HEGADAS-T module. Stability Class D.
TI7	TI7	Underprediction at 71 m, overprediction between 100 and 180 m, and underprediction from 229 to 500 m. Stability Class E.
TI8	TI8	Overprediction at 71 and 100 m and underprediction between 200 and 510 m. Stability Class B.
TI9	TI9	Underprediction at all distances. Stability Class F.
TI12	TI12	Underprediction at 71 and 150 m. Slightly overpredicts at 100 m, and again underpredicts at 361 and 500 m. Stability Class E.
TI13	TI13	Overprediction at all distances. Stability Class D.
TI17	TI17	Overprediction between 40 and 224 m and underprediction at 500 m. Stability Class D.
TI18	TI18	Overprediction at all distances. Stability Class D.
TI19	TI19	Overprediction at all distances. Stability Class D.

* An averaging time of 0.6 s was used for all runs.

Table 3.6 Predicted concentrations from the HGSYSTEM/UF₆ model and the measured concentrations for the continuous releases of dense gases

Trial	Distance (m)	Measured concentration (ppm)		Predicted concentration (ppm)		Ratio of predicted/measured	
		Mean	Peak	Mean	Peak*	Mean	Peak
GF1 (HF)	300	2.55×10^4	2.55×10^4	2.33×10^4	3.15×10^4	0.9	1.2
	1000	3.10×10^3	3.10×10^3	2.11×10^3	2.90×10^3	0.7	0.9
	3000	4.11×10^2	4.11×10^2	2.40×10^2	3.44×10^2	0.6	0.8
GF2 (HF)	300	1.94×10^4	1.94×10^4	1.17×10^4	1.58×10^4	0.6	0.8
	1000	2.39×10^3	2.39×10^3	1.05×10^3	1.45×10^3	0.4	0.6
GF3 (HF)	300	1.86×10^4	1.86×10^4	9.54×10^3	1.29×10^4	0.5	0.7
	1000	2.49×10^3	2.49×10^3	7.95×10^2	1.10×10^3	0.3	0.4
	3000	2.24×10^2	2.24×10^2	8.70×10^1	1.24×10^2	0.4	0.6
DT1 (NH ₃)	100	4.99×10^4	6.33×10^4	1.16×10^5	1.56×10^5	2.3	2.5
	800	8.84×10^3	1.10×10^4	7.90×10^3	1.13×10^4	0.9	1.0
DT2 (NH ₃)	100	8.32×10^4	1.10×10^5	1.21×10^5	1.63×10^5	1.5	1.5
	800	1.08×10^4	1.86×10^4	1.08×10^4	1.50×10^4	1.0	0.8
DT3 (NH ₃)	100	7.69×10^4	9.73×10^4	1.46×10^5	1.96×10^5	1.9	2.0
	800	7.09×10^3	1.56×10^4	1.37×10^4	1.92×10^4	1.9	1.2
DT4 (NH ₃)	100	5.73×10^4	8.43×10^4	9.86×10^4	1.33×10^5	1.7	1.6
	800	1.67×10^4	2.09×10^4	1.91×10^4	2.58×10^4	1.1	1.2
TC1 (Freon-12 +N ₂)	40	2.00×10^5	2.00×10^5	2.65×10^5	3.58×10^5	1.3	1.8
	53	1.29×10^5	1.29×10^5	1.64×10^5	2.21×10^5	1.3	1.7
	72	8.90×10^4	8.90×10^4	7.93×10^4	1.07×10^5	0.9	1.2
	90	6.20×10^4	6.20×10^4	5.05×10^4	6.82×10^4	0.8	1.1
	112	3.79×10^4	3.79×10^4	3.66×10^4	4.94×10^4	1.0	1.3
	158	2.62×10^4	2.62×10^4	2.12×10^4	2.86×10^4	0.8	1.1
	250	7.60×10^3	7.60×10^3	1.16×10^4	1.57×10^4	1.5	2.1
	335	5.00×10^3	5.00×10^3	7.96×10^3	1.07×10^4	1.6	2.1
	472	3.60×10^3	3.60×10^3	5.16×10^3	6.97×10^3	1.4	1.9
TC2 (Freon-12 +N ₂)	50	1.59×10^5	1.59×10^5	5.81×10^4	7.84×10^4	0.4	0.5
	90	7.40×10^4	7.40×10^4	2.01×10^4	2.71×10^4	0.3	0.4
	212	1.47×10^4	1.47×10^4	6.02×10^3	8.13×10^3	0.4	0.6
	250	6.70×10^3	6.70×10^3	4.80×10^3	6.48×10^3	0.7	1.0
	335	4.80×10^3	4.80×10^3	3.31×10^3	4.47×10^3	0.7	0.9
	472	2.40×10^3	2.40×10^3	2.19×10^3	2.96×10^3	0.9	1.2

* HGSYSTEM/UF₆ model does not output peak concentrations; therefore, the average predicted concentrations were multiplied by 1.35 to obtain the peak concentrations as suggested in Hanna, *et al.* (1994a).

Note: GF - Goldfish.
DT - Desert Tortoise.
TC - Thorney Island continuous release.

Table 3.7 Predicted concentrations from the HGSYSTEM/UF₆ model modules (HEGABOX & HEGADAS-T) and the measured concentrations for the instantaneous releases of a mixture of Freon-12 and N₂ at Thorney Island

Test series	Distance (m)	Observation (ppm)	Prediction (ppm)	Test series	Distance (m)	Observation (ppm)	Prediction (ppm)	Test series	Distance (m)	Observation (ppm)	Prediction (ppm)
T16	71	9.04×10^4	1.05×10^5	T17	71	1.32×10^5	1.02×10^5	T18	71	9.25×10^4	1.08×10^5
	141	3.67×10^4	3.97×10^4		100	5.92×10^4	6.49×10^4		100	6.11×10^4	6.65×10^4
	180	2.62×10^4	2.63×10^4		150	3.38×10^4	3.64×10^4		150	4.03×10^4	3.80×10^4
	283	9.76×10^3	1.09×10^4		180	2.54×10^4	2.72×10^4		200	2.81×10^4	2.44×10^4
	424	5.29×10^3	3.98×10^3		224	1.98×10^4	1.89×10^4		364	1.08×10^4	7.90×10^3
					361	1.19×10^4	7.50×10^3		412	6.92×10^3	5.67×10^3
					500	6.02×10^3	3.31×10^3		510	4.26×10^3	3.21×10^3
TI9	71	1.23×10^5	9.05×10^4	TI12	71	1.16×10^5	8.85×10^4	TI13	71	7.33×10^4	1.32×10^5
	100	7.06×10^4	5.45×10^4		150	3.17×10^4	3.04×10^4		100	6.46×10^4	8.91×10^4
	141	3.58×10^4	3.26×10^4		200	1.85×10^4	1.90×10^4		224	2.54×10^4	2.05×10^4
	180	2.65×10^4	2.31×10^4		361	9.99×10^3	6.20×10^3		316	1.25×10^4	1.25×10^4
	224	2.07×10^4	1.65×10^4		500	3.68×10^3	2.51×10^3		361	9.26×10^3	1.10×10^4
	316	1.14×10^4	9.40×10^3						412	7.29×10^3	7.65×10^3
	503	5.45×10^3	3.70×10^3								
TI17	40	1.27×10^5	2.04×10^5	TI18	40	2.42×10^5	2.69×10^5	TI19	40	1.84×10^5	2.25×10^5
	50	8.51×10^4	1.50×10^5		60	8.61×10^4	1.66×10^5		60	8.24×10^4	1.45×10^5
	71	4.76×10^4	9.46×10^4		70	6.27×10^4	1.36×10^5		71	7.22×10^4	1.23×10^5
	100	3.19×10^4	5.71×10^4		80	5.25×10^4	1.18×10^5		100	5.39×10^4	7.90×10^4
	141	1.49×10^4	3.52×10^4		100	4.08×10^4	9.18×10^4		224	1.36×10^4	1.70×10^4
	224	6.52×10^3	1.63×10^4		200	1.61×10^4	2.42×10^4		361	6.77×10^3	1.05×10^4
	500	3.33×10^3	2.34×10^3		224	1.10×10^4	2.40×10^4		583	2.99×10^3	4.57×10^3
					300	8.06×10^3	1.34×10^4				
					400	4.87×10^3	6.71×10^3				
					510	3.49×10^3	5.43×10^3				

Table 3.8 Model validation results for NH₃, HF, and a mixture of Freon-12 and N₂, using the HGSYSTEM/UF₆ model

Model statistics	GFA ^a	GFP ^b	DTA ^c	DTP ^d	TCA ^e	TCP ^f	TII ^g
Mean of prediction (P) (ppm)	6.10×10^3	8.26×10^3	6.74×10^4	9.09×10^4	4.91×10^4	6.62×10^4	5.52×10^4
Mean of observations (O) (ppm)	9.01×10^3	9.01×10^3	3.88×10^4	5.26×10^4	5.48×10^4	5.48×10^4	4.30×10^4
Fractional bias of the average	-0.39	-0.09	0.53	0.53	-0.11	0.19	0.25
S.D. of prediction (ppm)	7.74×10^3	1.04×10^4	5.56×10^4	7.49×10^4	7.11×10^4	9.59×10^4	6.07×10^4
S.D. of observations (ppm)	9.64×10^3	9.64×10^3	2.97×10^4	3.81×10^4	6.14×10^4	6.14×10^4	4.69×10^4
Fractional bias of standard deviations	-0.22	0.08	0.61	0.65	0.15	0.44	0.26
G.M. ^h of the P/O ratios	0.53	0.73	1.47	1.40	0.83	1.12	1.14
G.S.D. ⁱ of the P/O ratios	1.40	1.38	1.41	1.43	1.71	1.71	1.48
For paired data							
Predictions within a factor of 2 (%)	68.5	87.5	87.5	75.0	80.0	73.3	90.2
Slope of P vs. O line	0.75	1.01	1.78	1.81	1.05	1.42	1.29

^a GFA - Goldfish. - Average or mean (HF).

^b GFP - Goldfish. - Peak (HF).

^c DTA - Desert Tortoise. - Average or mean (NH₃).

^d DTP - Desert Tortoise. - Peak (NH₃).

^e TCA - Thorney Island. - Continuous release, average or mean (Freon-12 and N₂).

^f TCP - Thorney Island. - Continuous release, peak (Freon-12 and N₂).

^g TII - Thorney Island. - Instantaneous (Freon-12 and N₂).

^h Geometric mean.

ⁱ Geometric standard deviation.

Table 3.9 Details of the simulations conducted with the SAIC model module (SACRUNCH), using Goldfish data

Run name	Trial ID	Comments
GF1	GF1	Assumed that there are no droplets in the cloud, and the initial mixing ratio with ambient air is 1:10; (<i>i.e.</i> , an HF release rate of 27.7 kg s^{-1} and an air entrainment rate of 277.0 kg s^{-1}).
GF1A	GF1	Assumed 85% droplets in cloud (based on estimates from the TSCREEN model; USEPA, 1992a), and a mixing ratio of 1:5.
GF1B	GF1	Assumed 85% droplets in cloud and a mixing ratio of 1:10. This run estimates a much higher concentration at 300 m and underestimates the concentrations at distances of 1000 and 3000 m. FINAL RUN.
GF2	GF2	Assumed 85% droplets, 15% vapor in cloud, and a 1:10 mixing ratio.
GF3	GF3	Assumed 85% droplets, 15% vapor in cloud, and 1:10 initial mixing ratio.

Table 3.10 Details of the simulations conducted with the SAIC model module (SACRUNCH), using Desert Tortoise data

Run name	Trial ID	Comments
DT1	DT1	Primary assumptions are that all liquid flashes and the vapor are released at the boiling point of NH_3 . No droplets in cloud. Initial air entrainment rate assumed to be 797.0 kg s^{-1} ; (i.e., a 1:10 mixing ratio).
DT2	DT2	Same assumptions as in DT1.
DT3	DT3	Same assumptions as in DT1.
DT4	DT4	Same assumptions as in DT1.

Table 3.11 Details of the simulations conducted with the SAIC model module (SACRUNCH), using Thorney Island data for continuous releases

Run name	Trial ID	Comments
TC45	TC45	It is assumed that 75% liquid droplets are in cloud, based on the simulation of the TSCREEN model (USEPA, 1992a)*. Initial mixing ratio of 1:10 was assumed.
TC45D	TC45	Only stability class has been changed from E to D; this results in concentrations at close receptors being slightly higher while those at far receptors being slightly lower.
TC47	TC47	Same assumptions as in TC45.

* The modeler was not aware, during the conduct of the Run TC45, that the Thorney Island releases were in 100 percent vapor phase. Therefore, the TSCREEN model was used to obtain the input of 75 percent liquid droplets for Run TC45.

Table 3.12 Details of the simulations conducted with the SAIC model module (SADENZ), using Thorney Island data for instantaneous releases

Run name	Trial ID	Comments
TI6	TI6	Main assumptions are: (1) Release gas was at boiling temperature ^a ; (2) Ratio of gas release rate to initial air entrainment rate is 1:2 ^b . This ratio shows much better agreement than the 1:10 ratio that was used in the continuous releases. Concentration is lower than observation at 71 m, and the concentrations are higher than observations farther out.
TI7	TI7	Same assumptions as in TI6. Predicted concentrations are lower than observations at 71 and 100 m. At other distances, predicted concentrations are higher than observations.
TI8	TI8	Same assumptions as in TI6. Predicted concentrations are higher than observations beyond 200 m.
TI9	TI9	Same assumptions as in TI6. Predicted concentrations are higher than observations beyond 224 m.
TI12	TI12	Same assumptions as in TI6. Predicted concentrations are higher than observations beyond 200 m.
TI13	TI13	Same assumptions as in TI6. Predicted concentrations are higher than observations. Surface roughness is lower than other cases (0.01 m compared to 0.018 m).
TI17	TI17	Same assumptions as in TI6. Model overpredicts beyond 141 m.
TI18	TI18	Same assumptions as in TI6. Model overpredicts beyond 40 m. Similar to case TI13.
TI19	TI19	Same assumptions as in TI6. Similar behavior as in case TI13.

^aThe boiling point of the release gas was 243.4° K. The MDA (Hanna, *et al.*, 1991) reported that the release occurred at 291.8° K, the ambient temperature. Simulation of RUN TI6 using 291.8° K resulted in better agreement at 71 m and worse agreement at all other distances between predictions and measurements. The differences in predictions between the two sets of simulations were within 9 percent.

^bThe MDA (Hanna, *et al.*, 1991) also reported that a mixing ratio of 1:2 was used for the simulation of the "TRACE" model.

Table 3.13 Predicted concentrations from the SAIC model module (SACRUNCH) and the measured field concentrations for the continuous releases of dense gases

Trial	Distance (m)	Measured concentration (ppm)		Predicted concentration (ppm)		Ratio of predicted/measured	
		Mean	Peak	Mean	Peak	Average	Peak
GF1 (HF)	300	2.55×10^4	2.55×10^4	9.08×10^3	2.65×10^4	0.4	1.0
	1000	3.10×10^3	3.10×10^3	1.32×10^3	3.85×10^3	0.4	1.2
	3000	4.11×10^2	4.11×10^2	6.54×10^1	2.03×10^2	0.2	0.5
GF2 (HF)	300	1.94×10^4	1.94×10^4	5.23×10^3	1.53×10^4	0.3	0.8
	1000	2.39×10^3	2.39×10^3	4.88×10^2	1.51×10^3	0.2	0.6
GF3 (HF)	300	1.86×10^4	1.86×10^4	5.05×10^3	1.47×10^4	0.3	0.8
	1000	2.49×10^3	2.49×10^3	4.33×10^2	1.34×10^3	0.2	0.5
	3000	2.24×10^2	2.24×10^2	2.10×10^1	6.60×10^1	0.1	0.3
DT1 (NH ₃)	100	4.99×10^4	6.33×10^4	5.11×10^4	1.49×10^5	1.0	2.4
	800	8.84×10^3	1.10×10^4	3.41×10^3	9.93×10^3	0.4	0.9
DT2 (NH ₃)	100	8.32×10^4	1.10×10^5	5.43×10^4	1.58×10^5	0.7	1.4
	800	1.08×10^4	1.86×10^4	5.21×10^3	1.52×10^4	0.5	0.8
DT3 (NH ₃)	100	7.69×10^4	9.73×10^4	5.70×10^4	1.66×10^5	0.7	1.7
	800	7.09×10^3	1.56×10^4	4.81×10^3	1.40×10^4	0.7	0.9
DT4 (NH ₃)	100	5.73×10^4	8.43×10^4	5.01×10^4	1.46×10^5	0.9	1.7
	800	1.67×10^4	2.09×10^4	6.23×10^3	1.81×10^4	0.4	0.9
TC1 (Freon-12 +N ₂)	40	2.00×10^5	2.00×10^5	2.70×10^4	7.86×10^4	0.1	0.4
	53	1.29×10^5	1.29×10^5	2.05×10^4	5.98×10^4	0.2	0.5
	72	8.90×10^4	8.90×10^4	1.49×10^4	4.34×10^4	0.2	0.5
	90	6.20×10^4	6.20×10^4	1.32×10^4	3.85×10^4	0.2	0.6
	112	3.79×10^4	3.79×10^4	1.01×10^4	2.96×10^4	0.3	0.8
	158	2.62×10^4	2.62×10^4	7.49×10^3	2.18×10^4	0.3	0.8
	250	7.60×10^3	7.60×10^3	4.31×10^3	1.25×10^4	0.6	1.7
	335	5.00×10^3	5.00×10^3	2.76×10^3	8.03×10^3	0.6	1.6
TC2 (Freon-12 +N ₂)	472	3.60×10^3	3.60×10^3	1.65×10^3	4.82×10^3	0.5	1.3
	50	1.59×10^5	1.59×10^5	1.86×10^4	5.42×10^4	0.1	0.3
	90	7.40×10^4	7.40×10^4	1.23×10^4	3.57×10^4	0.2	0.5
	212	1.47×10^4	1.47×10^4	5.63×10^3	1.64×10^4	0.4	1.1
	250	6.70×10^3	6.70×10^3	4.81×10^3	1.40×10^4	0.7	2.1
	335	4.80×10^3	4.80×10^3	3.37×10^3	9.83×10^3	0.7	2.0
	472	2.40×10^3	2.40×10^3	2.24×10^3	6.54×10^3	0.9	2.7

Note: GF - Goldfish.
 DT - Desert Tortoise.
 TC - Thorney Island Continuous.

Table 3.14 Predicted concentrations from the SAIC model module (SADENZ) and the measured field concentrations for the instantaneous releases of a mixture of Freon-12 and N₂ at Thorney Island

Test series	Distance (m)	Observation (ppm)	Prediction (ppm)	Test series	Distance (m)	Observation (ppm)	Prediction (ppm)	Test series	Distance (m)	Observation (ppm)	Prediction (ppm)
T16	71	9.04×10^4	7.74×10^4	T17	71	1.32×10^5	8.56×10^4	T18	71	9.25×10^4	7.30×10^4
	141	3.67×10^4	4.54×10^4		100	5.92×10^4	6.10×10^4		100	6.11×10^4	5.21×10^4
	180	2.62×10^4	3.69×10^4		150	3.38×10^4	5.07×10^4		150	4.03×10^4	4.35×10^4
	283	9.76×10^3	2.21×10^4		180	2.54×10^4	4.15×10^4		200	2.81×10^4	2.87×10^4
	424	5.29×10^3	1.08×10^4		224	1.98×10^4	3.30×10^4		364	1.08×10^4	1.66×10^4
					361	1.19×10^4	1.86×10^4		412	6.92×10^3	1.17×10^4
					500	6.02×10^3	1.05×10^4		510	4.26×10^3	9.69×10^3
T19	71	1.23×10^5	5.76×10^4	T112	71	1.16×10^5	5.23×10^4	T113	71	7.33×10^4	1.24×10^5
	100	7.06×10^4	4.11×10^4		150	3.17×10^4	3.15×10^4		100	6.46×10^4	8.81×10^4
	141	3.58×10^4	3.44×10^4		200	1.85×10^4	2.13×10^4		224	2.54×10^4	4.51×10^4
	180	2.65×10^4	2.84×10^4		361	9.99×10^3	1.30×10^4		316	1.25×10^4	2.81×10^4
	224	2.07×10^4	2.31×10^4		500	3.68×10^3	8.05×10^3		361	9.26×10^3	2.30×10^4
	316	1.14×10^4	1.40×10^4						412	7.29×10^3	1.47×10^4
	503	5.45×10^3	8.52×10^3								
T117	40	1.27×10^5	6.41×10^4	T118	40	2.42×10^5	1.93×10^5	T119	40	1.84×10^5	1.63×10^5
	50	8.51×10^4	5.50×10^4		60	8.61×10^4	1.53×10^5		60	8.24×10^4	1.30×10^5
	71	4.76×10^4	4.34×10^4		70	6.27×10^4	1.31×10^5		71	7.22×10^4	1.11×10^5
	100	3.19×10^4	3.13×10^4		80	5.25×10^4	1.20×10^5		100	5.39×10^4	7.93×10^4
	141	1.49×10^4	2.64×10^4		100	4.08×10^4	9.18×10^4		224	1.36×10^4	4.18×10^4
	224	6.52×10^3	1.79×10^4		200	1.61×10^4	5.23×10^4		361	6.77×10^3	2.23×10^4
	500	3.33×10^3	6.76×10^3		224	1.10×10^4	4.52×10^4		583	2.99×10^3	9.03×10^3
					300	8.06×10^3	2.72×10^4				
					400	4.87×10^3	1.77×10^4				
					510	3.49×10^3	7.41×10^3				

Table 3.15 Model validation results for NH₃, HF, and a mixture of Freon-12 and N₂, using the SAIC model

Model statistics	DTA^a	DTP^b	GFA^c	GFP^d	TCA^e	TCP^f	TII^g
Mean of prediction (P) (ppm)	2.90×10^4	8.46×10^4	2.71×10^3	7.92×10^3	9423.3	2.89×10^4	4.96×10^4
Mean of observations (O) (ppm)	3.88×10^4	5.26×10^4	9.01×10^3	9.01×10^3	5.48×10^4	5.48×10^4	4.30×10^4
FB of the average	-0.29	0.47	-1.08	-0.13	-1.39	-0.62	0.14
S.D. of prediction (ppm)	2.42×10^4	7.05×10^4	3.13×10^3	9.12×10^3	7.41×10^3	2.16×10^4	4.23×10^4
S.D. of observations (ppm)	2.97×10^4	3.81×10^4	9.64×10^3	9.64×10^3	6.14×10^4	6.14×10^4	4.69×10^4
FB of standard deviations	-0.24	0.60	-1.02	-0.05	-1.57	-0.96	-0.10
G.M. ^h of the P/O ratios	0.22	0.67	0.61	1.25	0.31	0.92	1.47
G.S.D. ⁱ of the P/O ratios	1.62	1.58	1.45	1.50	1.98	1.97	1.69
For paired data							
Within a factor of 2 (%)	62.5	87.5	0.0	15.0	33.3	46.7	63.9
Slope of P vs. O line	0.77	1.70	0.31	0.92	0.15	0.44	1.02

^a DTA - Desert Tortoise. - Average or mean (NH₃).^b DTP - Desert Tortoise. - Peak (NH₃).^c GFA - Goldfish. - Average or mean (HF).^d GFP - Goldfish. - Peak (HF).^e TCA - Thorney Island. - Continuous release, average or mean (Freon-12 and N₂).^f TCP - Thorney Island. - Continuous release, peak (Freon-12 and N₂).^g TII - Thorney Island. - Instantaneous (Freon-12 and N₂).^h Geometric mean.ⁱ Geometric standard deviation.

Table 3.16 Release experiment/accident, source type, and the HGSYSTEM/UF₆ and SAIC modules used for model testing

Release experiment/accident location	Source type	Applied HGSYSTEM/UF ₆ modules	Applied SAIC modules
(1) Bordeaux, France	UF ₆ , point source	AEROPLUME and PGPLUME ^a	(A) SACRUNCH (B) SAPLUME
(2) Gore, Oklahoma	UF ₆ , volume source (puff & continuous)	(A) HEGADAS-S (only continuous release) (B) HEGABOX ^b and HEGADAS-T & HEGADAS-S	(A) SADENZ (only puff) ^c (B) SACRUNCH (only continuous) (C) SADENZ & SACRUNCH ^d
(3) Comurhex Plant	UF ₆ , continuous, ground-level source	HEGADAS-S	SACRUNCH

^a Model quickly transitions from AEROPLUME (dense gas jet model) to PGPLUME (passive gas module). The AERPLUME module generates input file for the PGPLUME module as an output.

^b HEGABOX module was run before HEGADAS-T to prepare the input file for HEGADAS-T. The HEGADAS-T module was used to simulate an instantaneous puff release. The HEGADAS-S module was used to simulate a continuous release. The results of the two simulations were combined to obtain the final prediction.

^c The release was simulated as an instantaneous puff as done by Kaiser (1993)

^d The SADENZ module was used to simulate an instantaneous puff release. The SACRUNCH module was used to simulate a continuous release. The results of the two simulations were combined to obtain the final prediction.

Table 3.17 Simulations of the UF₆ release experiments conducted in Bordeaux, France, using the HGSYSTEM/UF₆ model

Comments	
Run name	First release - 10 April 1986
UF6 1A	Assumptions: wind speed of 6.9 m s ⁻¹ , D stability class, release temperature of 333 °K, relative humidity of 100%, and surface roughness of 0.1 m. Averaging time of 3 minutes. This run was used for model validation.
UF6 1B	Same as UF61A except that the averaging time was changed to 10 minutes to match Hanna's model validation data (Hanna, <i>et al.</i> , 1994a) for the plume half-width.
Second release - 18 April 1987	
UF6 2A	Assumptions: wind speed of 3.3 m s ⁻¹ , C stability class, release temperature of 333 °K, relative humidity of 72.2%, and surface roughness of 0.1 m. Averaging time of 3 minutes. This run was used for model validation.
Third release - 5 June 1989	
UF6 3A	Assumptions: wind speed of 4.8 m s ⁻¹ , B stability class, release temperature of 333 °K, relative humidity of 54.3%, and surface roughness of 0.1 m. Averaging time of 3 minutes. This run was used for model validation.

Table 3.18 Simulations of the UF₆ release experiments conducted in Bordeaux, France, using the SAIC model

Comments	
Run name	First release - 10 April 1986
UF61.DAT	<p>SACRUNCH simulation: main assumptions for this run are: 79% solid particulate in the cloud before mixing with air; 21% vapor in cloud; 0% droplets in cloud; 1:1 initial mixing ratio between air and UF₆. This run was used for model validation.</p> <p>SAPLUME simulation: main assumptions for this run are: initial mixing ratio of 1:0 (no air introduced) and release height of 3.15 m; other assumptions the same as for the SACRUNCH simulation. This run was used for model validation.</p> <p>Other assumptions for both modules are consistent with those made for the HGSYSTEM/UF₆ model (Table 3.17).</p>
Second release - 18 April 1987	
UF62.DAT	<p>SACRUNCH simulation: main assumptions for this run are: 79% solid particulates in the cloud before mixing with air; 21% vapor in cloud; 0% droplets in cloud; and 1:1 initial mixing ratio. This run was used for model validation.</p> <p>SAPLUME simulation: main assumptions for this run are: initial mixing ratio of 1:0 (no air introduced) and release height of 3.15 m; other assumptions the same as for the SACRUNCH simulation. This run was used for model validation.</p> <p>Other assumptions for both modules are consistent with those made for the HGSYSTEM/UF₆ model (Table 3.17).</p>
Third release - 5 June 1989	
UF6F3.DAT	<p>SACRUNCH simulation: main assumptions for this run are: 79% solid particulates in the plume before mixing with air; 21% vapor in cloud; 0% droplets in cloud; 1:1 initial air mixing. This run was used for model validation.</p> <p>SAPLUME simulation: main assumptions for this run are: initial mixing ratio of 1:0 (no air introduced) and release height of 3.15 m; other assumptions the same as for the SACRUNCH simulation. This run was used for model validation.</p> <p>Other assumptions for both modules are consistent with those made for the HGSYSTEM/UF₆ model (Table 3.17).</p>

Table 3.19 Predicted concentrations of total uranium from the HGSYSTEM/UF₆ model for the continuous release of UF₆ from Bordeaux on April 10, 1986

Distance (m)	Observation (mg m ⁻³)	Total uranium concentration (mg m ⁻³) (UF61A ^a)		P/O ratio (UF61A)	Total uranium concentration (mg m ⁻³) (UF61B ^a)	
	at 1-m height	at 1-m height	at 3-m height	at 1-m height	at 1-m height	at 3-m height
10	4.34×10^2	4.90×10^2 ^b	1.88×10^3	1.10	3.67×10^2 ^b	1.36×10^3 ^b
20	2.62×10^2	2.32×10^2 ^b	7.16×10^2	0.89	2.00×10^2 ^b	4.70×10^2 ^b
40	9.30×10^1	1.68×10^2	2.32×10^2	1.81	1.40×10^2 ^b	1.52×10^2
100	1.00×10^1	6.76×10^1	6.12×10^1	6.76	4.42×10^1	4.07×10^1 ^b
500	1.50×10^0	4.00×10^0	4.00×10^0	2.67	2.30×10^0	2.30×10^0

^a UF61A was simulated with an averaging time of 3 minutes and UF61B was simulated with an averaging time of 10 minutes.

^b Indicates vertically and linearly interpolated values from model predictions.

Table 3.20 Predicted concentrations of total uranium from the HGSYSTEM/UF₆ model for the continuous release of UF₆ from Bordeaux on April 18, 1987

Distance (m)	Observation (mg m ⁻³)	Total predicted uranium concentration (mg m ⁻³) (UF62A)		P/O ratio
	at 1-m height	at 1-m height	at 3-m height	at 1-m height
10	5.43×10^2	5.07×10^2 *	1.73×10^3 *	0.9
20	2.81×10^2	3.56×10^2 *	6.37×10^2	1.3
40	1.12×10^2	2.36×10^2	2.28×10^2 *	2.1
70	4.30×10^1	1.15×10^2	1.06×10^2 *	2.7
100	2.40×10^1	6.37×10^1	6.04×10^1 *	2.7
200	7.40×10^0	1.81×10^1	1.77×10^1	2.5
500	1.20×10^0	3.20×10^0	3.20×10^0	2.7

* Indicates vertically and linearly interpolated values from model predictions.

Table 3.21 Predicted concentrations of total uranium from the HGSYSTEM/UF₆ model for the continuous release of UF₆ from Bordeaux on June 5, 1989

Distance, (m)	Observation at (mg m ⁻³)	Total predicted uranium concentration (mg m ⁻³) (UF63A)		P/O ratio
	at 1-m height	at 1-m height	at 3-m height	at 1-m height
10	2.31×10^2	2.48×10^2 *	6.95×10^2 *	1.1
20	1.54×10^2	1.85×10^2	2.33×10^2 *	1.2
40	6.12×10^1	9.56×10^1	8.79×10^1 *	1.6
70	2.65×10^1	3.96×10^1	3.76×10^1 *	1.5
100	1.61×10^1	2.10×10^1	2.03×10^1 *	1.3
200	4.90×10^0	5.70×10^0	5.70×10^0 *	1.2

* Indicates vertically and linearly interpolated values from model predictions.

Table 3.22 Predicted concentrations of total uranium from the SACRUNCH and SAPLUME modules of the SAIC model for the continuous releases of UF₆ from Bordeaux, at 1-m elevation.

Release 1, April 10, 1986						
Distance (m)	Observations (mg m ⁻³)	SACRUNCH Mean (mg m ⁻³)	SACRUNCH Mean P/O ratio	SACRUNCH Peak (mg m ⁻³)	SAPLUME (mg m ⁻³)	SAPLUME P/O ratio
10	4.34×10^2	2.43×10^3	5.6	7.09×10^3	1.21×10^3	2.8
20	2.62×10^2	8.91×10^2	3.4	2.60×10^3	7.13×10^2	2.7
40	9.30×10^1	1.10×10^2	1.2	3.22×10^2	3.64×10^2	3.9
100	1.00×10^1	1.36×10^1	1.4	3.97×10^1	8.18×10^1	8.2
500	1.50×10^0	6.00×10^{-1}	0.4	2.00×10^0	1.70×10^0	1.1
Release 2, April 18, 1987						
Distance (m)	Observations (mg m ⁻³)	SACRUNCH Mean (mg m ⁻³)	SACRUNCH Mean P/O ratio	SACRUNCH Peak (mg m ⁻³)	SAPLUME (mg m ⁻³)	SAPLUME P/O ratio
10	5.43×10^2	6.68×10^5	1231.1	1.91×10^6	1.48×10^3	2.7
20	2.81×10^2	4.94×10^2	1.8	1.44×10^3	9.12×10^2	3.2
40	1.12×10^2	1.70×10^2	1.5	4.95×10^2	4.91×10^2	4.4
70	4.30×10^1	4.85×10^1	1.1	1.42×10^2	2.47×10^2	5.7
100	2.40×10^1	2.25×10^1	0.9	6.56×10^1	7.46×10^1	3.1
200	7.40×10^0	4.40×10^0	0.6	1.32×10^1	1.39×10^1	1.9
500	1.20×10^0	8.00×10^{-1}	0.7	2.20×10^0	1.40×10^0	1.2

Table 3.22 (continued)

Release 3, June 5, 1989						
Distance (m)	Observations (mg m ⁻³)	SACRUNCH		SACRUNCH		SAPLUME (mg m ⁻³)
		Mean (mg m ⁻³)	P/O ratio	Mean (mg m ⁻³)	Peak (mg m ⁻³)	P/O ratio
10	2.31×10^2	5.03×10^3	21.8	1.46×10^4	1.39×10^3	6.0
20	1.54×10^2	4.33×10^2	2.8	1.26×10^3	8.14×10^2	5.3
40	6.12×10^1	5.73×10^1	0.9	1.67×10^2	4.23×10^2	6.9
70	2.65×10^1	1.78×10^1	0.7	5.19×10^1	1.21×10^2	4.6
100	1.61×10^1	7.20×10^0	0.4	2.08×10^1	2.15×10^1	1.3
200	4.90×10^0	1.50×10^0	0.3	4.40×10^0	5.70×10^0	1.2

Table 3.23 Predicted concentrations of total uranium from the RTM-96 model for the continuous releases of UF_6 from Bordeaux, at an elevation of 1 m

Distance (m)	First (10 April 1986) release			Second (18 April 1987) release			Third (5 June 1989) release		
	Observation (mg m^{-3})	RTM-96 (mg m^{-3})	P/O ratio	Observation (mg m^{-3})	RTM-96 (mg m^{-3})	P/O ratio	Observation (mg m^{-3})	RTM-96 (mg m^{-3})	P/O ratio
10	4.34×10^2	1.11×10^1	0.03	5.43×10^2	2.46×10^1	0.05	2.31×10^2	1.69×10^1	0.07
20	2.62×10^2	1.11×10^1	0.04	2.81×10^2	2.46×10^1	0.09	1.54×10^2	1.69×10^1	0.11
40	9.30×10^1	1.11×10^1	0.12	1.12×10^2	2.46×10^1	0.22	6.12×10^1	1.69×10^1	0.28
70	-	1.11×10^1	-	4.30×10^1	2.46×10^1	0.57	2.65×10^1	1.69×10^1	0.64
100	1.00×10^1	1.11×10^1	1.1	2.40×10^1	2.46×10^1	1.03	1.61×10^1	1.69×10^1	1.05
200	-	1.11×10^1	-	7.40×10^0	2.46×10^1	3.32	4.90×10^0	1.69×10^1	3.45
500	1.50×10^0	8.70×10^0	5.8	1.20×10^0	1.77×10^1	14.8	-	1.12×10^1	-

Table 3.24 Statistical analysis of the predictions and measurements for the Bordeaux releases

Model statistics	HGSYSTEM/UF ₆	HGSYSTEM/UF ₆ ^a	SAIC (SACRUNCH)	SAIC (SAPLUME)	RTM-96
Mean of prediction (P) (mg m ⁻³)	1.59×10^2	3.83×10^1	1.52×10^2	4.65×10^2	1.78×10^1
Mean of observations (O) (mg m ⁻³)	1.28×10^2	1.28×10^2	7.32×10^1	1.28×10^2	1.28×10^2
FB of the average	0.21	-1.08	0.70	1.14	-1.51
S.D. of prediction (mg m ⁻³)	1.56×10^2	3.45×10^1	2.49×10^2	4.91×10^2	5.50×10^0
S.D. of observations (mg m ⁻³)	1.57×10^2	1.57×10^2	8.93×10^1	1.57×10^2	1.57×10^2
FB of standard deviations	-0.00	-1.28	0.94	1.03	-1.86
GM ^b of the P/O ratios	1.72	0.32	0.97	3.09	0.31
GSD ^c of the P/O ratios	1.67	23.01	1.99	1.89	6.06
For paired data					
Within a factor of 2 (%)	61.1	44.4	66.7	27.8	28.0
Slope d(p)/d (O)	1.10	0.25	2.52	3.34	0.09

^a Hanna, *et al.* (1994a) used the HGSYSTEM/UF₆ model to estimate the concentrations of uranium in air. The statistics of their results are presented here.

^b Geometric mean.

^c Geometric standard deviation.

Note: For the SACRUNCH run of the SAIC model, points at 10 meters are excluded. Therefore, the mean and standard deviations for the observation data are different from those presented in the other columns. For the SAPLUME run of the SAIC model, all points are included.

Table 3.25a Predicted and measured concentrations of total uranium for the Gore, Oklahoma, release; source modeled as continuous release

Location identifier ^d	Distance (m)	Measured concentration (mg m ⁻³)		HEGADAS-S result ^a (mg m ⁻³)		HEGADAS-S result ^b (mg m ⁻³)		SACRUNCH result ^c (mg m ⁻³)		RTM-96 result ^e (mg m ⁻³)
		60-min. average	10-min. average	60-min. average	10-min. average	60-min. average	10-min. average	60-min. average	10-min. average	
A	160	2.00×10^1	1.20×10^2	6.45×10^2	8.46×10^2	3.01×10^2	3.09×10^2	1.84×10^3	2.64×10^3	3.16×10^2
I ^f	1490	3.70×10^0	2.21×10^1	1.13×10^1	1.69×10^1	1.11×10^1	1.44×10^1	2.38×10^0	3.40×10^0	2.28×10^1

^a Source was modeled as a continuous release from a pool of size 1.22 m × 0.61 m.

^b Source was modeled as a continuous release from a pool of size 150 m × 75 m because of presence of buildings. The UF₆ concentrations at 160 and 1490 m were predicted as 6.9 and 1.30×10^{-6} mg m⁻³, respectively.

^c Source was modeled as a continuous release with an initial source radius of 75 m. The UF₆ concentrations at 160 and 1490 m were predicted as 8.3 and 1.50×10^{-5} mg m⁻³, respectively.

^d Location identifiers are in Figure 3.21.

^e The RTM-96 model calculates just one output concentration for a given location irrespective of the type of release.

^f Actual measurements at the off-centerline location I were 2 and 12 mg m⁻³ for the 60- and 10-min. averaging times, respectively. The higher concentrations in the table represent the centerline concentrations at the two locations.

Table 3.25b Predicted concentrations of UO_2F_2 and HF for the Gore, Oklahoma, release; source modeled as continuous release

Location identifier ^f	Distance (m)	Concentration from NRC (1986a) ^a (mg m^{-3})		HEGADAS-S result ^b (mg m^{-3})		HEGADAS-S result ^c (mg m^{-3})		SACRUNCH result ^d (mg m^{-3})		RTM-96 result ^e (mg m^{-3})
		UO_2F_2	HF	UO_2F_2	HF	UO_2F_2	HF	UO_2F_2	HF	HF
5	2310	8.80×10^0	2.40×10^0	1.06×10^1	2.80×10^0	5.90×10^0	1.50×10^0	2.20×10^0	5.00×10^{-1}	2.5×10^0
17	2820	2.40×10^0	7.00×10^{-1}	6.80×10^0	1.80×10^0	3.90×10^0	1.00×10^0	1.60×10^0	4.00×10^{-1}	1.8×10^0

^a Concentrations presented in NRC (1986a) represent predictions made using the ADPIC model.

^b Source was modeled as a continuous release from a pool of size 1.22 m $\times$ 0.61 m. The UF_6 concentrations at 2310 and 2820 m were predicted as 3.3×10^{-8} and 3.0×10^{-9} mg m^{-3} , respectively.

^c Source was modeled as a continuous release from a pool of size 150 m $\times$ 75 m because of presence of buildings. The UF_6 concentrations at 2310 and 2820 m were predicted as 3.7×10^{-7} and 8.4×10^{-8} mg m^{-3} , respectively.

^d Source was modeled as a continuous release with an initial source radius of 75 m.

^e The RTM-96 model provides output concentrations of only total uranium and HF (see Section 3.2.1 for further details).

^f The location identifiers are provided in NRC (1986a).

Table 3.26a Predicted concentrations of total uranium from the HGSYSTEM/UF₆ model, using the combined puff and continuous-release approach for the Gore, Oklahoma, release

Location identifier ^a	Distance (m)	Observation (mg m ⁻³)	Predicted concentrations from HEGABOX/HEGADAS-T (puff) and HEGADAS-S (continuous) modules (mg m ⁻³)		
			U ^b (10-min. average)	U (puff)	U (continuous; 10-min. average)
A	160		1.20×10^2	2.46×10^3	7.83×10^1
I ^c	1490		2.21×10^1	9.54×10^1	3.60×10^0
					U (final, 10-min. average)
					2.26×10^2
					8.70×10^0

^a Location identifiers are in Figure 3.21.

^b Observed values for total uranium represent air monitoring data as presented in NRC (1986a).

^c Actual measurements at the off-centerline receptor 1 were 2 (mg m⁻³) and 12 (mg m⁻³) for the 60-minute and 10-minute sampling times, respectively. The higher concentrations represent the centerline concentrations for the two measurements.

Table 3.26b Predicted concentrations of UO_2F_2 and HF from the HGSYSTEM/ UF_6 model, using the combined puff and continuous-release approach for the Gore, Oklahoma, release

Location identifier ^b	Distance (m)	Reference calculation ^a (mg m^{-3})		Predicted concentrations from HEGABOX/HEGADAS-T (puff) and HEGADAS-S (continuous) modules (mg m^{-3})					
		UO_2F_2 (10-min. average)	HF (10-min. average)	UO_2F_2 (puff)	UO_2F_2 (cont.; 10-min. average)	UO_2F_2 (final, 10-min. average)	HF (puff)	HF (cont.; 10-min. average)	HF (final, 10-min. average)
5	2310	8.80×10^0	2.40×10^0	5.76×10^1	2.30×10^0	5.60×10^0	1.50×10^1	6.00×10^{-1}	1.50×10^0
17	2820	2.40×10^0	7.00×10^{-1}	3.97×10^1	1.50×10^0	3.70×10^0	1.03×10^1	4.00×10^{-1}	1.00×10^0

^a Values of UO_2F_2 and HF concentrations for reference calculations represent the results of modeling presented in NRC (1986a).

^b Location identifiers are in Figure 3.21.

Table 3.27a Predicted concentrations of total uranium from the SAIC model, using the combined puff and continuous-release approach for the Gore, Oklahoma, release

Location identifier ^a	Distance (m)	Observation (mg m ⁻³)		Predicted concentrations from HEGABOX/HEGADAS-T (puff) and HEGADAS-S (continuous) modules (mg m ⁻³)	
		U ^b (10-min. average)	U (puff)	U (continuous; 10-min. average)	U (final, 10-min. average)
A	160	1.20×10^2	1.19×10^5	6.45×10^2	1.12×10^4
I ^c	1490	2.21×10^1	5.27×10^2	8.30×10^{-1}	6.45×10^1

^a Location identifiers are in Figure 3.21.

^b Observed values for total uranium represent air monitoring data as presented in NRC (1986a).

^c Actual measurements at the off-centerline receptor I were 2 (mg m⁻³) and 12 (mg m⁻³) for the 60-minute and 10-minute sampling times, respectively. The higher concentrations represent the centerline concentrations for the two measurements.

Table 3.27b Predicted concentrations of UO_2F_2 and HF from the SAIC model, using the combined puff and continuous-release approach, for the Gore, Oklahoma, release

Location identifier ^b	Distance (m)	Reference calculation ^a (mg m^{-3})		Predicted concentrations from HEGABOX/HEGADAS-T (puff) and HEGADAS-S (continuous) modules (mg m^{-3})					
		UO_2F_2 (10-min. average)	HF (10-min. average)	UO_2F_2 (puff)	UO_2F_2 (cont.; 10-min. average)	UO_2F_2 (final, 10-min. average)	HF (puff)	HF (cont.; 10-min. average)	HF (final, 10-min. average)
5	2310	8.80×10^0	2.40×10^0	2.44×10^2	1.56×10^0	3.18×10^1	6.91×10^1	4.40×10^{-1}	9.00×10^0
17	2820	2.40×10^0	7.00×10^{-1}	1.29×10^2	1.25×10^0	2.09×10^1	3.65×10^1	3.60×10^{-1}	5.90×10^0

^a Values of UO_2F_2 and HF concentrations for reference calculations represent the results of modeling presented in NRC (1986a).

^b Location identifiers are in Figure 3.21.

Table 3.28 Predicted concentrations of HF for the release from the Comurhex Plant

Location identifier	Distance (m)	Predicted HF concentration (mg m ⁻³)			
		From reference calculation ^a	HGSYSTEM/UF ₆ (HEGADAS-S; 10-min. avg.)	SAIC ¹ (SACRUNCH)	RTM-96
Page 434, Doumenc (1978)	1200	2.4	2.1	0.42	3.1
Figure 4, page 227 Doumenc (1978)	7800-8200 ^b	0.001-0.1 ^b	0.09 ^c	0.02 ^d	0.1 ^c

^a HF concentrations were calculated from the predicted UF₆ concentrations from the SAIC model. The reaction of UF₆ with atmospheric moisture is assumed to be complete at 1200 m and beyond. Please see Section 3.2.1 for a discussion of the calculation of HF concentration from UF₆ concentration at complete reaction.

^b The concentrations were reported in Ducouret (1978) in the form of contour lines. The range of distances and concentrations represents the uncertainty in accurately reading the contours.

^c Predicted concentrations at 7800 m and 8200 m were averaged to obtain the reported value.

^d Prediction from the SAIC model was made at 7844 m.

Table 3.29 Notes on inputs for modeling continuous releases of heavy gases

HGSYSTEM/UF ₆ continuous release	SAIC continuous release
<p>DATAPROP - Inputs required:</p> <ul style="list-style-type: none"> Name of species, mole fractions <p>AEROPLUME - Inputs required:</p> <ul style="list-style-type: none"> Reservoir temperature (°C) (°F) Reservoir pressure (atm) Mass (discharge) flow rate (kg s⁻¹) Effective orifice diameter (m) Height of release (m) Duration of release (s) Angle of release to horizontal <p>AEROPLUME simulates near-field dispersion, and the code will automatically generate a link file for PGPLUME or for HEGADAS-S.</p> <p>HEGADAS-S - Inputs required:</p> <ul style="list-style-type: none"> Emission rate (kg s⁻¹) Pool length (m) Pool half-width (m) 	<p>SACRUNCH - Inputs required:</p> <ul style="list-style-type: none"> Release temperature The rate of release of gas by evaporation or other mechanisms being considered (kg s⁻¹) The initial entrainment flux of air or the mixing ratio The distance downwind at which the SACRUNCH calculations start (m) Percentage by mass that is in the form of liquid droplets at the atmospheric boiling point before mixing with air The initial velocity of the plume before mixing with air, assumed to be independent of weather conditions (m s⁻¹) For UF₆ releases - need to input initial fraction of UF₆ that is in the form of small, solid, particulate (before mixing with air) <p>SAPLUME - inputs required:</p> <ul style="list-style-type: none"> Release temperature Rate of release (kg s⁻¹) Initial air entrainment rate (kg s⁻¹) Percent droplets in release Percent solids in release Source height (m)

Table 3.30 Notes on inputs for modeling instantaneous releases of heavy gases

HGSYSTEM/UF₆ instantaneous releases	SAIC instantaneous releases
<p>DATAPROP - Inputs required:</p> <ul style="list-style-type: none"> Name of species, mole fractions <p>HEGABOX - near-field dispersion:</p> <ul style="list-style-type: none"> Size of spill (kg) Pool radius Initial wet pollutant temperature Dilution with ambient air (moles of wet pollutant plus pickup) Transition to HEGADAS-S or HEGADAS-T (far-field) will be made when the Richardson number reaches a critical value (normally 10). HEGABOX currently provides input file for HEGADAS-S or HEGADAS-T automatically. 	<p>SADENZ - Inputs required:</p> <ul style="list-style-type: none"> Release temperature of the air-gas mixture Mass of gas released (kg) Initial mass of air entrained in the source cylinder (kg) Initial density of the air-gas mixture (kg m⁻³) For UF₆ release - need to input initial fraction of UF₆ that is in the form of small, solid particulate (before mixing with air)

Table 3.31 Results of the sensitivity analysis for Bordeaux continuous release on April 10, 1986, using the AEROPLUME and PGPLUME modules from the HGSYSTEM/UF₆ model*

Input parameter	Values used as input			Output [Total uranium mean concentration (mg m ⁻³)]					
				at 10 m			at 500 m		
	Minimum	Nominal	Maximum	Result for minimum input	Result for nominal input	Result for maximum input	Result for minimum input	Result for nominal input	Result for maximum input
Release temp. (K)	299.7	333.0	366.3	4.73×10^2	4.90×10^2	4.57×10^2	3.8	4.0	3.9
Source height (m)	0.15	3.15	6.15	2.64×10^3	4.90×10^2	1.99×10^2	3.9	4.0	3.7
Stability	C	D	E	2.68×10^2	4.90×10^2	7.29×10^2	1.4	4.0	7.7
Wind speed (m s ⁻¹)	3.9	6.9	9.9	7.46×10^2	4.90×10^2	3.45×10^2	6.7	4.0	2.7
Relative humidity (%)	50	100	100	4.82×10^2	4.90×10^2	4.90×10^2	3.9	4.0	4.0
Surface roughness (m)	0.01	0.1	1.0	5.85×10^2	4.90×10^2	4.86×10^2	6.5	4.0	2.0
UF ₆ fraction as gas (f _{gas})	0.06	1.0	1.0	7.78×10^2	4.90×10^2	4.90×10^2	3.9	4.0	4.0

* The predicted concentrations of total uranium at each distance are most sensitive to the three highlighted parameters.

Table 3.32 Results of the sensitivity analysis for Gore continuous release, using the HEGADAS-S module from the HGSYSTEM/UF₆ model*

Input parameter	Values used as input			Output [Total uranium mean concentration (mg m ⁻³)]					
	Minimum	Nominal	Maximum	at 160 m			at 1490 m		
				Result for minimum input	Result for nominal input	Result for maximum input	Result for minimum input	Result for nominal input	Result for maximum input
Release temp. (K)	326.7	363.0	399.3	7.93×10^1	7.83×10^1	7.73×10^1	3.6	3.6	3.6
Source size (m × m)	75 × 37.5	150 × 75	300 × 150	1.07×10^2	7.83×10^1	8.44×10^1	4.1	3.6	2.9
Stability	C	D	E	4.68×10^1	7.83×10^1	1.25×10^2	0.4	3.6	9.5
Wind speed (m s ⁻¹)	5	8	11	1.40×10^2	7.83×10^1	5.37×10^1	7.2	3.6	2.3
Relative humidity (%)	10	40	70	7.84×10^1	7.83×10^1	7.82×10^1	3.6	3.6	3.6
Surface roughness (m)	0.01	0.1	1.0	1.30×10^2	7.83×10^1	3.38×10^1	6.4	3.6	1.4

* The predicted concentrations of total uranium at each distance are most sensitive to the three highlighted parameters.

Table 3.33 Results of the sensitivity analysis for Bordeaux continuous release on April 10, 1986, using the SAPLUME module from the SAIC model*

Input parameter	Values used as input			Output [Total uranium mean concentration (mg m ⁻³)]					
				at 10 m			at 500 m		
	Minimum	Nominal	Maximum	Result for minimum input	Result for nominal input	Result for maximum input	Result for minimum input	Result for nominal input	Result for maximum input
Release temp. (K)	299.7	333.0	366.3	1.24×10^3	1.21×10^3	1.17×10^3	1.7	1.7	1.6
Source height (m)	1.15	3.15	6.15	2.35×10^3	1.21×10^3	1.24×10^3	1.4	1.7	2.0
Stability	C	D	E	1.21×10^3	1.21×10^3	1.21×10^3	0.7	1.7	3.8
Wind speed (m s ⁻¹)	3.9	6.9	9.9	1.40×10^3	1.21×10^3	1.08×10^3	2.9	1.7	1.2
Relative humidity (%)	50	100	100	1.24×10^3	1.21×10^3	1.21×10^3	1.6	1.7	1.7
Momentum flux (kg-m s ⁻²)	165.6	331.0	662.0	1.29×10^3	1.21×10^3	1.09×10^3	1.6	1.7	1.7
Surface roughness (m)	0.01	0.1	1.0	1.23×10^3	1.21×10^3	1.15×10^3	1.7	1.7	1.6
Mixing ratio	1:1	1:0	1:10	1.25×10^3	1.21×10^3	1.26×10^3	1.7	1.7	1.7
Percent solids	0	0	50	1.21×10^3	1.21×10^3	1.22×10^3	1.7	1.7	1.7
Percent droplets	0	0	50	1.21×10^3	1.21×10^3	1.21×10^3	1.7	1.7	1.7

* The predicted concentrations of total uranium at each distance are most sensitive to the three highlighted parameters.

Table 3.34 Results of the sensitivity analysis for Gore continuous release, using the SACRUNCH module from the SAIC model^a

Input parameter	Values used as input			Output [Total uranium mean concentration (mg m ⁻³)]					
	Minimum	Nominal	Maximum	at 160 m			at 1490 m		
				Result for minimum input	Result for nominal input	Result for maximum input	Result for minimum input	Result for nominal input	Result for maximum input
Release temp. (K)	326.7	363.0	399.3	5.31×10^2	6.45×10^2	6.49×10^2	0.81	0.83	0.82
Source radius (m)	37.5	75	150	6.45×10^2	6.45×10^2	6.45×10^2	0.83	0.83	0.83
Stability	C	D	E	3.77×10^2	6.45×10^2	7.48×10^2	0.26	0.83	1.88
Wind speed (m s ⁻¹)	5	8	11	9.11×10^2	6.45×10^2	4.21×10^2	1.35	0.83	0.59
Relative humidity (%)	10	40	60 ^b	1.13×10^2	6.45×10^2	9.01×10^1	0.75	0.83	0.74
Surface roughness (m)	0.01	0.1	1.0	1.02×10^3	6.45×10^2	4.49×10^2	0.95	0.83	0.61
Initial plume vel. (m s ⁻¹)	11	22	30	5.12×10^2	6.45×10^2	7.00×10^2	0.81	0.83	0.83
Initial plume distance (m)	0	10	20	4.08×10^2	6.45×10^2	6.45×10^2	0.83	0.83	0.83
Percent solids	30	80	85	7.31×10^1	6.45×10^2	5.34×10^2	0.73	0.83	0.81
Percent droplets	0	30	60	5.34×10^2	6.45×10^2	6.41×10^2	0.81	0.83	0.83
Mixing ratio	1:5	1:10	1:20	6.73×10^2	6.45×10^2	5.21×10^2	0.83	0.83	0.81

^a The predicted concentrations of total uranium at each distance are most sensitive to the three highlighted parameters.

^b At 70 percent relative humidity, the SACRUNCH module terminates without solution.

Table 3.35 Results of the sensitivity analysis for Gore instantaneous (puff) release, using the SADENZ module from the SAIC model^a

Input parameter	Values used as input			Output [Total uranium mean concentration (mg m ⁻³)]					
				at 160 m			at 1490 m		
	Minimum	Nominal	Maximum	Result for minimum input	Result for nominal input	Result for maximum input	Result for minimum input	Result for nominal input	Result for maximum input
Release temp. (K)	326.7	363.0	399.3	1.22×10^5	1.19×10^5	1.25×10^5	5.17×10^2	5.27×10^2	3.50×10^2
Source radius (m)	37.5	75	150	1.62×10^5	1.19×10^5	3.48×10^4	6.94×10^2	5.27×10^2	3.62×10^2
Stability	C	D	E	1.16×10^5	1.19×10^5	1.22×10^5	2.75×10^2	5.27×10^2	7.23×10^2
Wind speed (m s ⁻¹)	5	8	11	1.56×10^5	1.19×10^5	8.33×10^4	1.35×10^3	5.27×10^2	6.44×10^2
Relative humidity (%)	10	40	60 ^b	1.31×10^5	1.19×10^5	1.24×10^5	4.68×10^2	5.27×10^2	3.34×10^2
Initial puff density (kg m ⁻³)	2.51	4.58	12.88	1.19×10^5	1.19×10^5	1.19×10^5	5.27×10^2	5.27×10^2	5.27×10^2
Mixing ratio	1:1	1:2	1:10	1.90×10^5	1.19×10^5	3.80×10^4	4.30×10^2	5.27×10^2	6.39×10^2
Percent solids	15	35	60	1.22×10^5	1.19×10^5	1.26×10^5	3.51×10^2	5.27×10^2	5.20×10^2
Surface roughness (m)	0.01	0.1	1.0	1.08×10^5	1.19×10^5	1.30×10^5	5.80×10^2	5.27×10^2	4.02×10^2

^a The predicted concentrations of total uranium at each distance are most sensitive to the three highlighted parameters.

^b At 70 percent relative humidity, the SADENZ module terminates without solution.

Table 3.36 Results of the sensitivity analysis for Bordeaux continuous release on April 10, 1986, using the RTM-96 model*

Input parameter	Values used as input			Output [Total uranium mean concentration (mg m^{-3})]					
				at 10 m			at 500 m		
	Minimum	Nominal	Maximum	Result for minimum input	Result for nominal input	Result for maximum input	Result for minimum input	Result for nominal input	Result for maximum input
Stability	C	D	E	11.1	11.1	11.1	7.3	8.7	9.3
Wind speed (m s^{-1})	3.9	6.9	9.9	19.6	11.1	7.7	15.5	8.7	6.1

* The predicted concentrations of total uranium at each distance are most sensitive to the three highlighted parameters.

Table 3.37 Results of the sensitivity analysis for Gore continuous release, using the RTM-96 model*

Input parameter	Values used as input			Output [Total uranium mean concentration (mg m ⁻³)]					
				at 160 m			at 1490 m		
	Minimum	Nominal	Maximum	Result for minimum input	Result for nominal input	Result for maximum input	Result for minimum input	Result for nominal input	Result for maximum input
Stability	C	D	E	315.7	315.7	315.7	8.0	22.8	43.2
Wind speed (m s ⁻¹)	5	8	11	505.0	315.7	229.6	36.4	22.8	16.6

* The predicted concentrations of total uranium at each distance are most sensitive to the three highlighted parameters.

Figure 3.1 Scattergram for HGSYSTEM/ UF_6 predictions against observations for mean HF concentrations for Goldfish data.

Figure 3.2 Scattergram for HGSYSTEM/ UF_6 predictions against observations for peak HF concentrations for Goldfish data.

Figure 3.3 Scattergram for HGSYSTEM/UF₆ predictions against observations for mean NH₃ concentrations for Desert Tortoise data.

Figure 3.4 Scattergram for HGSYSTEM/ UF_6 predictions against observations for peak NH_3 concentrations for Desert Tortoise data.

Figure 3.5 Scattergram for HGSYSTEM/ UF_6 predictions against observations for mean concentrations of a Freon-12 and N_2 mixture for the continuous release data from Thorney Island.

Figure 3.6 Scattergram for HGSYSTEM/ UF_6 predictions against observations for peak concentrations of a Freon-12 and N_2 mixture for the continuous release data from Thorney Island.

Figure 3.7 Scattergram for HGSYSTEM/ UF_6 predictions against observations for concentrations of a Freon-12 and N_2 mixture for the instantaneous release data from Thorney Island.

Figure 3.8 Fractional bias plot for predicted concentrations from the HGSYSTEM/UF₆ model.

Note:

- DTA - Desert Tortoise - average (NH₃).
- DTP - Desert Tortoise - peak (NH₃).
- GFA - Goldfish - average (HF).
- GFP - Goldfish - peak (HF).
- TCA - Thorney Island - average (Freon-12 and N₂ mixture).
- TCP - Thorney Island - peak (Freon-12 and N₂ mixture).
- TII - Thorney Island - instantaneous (Freon-12 and N₂ mixture).

Figure 3.9 Scattergram for SAIC predictions against observations for mean HF concentrations for Goldfish data.

Figure 3.10 Scattergram for SAIC predictions against observations for peak HF concentrations for Goldfish data.

Figure 3.11 Scattergram for SAIC predictions against observations for mean NH_3 concentrations for Desert Tortoise data.

Figure 3.12 Scattergram for SAIC predictions against observations for peak NH_3 concentrations for Desert Tortoise data.

Figure 3.13 Scattergram for SAIC predictions against observations for mean concentrations of a Freon-12 and N_2 mixture for the continuous release data from Thorney Island.

Figure 3.14 Scattergram for SAIC predictions against observations for peak concentrations of a Freon-12 and N_2 mixture for the continuous release data from Thorney Island.

Figure 3.15 Scattergram for SAIC predictions against observations for concentrations of a Freon-12 and N_2 mixture for the instantaneous release data from Thorney Island.

Figure 3.16 Fractional bias plot for predicted concentrations from the SAIC model.

Note:

DTA - Desert Tortoise - average (NH_3).

DTP - Desert Tortoise - peak (NH_3).

GFA - Goldfish - average (HF).

GFP - Goldfish - peak (HF).

TCA - Thorney Island - average (Freon-12 and N_2 mixture).

TCP - Thorney Island - peak (Freon-12 and N_2 mixture).

TII - Thorney Island - instantaneous (Freon-12 and N_2 mixture).

Figure 3.17 Scattergram for HGSYSTEM/UF₆ predictions (averaging time of 3 min.) against observations for total uranium concentrations for data from Bordeaux releases.

Figure 3.18 Scattergram for HGSYSTEM/UF₆ predictions from the simulations of Hanna, *et al.* (1994a) against observations for total uranium concentrations for data from Bordeaux releases.

Figure 3.19 Scattergram for SACRUNCH predictions against observations for total uranium concentrations for data from Bordeaux releases.

Figure 3.20 Fractional bias plot for predicted total uranium concentrations with the Bordeaux data, using the HGSYSTEM/UF₆, SAIC, and RTM-96 models.

* Using results from the simulations of Hanna, *et al.* (1994a). At distances close to the source (≤ 30 m), Hanna, *et al.* (1994a) severely underpredicted the observations. At these distances, the predictions in this study (at 1-m height) were obtained from linear interpolation of model outputs at heights above and below the 1-m height. The linear interpolation is justified because of the close proximity to the source where the plume would still be well-mixed and not yet Gaussian in the internal distribution of contaminants. Therefore, the different methods of interpolation used by the two modelers could be the reason for the differences in predicted values at distances close to the source.

Figure 3.21 Locations of routine monitoring of air, surface water, soil, and vegetation USNRC (1968a), at Gore, Oklahoma.

Figure 3.22 Movement of the UF_6 -cloud at 160 m from the source as modeled by the HEGADAS-T module from the HGSYSTEM/ UF_6 model for Gore, Oklahoma, release.

Figure 3.23 Concentration of total uranium at 160 m as a function of time during the puff passage at that location as predicted by the HEGADAS-T module of the HGSYTEM/UF₆ model for the Gore, Oklahoma, accident modeled as an instantaneous puff release.

Figure 3.24 P/O ratios for the mean values for all simulations conducted with all models for all releases of heavy gases other than UF₆.

Figure 3.25 P/O ratios for the peak values for all simulations conducted with all models for all releases of heavy gases other than UF₆.

Figure 3.26 P/O ratios for all simulations conducted with all models for all UF₆ releases.

Gore – 1: continuous-release modeling with no building effects; 2: continuous-release modeling with building effects; and 3: combined puff and continuous-release modeling; and Bordeaux – 1: SACRUNCH runs, and 2: SAPLUME runs. Triangles for the Bordeaux simulations represent P/O ratios at distances less than 400 m (0.25 miles) from the source.

Figure 3.27 Results of the sensitivity analysis for Bordeaux release of April 10, 1986, using the AEROPLUME and PGPLUME modules from HGSYSTEM/UF₆ model at 10 m: range of predicted total uranium concentrations from variations in input parameter about its nominal value.

Figure 3.28 Results of the sensitivity analysis for Bordeaux release of April 10, 1986, using the AEROPLUME and PGPLUME modules from HGSYSTEM/UF₆ model at 500 m: range of predicted total uranium concentrations from variations in input parameter about its nominal value.

Figure 3.29 Results of the sensitivity analysis for the Gore accident (continuous-release part) using the HEGADAS-S module from the HGSYSTEM/UF₆ model at 160 m: range of predicted total uranium concentrations from variations in input parameter about its nominal value.

Figure 3.30 Results of the sensitivity analysis for the Gore accident (continuous-release part) using the HEGADAS-S module from the HGSYSTEM/UF₆ model at 1490 m: range of predicted total uranium concentrations from variations in input parameter about its nominal value.

Figure 3.31 Results of the sensitivity analysis for Bordeaux release of April 10, 1986, using the SAPLUME module from the SAIC model at 10 m: range of predicted total uranium concentrations from variations in input parameter about its nominal value.

Figure 3.32 Results of the sensitivity analysis for Bordeaux release of April 10, 1986, using the SAPLUME module from the SAIC model at 500 m: range of predicted total uranium concentrations from variations in input parameter about its nominal value.

Figure 3.33 Results of the sensitivity analysis for the Gore accident (continuous-release part) using the SACRUNCH module from the SAIC model at 160 m: range of predicted total uranium concentrations from variations in input parameter about its nominal value.

Figure 3.34 Results of the sensitivity analysis for the Gore accident (continuous-release part) using the SACRUNCH module from the SAIC model at 1490 m: range of predicted total uranium concentrations from variations in input parameter about its nominal value.

Figure 3.35 Results of the sensitivity analysis for the Gore accident (puff-release part) using the SADENZ module from the SAIC model at 160 m: range of predicted total uranium concentrations from variations in input parameter about its nominal value.

Figure 3.36 Results of the sensitivity analysis for the Gore accident (puff-release part) using the SADENZ module from the SAIC model at 1490 m: range of predicted total uranium concentrations from variations in input parameter about its nominal value.

Figure 3.37 Results of the sensitivity analysis using the RTM-96 module: range of predicted total uranium concentrations from variations in input parameter about its nominal value.

4 APPLICABILITY EVALUATION

As described in Section 1, the applicability of each model to the four categories -- integrated safety analysis, emergency response planning, post-accident analysis, and site-specific factors -- was evaluated. It should be kept in mind that a single model may be suitable for more than one category. The criteria developed to evaluate the model applicability are identified in Nair, *et al.* (1997). These criteria were also classified into those requiring qualitative (yes/no) evaluation and those requiring quantitative (evaluating how well the model handles the criteria) evaluation. In the following discussion, the criteria are presented consecutively without regard to the nature of evaluation. Tables 4.1, 4.3, 4.5, and 4.7 include the complete lists of criteria and the maximum score that could be awarded to each criterion.

4.1 Applicability to ISA

Criterion 1. *Does the model have an output that can be compared to the NRC accident criteria?*

This is a qualitatively evaluated criterion requiring a 'yes' or 'no' response (Nair, *et al.*, 1997). The NRC and EPA criteria for health impacts from exposure to radioactive uranium are given in terms of protective action guides (PAGs). The PAGs represent total whole-body doses to the exposed individuals (US NRC, 1996). For chemical toxicity of uranium, the criteria are defined in terms of specific health effects and the intakes (expressed as grams of uranium intake) above which these effects are likely to be manifested (US NRC, 1996). For the

chemical toxicity of HF, the criteria above which specific health effects are manifested are given as concentrations of HF in air (g m^{-3}). Models providing estimates of all three quantities for direct comparison with the NRC criteria were given the full 20 points; those providing estimates of two quantities were given 14 points, and those providing estimates of just one quantity were given 7 points. However, if estimates of the concentrations of UF_6 , UO_2F_2 , and HF in air are given by a model, it was awarded a minimum of 15 points because the concentrations can be used to estimate intakes and doses.

The HGSYSTEM/ UF_6 model was awarded 15 points. The SAIC model was awarded 18 points because it provides estimates of the areas that are impacted when the UF_6 concentration exceeds the hazard levels for total uranium and HF exposures. The RTM-96 model was awarded 20 points. DEGADIS, SLAB, and AFTOX models were each awarded 7 points. The Chlorine Institute methodology was awarded 5 points because it provides only a graphical comparison to determine approximate geographical areas of concern around the facility for two or three specific concentration levels of chlorine in the atmosphere.

Criterion 2. *Does the model account for variable room ventilation rates to translate an internal release into an external release?*

This is a quantitatively evaluated criterion to check for the presence of the feature in a model and to evaluate how the feature is handled by the model. UF_6 accidents involving pipeline leaks, valve failures, or tank ruptures could potentially occur inside

a building. Subsequently, a significant portion of reactions of UF_6 with water vapor could proceed within the building. Ventilation allows for the removal to the outside of unreacted UF_6 and its reaction products. The vents on the building then become a continuous external release to the atmosphere. The characteristics of the external continuous (but not necessarily steady) release can be modeled correctly only if the UF_6 reactions and thermodynamics within the building and the building ventilation rates are correctly handled by the source term evaluation component of a model. None of the models currently possesses this feature. A minimum of 10 points out of 20 was awarded to a model even if this feature were absent, provided that the model can handle an external continuous elevated release once the source term for the release is estimated by another model or by external calculation. This ensured that the model can analyze dispersion from a stack or a vent release from a building once the source term from the building is provided to the model. Furthermore, if a model also accounted for the effects of the presence of buildings on air concentrations within the plume, it was awarded additional points.

The HGSYSTEM/ UF_6 model was awarded 15 points because in its analysis of the plume concentrations near the source, the model accounts for the presence of buildings and the effects of various configurations of buildings on the concentration distribution within the plume, as discussed in Section 2.2. The SAIC, DEGADIS, SLAB, and AFTOX models were awarded 10 points each for handling an elevated release. The RTM-96 model was awarded 0 points because it cannot handle an

elevated release. The Chlorine Institute methodology was awarded 5 points although it is not clear if it can handle elevated releases at heights comparable to the heights of typical building vents.

Criterion 3. *Can the model handle each of the failure modes and scenarios identified in source term evaluation criteria development so that a priori safety analysis can be conducted?*

The HGSYSTEM/ UF_6 and SAIC models can handle all release modes and scenarios; however, the source term in some cases may have to be developed externally. Since the latter issue has already been addressed in Section 2.1, it is not scored here. The HGSYSTEM/ UF_6 and SAIC models were awarded the full 30 points each. The DEGADIS, SLAB, and AFTOX models and the Chlorine Institute methodology cannot handle UF_6 -specific release thermodynamics and chemistry. They were each awarded 20 points. The RTM-96 model provides a single approach to all situations of release for a bounded analysis of a UF_6 release. However, because documentation is inadequate to defend the approach, the model was awarded only 25 points.

Criterion 4. *Can the model handle each of the evaluation components identified in atmospheric dispersion modeling so that a priori safety analysis can be conducted?*

Scoring for this criterion was based on a maximum score of 30 points being awarded to the model with the most capabilities and 10 points to the one possessing minimum capabilities. Models falling in between were awarded 15, 20, or 25 points based on capabilities. Both ability to model

a specific dispersion feature by the model and treatment of the feature were taken into consideration. The scoring was based on the results of the dispersion component analysis presented in Section 2.2.

The HGSYSTEM/UF₆ model was awarded 30 points for possessing the maximum capabilities. The SAIC model was awarded 25 points. The RTM-96 model was awarded 15 points primarily because it was intended to provide a screening-level bounding assessment, even though it did not possess many of the capabilities of the HGSYSTEM/UF₆ and SAIC models. DEGADIS and SLAB models were awarded 20 points each for providing a number of dispersion features specific to dense gases. However, they cannot handle UF₆-specific dispersion, as discussed earlier in Section 2.2. The Chlorine Institute methodology was awarded 15 points for its ability to handle dense gas dispersion and for providing a screening-level assessment without accounting for UF₆-specific dispersion analysis. The AFTOX model provided the least UF₆-specific dispersion capabilities, and it was awarded only 10 points.

Criterion 5. *Can the model be simulated under a worst-case, acute-release mode to evaluate worst-case concentrations of UF₆ and its reaction products in each risk zone (within the site boundary or facility, inside a facility building, and outside the site boundary) to support an integrated safety analysis?*

The features of primary concern in a worst-case situation are building wake effects, canyon effects between two buildings, near-source and far-field dispersion. All models

currently being evaluated have been developed for evaluating impacts outside a building. Therefore, none of the models handles release and dispersion scenarios within a building. Since this feature was specifically addressed in Criterion 2, it is not evaluated here. The HGSYSTEM/UF₆ model was awarded the full 20 points for possessing the most features to conduct a worst-case evaluation. The SAIC model does not include effects from the presence of buildings or canyon effects. However, it provides air concentrations within buildings downwind of the source for accounting for sheltering effects of staying indoors. The SAIC model was awarded 15 points. The RTM-96 model presents a screening-level methodology to calculate worst-case concentrations. However, because of the Gaussian nature of its dispersion analysis, it is not obvious that the model will consistently produce worst-case estimates. It was awarded 12 points. All of the other models were awarded the minimum 10 points for providing various capabilities with respect to dense-gas modeling, but lacking the abilities to conduct a UF₆-specific worst-case analysis.

Criterion 6. *Can the model be simulated within an uncertainty analysis framework to evaluate a range of probable concentrations and realistic upper- and lower-bound concentrations of UF₆ and its reaction products in each risk zone (within the site boundary or facility, inside a facility building, and outside the boundary) to support an integrated safety analysis?*

None of the models has built-in capabilities to handle uncertainty analysis. The SAIC model can handle multiple receptors located in different directions in a single run, thereby

providing several realistic estimates in a single run. The SAIC model was assigned 15 points out of 20. All other models were assigned a minimum of 10 points each because individual runs can be made to assess results from various alternative scenarios.

Criterion 7. *Can the model be simulated to include similar degrees of biases in both source term and dispersion so that their combined use leads to defensible and expected bias in the estimates of the output?*

For safety analysis, the biases are normally directed toward obtaining worst-case predictions. Most of the models being evaluated fit into this category. Since all models rely on external calculations of the source term (except for the handling of certain specific-release types), they can all be used to simulate worst-case scenarios. The HGSYSTEM/UF₆ and SAIC models were each awarded the full 10 points. The RTM-96 model is a screening-level approach especially designed to produce worst-case predictions. However, no justifications for the choice of specific modeling assumptions for the source term or dispersion analysis are provided in the current documentation, making it difficult to judge the consistency of biases for handling the source terms or dispersion. Consequently, the RTM-96 model was awarded 5 points. DEGADIS, SLAB, and AFTOX models were not designed to handle UF₆. Therefore, even though biases for source term and dispersion can be handled consistently by these models, the calculations may not result in the propagation of the biases to the model predictions in a consistent manner. DEGADIS and SLAB models were awarded 4 points, and the AFTOX model

was awarded 3 points because it cannot handle dense gas releases. Documentation for the Chlorine Institute methodology does not provide sufficient information for the biases to be evaluated. It was awarded 0 points.

Criterion 8. *Can the model be easily modified to accommodate an accident whose release/dispersion characteristics are different from the range of characteristics that the model was developed for? Or, in other words, is the model modular in structure?*

Modification of the models in this criterion is not intended to represent a modification of the source code. It indicates only that a specific set of input parameters can represent more than one scenario. Both HGSYSTEM/UF₆ and SAIC models were developed to address most of the scenarios anticipated during a UF₆ release, even though the source terms may have to be calculated externally. Each model was awarded the full 10 points. The RTM-96 model was awarded 7.5 points because it treats all releases in a similar fashion irrespective of the nature of release, even though it produces varying degrees of biases for different scenarios. DEGADIS, SLAB, and AFTOX models were all awarded 5 points for providing the flexibility to handle various accidental scenarios, even though they were not designed to handle UF₆-specific characteristics. The Chlorine Institute methodology has the capability to handle various types of release/dispersion characteristics, but it is inflexible in terms of handling a new release/dispersion situation. It was awarded 2 points.

Criterion 9. *Can the model be used to calculate concentrations of UF₆ and reaction products in the control room from releases in a UF₆-handling facility?*

The SAIC model provides the capability to estimate reduced concentrations, within a room, from an external air concentration. However, the criterion pertains to increasing concentrations within a control room within the same building in which an accident occurs, because of transport through a ventilation system. None of the models provides this capability. All models were awarded 0 points out of 5.

4.2 Applicability to Emergency Planning

Criterion 1. *Does the model have an output that can be compared to the NRC accident criteria?*

The response to this criterion is identical to that for Criterion 1 in Section 4.1. Since a distinction has not been made between separate assessment endpoints for the integrated safety analysis and emergency response planning, the assumption made in evaluating this criterion is that both assessments have the same endpoints and the same sets of NRC regulatory criteria. Accordingly, the HGSYSTEM/UF₆ model was awarded 15 points out of 20; the SAIC model was awarded 18 points; the RTM-96 model was awarded 20 points; DEGADIS, SLAB, and AFTOX models were awarded 7 points each, and the Chlorine Institute methodology was awarded 5 points.

Criterion 2. *Can the model handle short-term meteorology (e.g., 15-minute or hourly meteorology information) so that it*

can be simulated under various atmospheric conditions for various lengths of time to evaluate concentrations to dense population groups around the release facility under various conditions of release?

The purpose of this criterion is not to test whether the models can be run in a real-time mode, because emergency response planning does not require a real-time application. For a long-duration accident, the wind directions and stability conditions could change dramatically during the accident. Most dispersion models account for these changes by providing adjustments for plume meander. Typical meteorological information is recorded on an hourly basis and sometimes at 10-minute intervals. Changes in meteorological parameters over shorter time intervals normally would not be recorded by the measuring instruments. It should be kept in mind that typical long-term UF₆ accidents have not lasted for more than about 20-30 minutes. Therefore, the use of shorter-term meteorological information may actually be unwarranted. Accordingly, for evaluating this criterion, the focus has been redirected to checking how much site-specific meteorological information a model can accept to yield site-specific concentrations of UF₆ and its reaction products in air.

The HGSYSTEM/UF₆ model accepts one set of values of wind speed, wind direction, and stability class. Consequently, time averaging provides the only means of assessing the effects from changes in wind direction. When more than one set of information at two different times is available for a continuous/steady-state release, more than one run can be made and results superimposed by appropriately

accounting for the fraction of time taken by each meteorological category. The need for this adjustment, however, is rare for short-duration UF_6 accidents. For transient releases, the model assumes that a single set of meteorological conditions prevails throughout the duration of the accident. Typical transient releases are of the order of 1-2 minutes, and the assumption seems appropriate. The HGSYSTEM/ UF_6 model was awarded 15 out of 20 points.

The SAIC model can accommodate wind flow in several directions at various speeds and under different stability classes, along with the joint probabilities of the occurrence of each wind speed, wind direction, and stability category. However, in all other aspects, it is similar to the HGSYSTEM/ UF_6 model. It was awarded 17.5 points.

The RTM-96 model allows the same level of meteorological input as does the HGSYSTEM/ UF_6 model. It was also awarded 15 points.

The DEGADIS and SLAB models provide capabilities similar to HGSYSTEM/ UF_6 . However, their usefulness to handle UF_6 -specific issues is limited. They were each awarded 12 points. The AFTOX model has similar capabilities as the HGSYSTEM/ UF_6 model. However, its usefulness for UF_6 -specific issues is more limited than DEGADIS and SLAB models because it was not designed to handle dense gas releases. It was awarded 10 points. The Chlorine Institute methodology has capabilities similar to the DEGADIS and SLAB models, but it is a graphical procedure valid primarily for chlorine. It was awarded only 10 points.

Criterion 3. *Can the model be simulated under a transient mode?*

This criterion is related to Criterion 1 in Section 2.2. Models were evaluated and scored in a similar manner. The HGSYSTEM/ UF_6 model was awarded the full 20 points, the SAIC model was awarded 16 points, the RTM-96 model was awarded 14 points, and the other models were awarded 10 points each.

Criterion 4. *Can the model outputs be easily converted to concentration isopleths, for UF_6 and its reaction products to be superimposed on a population map of the region surrounding the facility?*

The HGSYSTEM/ UF_6 model provides air concentrations as a function of downwind distance, lateral distance, and vertical elevation. However, it assumes that the downwind transport is strictly along the assumed wind direction. Since the duration of usual UF_6 accidents is small, the change in wind direction can be assumed to be accounted for in the calculations of time-averaged concentrations. The concentrations can be superimposed on a population map. The HGSYSTEM/ UF_6 model was awarded the full 10 points. For similar reasons, the SAIC model was also awarded 10 points.

Outputs from RTM-96, SLAB, and AFTOX models cannot be used to directly prepare concentration contours without further modification of the output and invoking the Gaussian plume assumptions. They were awarded 0 points each. The Chlorine Institute methodology provides graphical outputs for chlorine that can be directly superimposed on population maps.

However, because it cannot be directly used for UF_6 releases, the methodology was awarded 5 points.

The DEGADIS model was awarded 10 points for providing concentrations as a function of downwind distance along with an estimate of the standard deviation of the diffusion coefficient in the lateral direction.

Criterion 5. *Does the model have the capability to provide concentrations of UF_6 and its reaction products in the vicinity of the accident, to plan for worker safety?*

This criterion addresses the issues of evaluating concentrations within the building where the release occurred as well as in the vicinity of the buildings, accounting for the presence of the buildings. None of the models provides the capabilities to predict the concentrations of UF_6 and its reaction products within buildings. Usually fuel processing plants contain large buildings where the effects of buildings on contaminant plumes cannot be ignored. The HGSYSTEM/ UF_6 and RTM-96 models provide concentration adjustments for the presence of buildings. The HGSYSTEM/ UF_6 model also allows for the evaluations of the effects of different building configurations on the plume (e.g., building wake effects, canyon effects). The HGSYSTEM/ UF_6 model was awarded the full 30 points, and the RTM-96 model was awarded 25 points. None of the other models handles the presence of buildings in the vicinity of the source. Because SAIC estimates UF_6 -specific concentrations (please see Section 3.2.1 for a full discussion of outputs from the SAIC model), it was awarded 15 points. All other models were awarded the minimum 10 points.

Criterion 6. *Does the model calculate or allow for the calculations of the mitigation time within which corrective actions can be safely carried out?*

None of the models possesses this capability. All models were awarded 0 points out of 10.

Criterion 7. *Does the model account for variable room ventilation rates to translate an internal instantaneous release into an external release?*

This criterion was addressed earlier in Section 4.1. The evaluation scores presented there for applicability to integrated safety analysis are also applicable for emergency response planning. Accordingly, the HGSYSTEM/ UF_6 model was awarded 15 points out of 20, the SAIC model was awarded 10, the RTM-96 model was awarded 0, the Chlorine Institute methodology was awarded 5, and the DEGADIS, SLAB, and AFTOX models were awarded 10 points each.

Criterion 8. *Can the model handle each of the failure modes and scenarios identified in source-term evaluation criteria development so that a priori safety response planning for an accident can be conducted?*

This criterion is identical to Question 3 in Section 4.1, and the models were evaluated in a like fashion. Accordingly, the HGSYSTEM/ UF_6 and SAIC models were awarded the full 30 points each; DEGADIS, SLAB, and AFTOX models, and the Chlorine Institute methodology were all awarded 20 points each; and the RTM-96 model was awarded 25 points.

Criterion 9. *Can the model handle each of the evaluation components identified in atmospheric dispersion modeling so that a priori response planning for an accident can be conducted?*

This criterion is identical to Question 4 in Section 4.1 and was evaluated in a like fashion. The HGSYSTEM/UF₆ model was awarded the full 30 points, the SAIC model was awarded 25 points, the RTM-96 model was awarded 15 points, the DEGADIS and SLAB models were both awarded 20 points, the Chlorine Institute methodology was awarded 15 points, and the AFTOX model was awarded 10 points.

Criterion 10. *Does the model provide realistic estimates of the concentrations to ensure that the planned emergency response is appropriate?*

The HGSYSTEM/UF₆ and SAIC models are developed to provide realistic or conservative estimates of the concentrations by using appropriate input parameters so that the planned emergency response can be considered appropriate. The SAIC model also takes into account direction-specific changes in wind speeds and the probabilities of occurrence of different stability classes. However, the usefulness of the joint-frequency distributions of wind speed, wind direction, and stability, is questionable when dealing with a specific accident of short duration. Neither model is designed to be simulated under an uncertainty analysis framework. Therefore, quantitative confidence intervals on the predicted concentrations and the degree of confidence that can be placed on a given predicted value of concentration cannot be estimated. Each model was awarded 15 points out of 20.

The RTM-96 model was designed to provide upper-bound estimates of air concentrations. Therefore, it cannot be used to obtain realistic estimates to determine the appropriateness of the emergency response planning. However, it can be used to ensure that the emergency plan put in place is adequate. The RTM-96 model was awarded 12 points.

All other models were given the minimum 10 points because they did not possess the capabilities to handle UF₆-specific dynamics.

Criterion 11. *Can the model be simulated under an uncertainty analysis framework to plan for a range of emergency responses with varying budgetary allocation depending on severity of predicted impacts?*

None of the models has built-in capabilities to handle an uncertainty analysis. The range of emergency actions that can possibly be taken for mitigating the effects from a given accident cannot, therefore, be predetermined for emergency response planning. However, in lieu of uncertainty analysis, if sufficient validation information using field data from actual releases of UF₆ exists, such information can be used to determine the degree of confidence or conservatism built into a model. In addition, the models could be used in a sensitivity analysis mode to estimate how much the predicted concentrations change for a specific change in an input parameter. However, extensive information regarding such validation using UF₆ accidents is practically nonexistent.

The HGSYSTEM/UF₆, SAIC, and RTM-96 models were awarded 12 points each out of 20 for providing results (in a purely

deterministic framework) for UF_6 -specific applications. All other models, not specifically designed for UF_6 , were awarded the minimum 10 points.

Criterion 12. *Can the model be easily modified to accommodate an accident whose release/dispersion characteristics are different from the range of characteristics that the model was developed for? Or, in other words, is the model modular in nature?*

This criterion is identical to Criterion 8 in Section 4.1 for the integrated safety analysis, and the same response is applicable. Accordingly, the HGSYSTEM/ UF_6 and SAIC models were awarded the full 10 points each; the RTM-96 model was awarded 7.5 points; the DEGADIS, SLAB, and AFTOX models were awarded 5 points each; and the Chlorine Institute methodology was awarded 2 points.

Criterion 13. *Can the model be used to calculate concentrations of UF_6 and reaction products in the control room from releases in a UF_6 -handling facility?*

The SAIC model provides the capability to estimate reduced concentrations within a room from an external air concentration. However, the criterion pertains to concentrations within a control room within the same building that an accident occurs because of ventilation system. None of the models provides this capability. All models were awarded 0 points out of 5.

4.3 Applicability to PAA

Criterion 1. *Does the model allow input of measured and realistic values such that the location of areas of maximum or critical impacts can be determined?*

Realistic input of measured or realistic values is critical for the accurate calculations of source terms and concentrations at the receptor locations. Both HGSYSTEM/ UF_6 and SAIC models allow the input of realistic values for input parameters (e.g., wind-speed and direction, stability class, ambient temperature, atmospheric humidity, release pressure, and temperature). In many situations, such data during the occurrence of an accident may be available from various sources.

Both the SAIC and HGSYSTEM/ UF_6 models allow for the determination of the distribution of contaminant concentrations surrounding a source when realistic meteorological and source data are provided. Both were awarded the full 20 points. The RTM-96 model was awarded 15 points because it would require a large set of hand calculations before the area of maximum or critical impacts can be determined. The DEGADIS, SLAB, and AFTOX models were each awarded 15 points as they do not possess the capabilities to produce areas of maximum impacts for UF_6 and its reaction products. The Chlorine Institute methodology provides a graphical delineation of the area affected by a release of chlorine, but its applicability to a UF_6 release is not readily defensible. The Chlorine Institute methodology was awarded 10 points.

Criterion 2. *Can the model handle each of the failure modes and scenarios identified in source term evaluation criteria development so that the source term for the accident can be adequately evaluated?*

This criterion is identical to Question 3 in Section 4.1, and the models were evaluated in a like fashion. Accordingly, the HGSYSTEM/UF₆ and SAIC models were awarded the full 30 points; DEGADIS, SLAB, and AFTOX models, and the Chlorine Institute methodology were all awarded 20 points; and the RTM-96 model was awarded 25 points.

Criterion 3. *Can the model handle each of the evaluation components identified in atmospheric dispersion modeling so that the concentrations of UF₆ and its reaction products can be adequately evaluated?*

This criterion is identical to Question 4 in Section 4.1, and the models were evaluated in a like fashion. The HGSYSTEM/UF₆ model was awarded the full 30 points; the SAIC model was awarded 25 points; the RTM-96 model was awarded 15 points; the DEGADIS and SLAB models were each awarded 20 points; the Chlorine Institute methodology was awarded 15 points; and the AFTOX model was awarded 10 points.

Criterion 4. *Can the model be simulated under transient conditions?*

This criterion is related to Criterion 1 in Section 2.2. The models were evaluated and scored in a similar manner. The HGSYSTEM/UF₆ model was awarded the full 20 points; the SAIC model was awarded 16 points; the RTM-96 model was awarded

14; and each of the other models was awarded 12 points.

Criterion 5. *Can the model be simulated under an uncertainty analysis framework to obtain a range of possible concentration distributions for UF₆ and its reaction products?*

None of the models has built-in capabilities to handle an uncertainty analysis. Degrees of realism in terms of predicting long-term health impacts for a given accident cannot, therefore, be predetermined. However, in lieu of an uncertainty analysis, if sufficient validation information using field data from actual releases of UF₆ exists, such information can be used to determine the degree of confidence or conservatism built into the model. However, extensive information regarding such validation data from prior UF₆ accidents is practically nonexistent.

The HGSYSTEM/UF₆, SAIC, and RTM-96 models were each awarded 12 points out of 20 for providing results (in a purely deterministic framework) for UF₆-specific applications. All other models, not specifically designed for UF₆, were awarded the minimum 10 points each.

Criterion 6. *Can the model be easily modified to accommodate an accident whose release/dispersion characteristics are different from the range of characteristics that the model was developed for? Or, in other words, is the model modular in nature?*

This criterion is identical to Criterion 8 in Section 4.1 for integrated safety analysis.

Accordingly, HGSYSTEM/UF₆ and SAIC models were each awarded the full 10 points; the RTM-96 model was awarded 7.5 points; the DEGADIS, SLAB, and AFTOX models were awarded 5 points each; and the Chlorine Institute methodology was awarded 2 points.

Criterion 7. *Can the model output be easily compared with monitoring data to evaluate the accuracy of predictions? (This could include not only air quality data, but also data from vegetation, soil, etc.)*

None of the models evaluated here estimates the concentration of UF₆ and its reaction products in any medium other than air. The HGSYSTEM/UF₆ model provides predictions of the concentrations of UF₆ and all of its reaction products in air. It also provides predictions for the deposition rates. Thus, concentrations on soil or vegetation can be compared with time-integrated values of predicted deposition rates. The HGSYSTEM/UF₆ model was awarded the full 10 points. The SAIC model provides predictions of total uranium concentrations but not of the individual species (UF₆, HF, and UO₂F₂). (The SAIC model outputs the concentrations of UF₆ as if it does not enter into any chemical reaction so that the output concentrations can be used to estimate total uranium concentrations; see Section 3.2.1 for a full discussion of outputs from the SAIC model.) It also does not predict wet deposition rates. The SAIC model was awarded 6 points. The RTM-96 model provides predictions of the impacts from total uranium and HF in air without any accompanying predictions for uranium concentrations or deposition rates, so it was awarded 6 points. Each of the other models

was awarded only 5 points, because they do not possess the capabilities for modeling UF₆ releases.

Criterion 8. *Can the model be used to calculate concentrations of UF₆ and reaction products in the control room from releases in a UF₆-handling facility?*

This criterion is identical to Criterion 13 in Section 4.2. None of the models provides this capability. Accordingly, all models were awarded 0 points.

4.4 Applicability to Site-Specific Factors

Criterion 1. *Ability to include environmental pathways analysis to evaluate health impacts on humans.*

The intent of this criterion is to evaluate whether the results from a model can be directly used to assess health impacts, primarily on humans. The HGSYSTEM/UF₆ model does not make any predictions to support environmental pathways analysis other than concentrations in air and deposition rates. However, because it provides UF₆-specific results, it was awarded 15 points out of 30. The SAIC model allows for the prediction of areas where the concentrations of total uranium and HF in air are above the regulatory criteria, which are based on potential health impacts. It does not, however, conduct a pathways analysis. The SAIC model was awarded 25 points. The RTM-96 model directly provides estimates of radiological and chemically toxic health effects on a human. It was awarded 25 points also because it represents a screening-level approach. None of the other models

provides any health impact analysis, and they were awarded the minimum 10 points each.

Criterion 2. *Ability to handle the presence of snow or rain either on the ground or actively falling.*

The HGSYSTEM/UF₆ model was the only one that allowed for the scavenging of contaminants during rain and snow, and it also included in-cloud scavenging during fogs. It was awarded 8 points out of 10. Two points were deducted primarily because these processes do not remove the contaminants from the plume within the model. All other models were awarded 0 points for not providing this capability.

Criterion 3. *Ability to model complex terrain.*

None of the models evaluated provides the capability to handle air flow and dispersion in the presence of complex terrain. This criterion pertains directly to topography rather than to factors affecting surface roughness. All models were awarded the minimum 10 points out of 20.

Criterion 4. *Ability to simulate long-term effects of deposition on agricultural areas.*

None of the evaluated modes provides this capability. As in the previous criterion, all models were awarded the minimum 10 points out of 20. This criterion was included to address the deleterious effects of HF on vegetation and crops.

Criterion 5. *Ability to handle population effects (e.g., for densely populated urban areas).*

Only the SAIC model provides the capability to estimate the impacts on a population group on a sector-by-sector basis at different downwind distances. Therefore, it can be used to estimate the effects on populations in various sectors (using the available meteorological data for each sector) to identify the most sensitive population subgroup. It was awarded the full 10 points. The HGSYSTEM/UF₆ model calculates the concentration distributions of reactants and products on a plane perpendicular to the principal wind direction. It was awarded 3 points because only one sector can be handled at a time; within a sector, the lateral distribution of concentrations can be predicted. The Chlorine Institute methodology was awarded 2 points for providing contours of concentrations, which can be used with the population data to estimate the impacts of a UF₆ release on different population groups. All other models were awarded 0 points because they provide only estimates of single-value air concentrations, and only at one or more distances in a given sector. For these models, multiple runs would have to be conducted to obtain the concentration distribution; to estimate the impacts on population groups, further analysis would have to be conducted.

Criterion 6. *Ability to conduct a human or an ecological health impact assessment.*

Only the RTM-96 model provides outputs in the units of dose or intake both for radiological and chemically toxic impacts, respectively. It was awarded the full 10 points. The SAIC model provides an indirect measure of health impacts by providing an estimate of the area within which the air concentration may have

exceeded the regulatory limits of concern to human health. It was awarded 8 points. The Chlorine Institute methodology does the same; however, it does not model UF_6 -specific dispersion. It was awarded 2 points. All other models were awarded 0 points.

4.5 Results of the Applicability Evaluations

Tables 4.1, 4.3, 4.5, and 4.7 summarize the scores awarded for each criterion to each model from the evaluations of the applicability of models to integrated safety analysis, emergency planning, post-accident analysis, and site-specific factors, respectively. Tables 4.2, 4.4, 4.6, and 4.8 present the total scores awarded to each model under each applicability category.

Table 4.1 Scores awarded to models for their applicability to integrated safety analysis

Criteria	Maximum score	HGSYSTEM/ SAIC RTM-96 DEGADIS SLAB AFTOX CIM*	UF ₆					
(1) Does the model have an output that can be compared to the NRC accident criteria?	20	15	18	20	7	7	7	5
(2) Does the model account for variable room ventilation rates to translate an internal release into an external release?	20	15	10	0	10	10	10	5
(3) Can the model handle each of the failures modes and scenarios identified in source-term evaluation criteria development so that <i>a priori</i> safety analysis can be conducted?	30	30	30	25	20	20	20	20
(4) Can the model handle each of the evaluation components identified in atmospheric dispersion modeling so that <i>a priori</i> safety analysis can be conducted?	30	30	25	15	20	20	10	15
(5) Can the model be simulated under a worst-case, acute-release mode to evaluate worst-case concentrations of UF ₆ and its reaction products in each risk zone (within the site boundary or facility, inside a facility building, and outside the site boundary) to support an integrated safety analysis?	20	20	15	12	10	10	10	10
(6) Can the model be simulated within an uncertainty analysis framework to evaluate a range of probable concentrations and realistic upper- and lower-bound concentrations of UF ₆ and its reaction products in each risk zone (within the site boundary or facility, inside a facility building, and outside the site boundary) to support an integrated safety analysis?	20	10	15	10	10	10	10	10
(7) Can the model be simulated to include similar degrees of biases in both source term and dispersion so that their combined use leads to defensible and expected bias in the estimates of the output?	10	10	10	5	4	4	3	0
(8) Can the model be easily modified to accommodate an accident whose release/ dispersion characteristics are different from the range of characteristics that the model was developed for? (Is the model modular in structure?)	10	10	10	7.5	5	5	5	2

* Chlorine Institute methodology.

Table 4.1 (continued)

Criteria	Maximum score	HGSYSTEM/ UF ₆	SAIC	RTM-96	DEGADIS	SLAB	AFTOX	CIM*
(9) Can the model be used to calculate concentrations of UF ₆ and reaction products in the control room from releases in a UF ₆ -handling facility?	5	0	0	0	0	0	0	0
Total score	165	140	133	94.5	86	86	75	67

* Chlorine Institute methodology.

Table 4.2 **Summary of model scores for
applicability to integrated safety
analysis**

Model name	Total score	Rank
HGSYSTEM/UF6	140	1
SAIC	133	2
RTM-96	94.5	3
DEGADIS	86	4
SLAB	86	4
AFTOX	75	6
Chlorine Institute methodology	67	7

Table 4.3 Scores awarded to models for their applicability to emergency response planning

Criteria	Maximum score	HGSYSTEM/ UF ₆	SAIC	RTM- 96	DEGADIS	SLAB	AFTOX	CIM*
(1) Does the model have an output that can be compared to the NRC accident criteria?	20	15	18	20	7	7	7	5
(2) Can the model handle short-term meteorology (e.g., 15-minute or hourly meteorology information) so that it can be simulated under various atmospheric conditions for various lengths of time to evaluate concentrations to dense population groups around the release facility under various conditions of release?	20	15	17.5	15	12	12	10	10
(3) Can the model be simulated under a transient mode?	20	20	16	14	10	10	10	10
(4) Can the model outputs be easily converted to concentration isopleths, for UF ₆ and its reaction products to be superimposed on a population map of the region surrounding the facility?	10	10	10	0	10	0	0	5
(5) Does the model have the capability to provide concentrations of UF ₆ and its reaction products in the vicinity of the accident to plan for worker safety?	30	30	15	25	10	10	10	10
(6) Does the model calculate or allow for the calculation of the mitigation time within which corrective or protective actions can be safely carried out?	10	0	0	0	0	0	0	0
(7) Does the model account for variable room ventilation rates to translate an internal instantaneous release into an external release?	20	15	10	0	10	10	10	5
(8) Can the model handle each of the failure modes and scenarios identified in source-term evaluation criteria development so that <i>a priori</i> response planning for a potential accident can be conducted?	30	30	30	25	20	20	20	20

* The Chlorine Institute methodology.

Table 4.3 (continued)

Criteria		Maximum score	HGSYSTEM/ UF ₆	SAIC	RTM- 96	DEGADIS	SLAB	AFTOX	CIM*
(9)	Can the model handle each of the evaluation components identified in atmospheric dispersion modeling so that <i>a priori</i> response planning for a potential accident can be conducted?	30	30	25	15	20	20	10	15
(10)	Does the model provide realistic estimates of the concentrations to ensure that the planned emergency response is appropriate?	20	15	15	12	10	10	10	10
(11)	Can the model be simulated under an uncertainty analysis framework to plan for a range of emergency responses with varying budgetary allocation depending on severity of predicted impacts?	20	12	12	12	10	10	10	10
(12)	Can the model be easily modified to accommodate an accident whose release/dispersion characteristics are different from the range of characteristics that the model was developed for? (Is the model modular in structure?)	10	10	10	7.5	5	5	5	2
(13)	Can the model be used to calculate concentrations of UF ₆ and reaction products in the control room from releases in a UF ₆ -handling facility?	5	0	0	0	0	0	0	0
Total score		245	202	178.5	145.5	124	114	102	102

* The Chlorine Institute methodology.

Table 4.4 **Summary of model scores for
applicability to emergency response
planning**

Model name	Total score	Rank
HGSYSTEM/UF ₆	202	1
SAIC	178.5	2
RTM-96	145.5	3
DEGADIS	124	4
SLAB	114	5
AFTOX	102	6
Chlorine Institute methodology	102	6

Table 4.5 Scores awarded to models for their applicability to post-accident analysis

Criteria	Maximum score	HGSYSTEM/ UF ₆	SAIC	RTM-96	DEGADIS	SLAB	AFTOX	CIM*
(1) Does the model allow the input of measured and realistic values such that the location of areas of maximum or critical impacts can be determined?	20	20	20	15	15	15	15	10
(2) Can the model handle each of the failure modes and scenarios identified in source-term evaluation criteria development so that the source-term for the accident can be adequately evaluated?	30	30	30	25	20	20	20	20
(3) Can the model handle each of the evaluation components identified in atmospheric dispersion modeling so that the concentrations of UF ₆ and its reaction products can be adequately estimated for the accident in question?	30	30	25	15	20	20	10	15
(4) Can the model be simulated under transient conditions?	20	20	16	14	12	12	12	12
(5) Can the model be simulated under an uncertainty analysis framework to obtain a range of possible concentration distribution of UF ₆ and its reaction products?	20	12	12	12	10	10	10	10
(6) Can the model be easily modified to accommodate an accident whose release/dispersion characteristics are different from the range of characteristics that the model was developed for? (Is the model modular in structure?)	10	10	10	7.5	5	5	5	2
(7) Can the model output be easily compared with monitoring data to evaluate the accuracy of predictions? (This could include not only air-quality data, but also data from vegetation, soil, etc.)	10	10	6	6	5	5	5	5
(8) Can the model be used to calculate concentrations of UF ₆ and reaction products in the control room from releases in a UF ₆ -handling facility?	5	0	0	0	0	0	0	0
Total score	145	132	119	94.5	87	87	77	74

* Chlorine Institute methodology.

**Table 4.6 Summary of model score applicability
to post-accident analysis**

Model name	Total score	Rank
HGSYSTEM/UF ₆	132	1
SAIC	119	2
RTM-96	94.5	3
DEGADIS	87	4
SLAB	87	4
AFTOX	77	6
Chlorine Institute methodology	74	7

Table 4.7 Scores awarded to models for their applicability to site-specific factors

Criteria	Maximum score	HGSYSTEM/ UF ₆	SAIC	RTM-96	DEGADIS	SLAB	AFTOX	CIM*
(1) Ability to include environmental pathways analysis to evaluate health impacts to humans	30	15	25	25	10	10	10	10
(2) Ability to handle the presence of snow or rain either on the ground or actively falling	10	8	0	0	0	0	0	0
(3) Ability to model complex terrain	20	10	10	10	10	10	10	10
(4) Ability to simulate long-term effects of deposition on agricultural areas	20	10	10	10	10	10	10	10
(5) Ability to model population effects (e.g., for densely populated urban areas)	10	3	10	0	0	0	0	2
(6) Ability to conduct a human or an ecological health impact assessment	10	0	10	8	0	0	0	2
Total score	100	46	65	53	30	30	30	34

* Chlorine Institute methodology.

**Table 4.8 Summary of model scores applicability
to site-specific factors**

Model name	Total score	Rank
SAIC	65	1
RTM-96	53	2
HGSYSTEM/UF ₆	46	3
DEGADIS	30	7
SLAB	30	7
AFTOX	30	7
Chlorine Institute methodology	34	4

5 USER INTERFACE AND MODEL QUALITY ASSURANCE AND QUALITY CONTROL EVALUATIONS

To a large extent, a model's usefulness depends on the clarity of its documentation, ease of preparation of input parameters, and ease of understanding of the output presentation. The documentation QA/QC issues increases the credibility of the model and ensures that the model has been well-tested. A number of criteria were developed (Nair, *et al.*, 1997) to evaluate the user interface and QA/QC issues associated with UF_6 release and dispersion models. These criteria and the associated maximum scores are included in Tables 5.1 and 5.3. The processes used to conduct the evaluation are described in the following sections.

5.1 User Interface

Criterion 1. *Clear documentation.*

Clarity of documentation is the key to providing a clear understanding of the theoretical foundations of a model and its usage. The HGSYSTEM/ UF_6 model consists of three manuals [the User's Manual, (Post, 1994); technical documentation (Hanna, *et al.*, 1994a); and documentation specific to UF_6 (Hanna, *et al.*, 1994b)]. The first two documents are extremely clear; however, they do not directly relate to UF_6 -specific releases, reactions, and transport. The third document is UF_6 -specific; however, it relies on the first two documents to provide the complete description of the model. The documentation for the HGSYSTEM/ UF_6

model could be rewritten with the purpose of providing a clear description of all aspects of modeling a UF_6 release into the atmosphere. Exhaustive model documentation of the theoretical foundations is also provided. To completely understand the model, the user has to go back and forth several times between the three documents. The HGSYSTEM/ UF_6 model was awarded 15 points out of the maximum 20.

In most areas, documentation for the SAIC model is very clear. However, estimations of the initial plume size, the initial chemistry of the plume, and air entrainment for the analysis of continuous releases of UF_6 are not explicitly provided -- the analysis is intended to be carried out by the user. The SAIC model was awarded 19 points.

The RTM-96 model is an easily understood, screening-level hand-calculation method. However, its defensibility in terms of providing an upper-bound estimate of health impact is not substantiated in the model documentation. The documentation of the model refers the reader to NRC (1988) to provide the basis for the conservatism structured into the model. However, NRC (1988) does not provide a sound rationale to support the claim to the built-in conservatism of the RTM-96 model. Likewise, the numerous assumptions made regarding the release fractions of uranium and HF and in the treatment of transport (as a neutrally buoyant plume) are not very well defended. The RTM-96 model was awarded 15 points because it is a screening-level model.

The DEGADIS and AFTOX models were awarded 12 points each for providing clear documentation but not being suitable for

UF₆-specific analysis. Documentation for the SLAB model is very poor in quality. The SLAB model was awarded 10 points. Documentation for the Chlorine Institute methodology is extremely brief and does not provide all of the equations used to model the release and transport. It was also a screening-level approach. Therefore, the Chlorine Institute methodology was awarded 7 points, more than what it would have been awarded if it were intended to be a detailed model.

Criterion 2. Complete documentation.

Ten items were identified in the checklist presented in Nair, *et al.* (1997) to determine the completeness of model documentation. These are as follows: (a) statement of the model objective; (b) theoretical basis for all approaches and assumptions; (c) assumptions made; (d) limitations of application; (e) modeling approach; (f) instructions for preparing an input file; (g) example problem; (h) presentation of output format; (i) presentation of verification study; and (j) presentation of validation study. If a model provided adequate documentation for an item, it was awarded 2 points. Inadequate documentation resulted in a model awarded of 0 to 2 points for the item under consideration.

The documentation for the HGSYSTEM/UF₆ model did not provide a complete set of example problems for UF₆ releases. However, it provided another set of example problems without documentation in the disks sent with the code. The problems presented in the model documentation were not accompanied by sample input files. For these reasons, for the item (g), "example problem," the HGSYSTEM/UF₆ model was

awarded 1 point. Similarly, the item (d), "limitations of application," was not clearly presented, although the document addresses the limitations over the three documents in various places. The model was awarded 1 point for item (d). The model was awarded 2 points each for all other items. The HGSYSTEM/UF₆ model was awarded a total of 18 points for completeness.

The SAIC model was awarded 19 points, based on similar considerations as for the HGSYSTEM/UF₆ model. Sample input files did not reflect the example problem discussed in the documentation. However, sample input files were provided both in disks and in the documentation. Model limitations were not clearly described for UF₆-specific applications. However, selection of a particular code (SAPLUME, SACRUNCH, and SADENZ) within SAIC for a given application was much easier for the SAIC model than for the HGSYSTEM/UF₆ model. The SAIC model was awarded 1.5 points for items (d) and (g). It was awarded the full 2 points for all other items.

The RTM-96 model does not provide any documentation for the theoretical approach used in the model. The model presents the assumptions made in its mathematical formulations without any accompanying theoretical basis. It refers the reader to NRC (1988) for the theoretical basis of the model. However, NRC (1988) does not provide any conclusive rationale to establish that the model will yield a conservative set of predictions irrespective of the conditions of release and dispersion. The model was awarded 1 point for item (b) for providing partial documentation. For item (d), "limitations of application," the model was awarded 1 point for not identifying any

limitation, but for being capable of modeling most ground-level releases at a screening level. The model does not provide any documentation of example problems. However, it provides a step-by-step calculation approach where the user can fill in the blanks provided by the model and obtain the required result. Accordingly, the model was awarded 1 point for item (g). The model does not provide any verification or validation documentation, and therefore was awarded 0 points each for items (i) and (j). The RTM-96 model was awarded 2 points each for all other items, for a total of 13 points.

The DEGADIS, SLAB, and AFTOX models and the Chlorine Institute methodology are limited in their applicability to UF_6 , as described in the evaluations in previous sections. Therefore, the drawbacks of these models with respect to completeness of documentation are not discussed here in detail. DEGADIS and SLAB models were awarded 16 points each. The AFTOX model was awarded 12 points, and the Chlorine Institute methodology was awarded 2 points.

Criterion 3. *Correctness of documentation.*

Simulations were conducted only for the HGSYSTEM/ UF_6 , SAIC, and RTM-96 models. Therefore, a full in-depth test of correctness of documentation could be carried out only for these three models. Part of the subjective scoring involved the presentation of the theoretical bases for using specific approaches and algorithms, and the clarity of presentation. The HGSYSTEM/ UF_6 model was awarded 9 points out of 10; the RTM-96 model was

awarded 8 points; the DEGADIS and SLAB models were awarded 7 points each; the AFTOX model was awarded 10 points; and the Chlorine Institute methodology was awarded 5 points.

The methodology presented in the SAIC model to estimate the health effects from HF exposure is erroneous. The model estimates the health hazards from HF from the output UF_6 concentrations instead of actual HF concentrations. As discussed in Section 3.2.1, the output UF_6 concentration represents all of the UF_6 released at the source without accounting for the reaction of UF_6 with atmospheric moisture. Therefore, the output UF_6 concentration can be used to calculate the total uranium, but it cannot be used to estimate HF concentration and the hazard level from HF except when all of UF_6 has been converted to UO_2F_2 and HF within the plume (see Section 3.2.1 for a full explanation). The model documentation states clearly that UF_6 concentration is output by the model; however, it does not caution the reader that the UF_6 concentration represents UF_6 as if it did not enter into any reaction.

The SACRUNCH and SAPLUME modules within the SAIC model use an averaging time for the calculation of time-averaged concentration of a contaminant in the plume. In the SAIC documentation, the averaging time is defined as the plume passage time in one place and as release duration in the model input descriptions. The reader should be aware that the SAIC model does incorporate the effect of time-averaging for a continuous, steady state, buoyant plume through the release-duration parameter. The release duration is not used for anything else by the model. These erroneous descriptions

of averaging time should be corrected in the model documentation. Potential for erroneous use cannot be ruled out if the user is not aware of this mistake in the model documentation. The SAIC model was awarded 5 points.

Criterion 4. Computer Use.

All of the models requiring the use of a computer could be run on an IBM-PC or equivalent. They were each awarded the full 10 points. The RTM-96 model and Chlorine Institute methodology do not require the use of a computer. They were also awarded 10 points, even though the criterion is not directly applicable to them. The run time for the HGSYSTEM/UF₆ model is longer than the SAIC model, although both run reasonably fast on a 486-PC. The HGSYSTEM/UF₆ model runs very slowly on a 386-PC.

Criterion 5. Model input scheme and input-stream preparation.

Only the HGSYSTEM/UF₆, SAIC, and RTM-96 models were used for simulation testing. Therefore, their evaluations are addressed in greater detail than those for the other models, for which the model documentation was relied on to derive the conclusions regarding model input scheme and input preparation. Further discussions are provided in Section 3.3 for the problems that were encountered during the preparation of input files for the simulations that were performed using the models.

Both the HGSYSTEM/UF₆ and SAIC models provide very clear documentation of the input scheme. The documentation of the input scheme of the HGSYSTEM/UF₆

model could be significantly improved by providing the UF₆-specific input scheme in a single document. Currently, the documentation of the input scheme for simulating releases of dense gases is presented in the generic user's manual, and the UF₆-specific documentation is provided in Hanna, *et al.* (1994a).

Preparation of input streams or input data sets for these models is quite straightforward. However, there may be certain accidents for which, unless some *a priori*, external analysis is carried out, certain parameters may not be easy to quantify. For the HGSYSTEM/UF₆ model, such parameters would include the release rate and fractions in various phases. For the SAIC model, such parameters include the release rate, fractions in various phases, initial quantity of air entrained into the plume, and the distance from the source that the plume has traveled at which point the initial condition of the dispersion model is applicable. Both models provide sample files on disk that can be easily edited for new runs. Clear guidelines for the preparation of other supporting files for the HGSYSTEM/UF₆ model are also provided in the user's manual. However, very little guidance is provided for either model regarding the choice of parameter values when sufficient data do not exist. It would be extremely useful to provide such default information for all major UF₆-related accident scenarios, as discussed in Nair, *et al.* (1997).

In the HGSYSTEM/UF₆ model, the selection of a particular code (e.g., AEROPLOUME, HEGABOX, HEGADAS, or PGPLUME) for a particular application is primarily the user's choice, even though

some guidelines are provided within the documents. Transition from one module to another is not automatic as in the SAIC model, even though a relevant input file for the next module is automatically prepared whenever a transition is warranted. The input file to the next module had to be modified by the user before the transition could be made. This is rather cumbersome and could be easily avoided by accommodating a few programming modifications in the modules. The HGSYSTEM/UF₆ model was awarded 40 points out of 50, and the SAIC model was awarded 45 points.

The RTM-96 model is a hand-calculation, not requiring any input file preparation. Therefore, the criterion is not directly relevant. However, the hand-calculations can be conducted for any UF₆ release with the directions provided in the documentation. The model was awarded 45 points because very little justification is provided for the approach presented in the documentation.

The DEGADIS model was awarded 25 points, the SLAB model was awarded 30 points, and the AFTOX model was awarded 35 points. None of these models could be directly applied to UF₆. The Chlorine Institute methodology is a graphical procedure that can be used quite easily. However, it cannot be directly used for UF₆, and it provides very little justification for the implemented theoretical approach. The Chlorine Institute methodology was awarded 25 points.

Criterion 6. *Model simulation.*

Both the HGSYSTEM/UF₆ and SAIC models were easy to run. The HGSYSTEM/UF₆ model provided adequate rationale whenever unexpected terminations occurred, and it provided useful indications to successfully conduct a model simulation. The only problem identified in the runs performed for this study was when an input file was generated by one module to be used by the next module (*e.g.*, AEROPLUME followed by PGPLUME). The user had to change a few parameter values before the simulation could be correctly carried out. The HGSYSTEM/UF₆ model was awarded 15 points out of 20. For the simulations performed in this study, problems were experienced with the SAIC modules hanging up or ending calculations erroneously and not providing error messages. The SAIC model was also awarded 10 points.

The RTM-96 model does not represent a computer simulation. However, the hand calculations using the documentation were easily performed. Automating the model, however, would make it more useful and easier to use. The RTM-96 model was awarded 15 points.

No simulations were conducted using the DEGADIS, SLAB, and AFTOX models or the Chlorine Institute methodology. They were each awarded the minimum 10 points, as none of them could be readily used for modeling a UF₆ release.

Criterion 7. Model output scheme.

Outputs of the HGSYSTEM/UF₆ model were very clearly presented. They provided the concentrations of all reactants and products generated during the UF₆ release and transport. The model also provided post-processors for plotting the data. However, these were not tested. The model was awarded 18 points out of 20. The SAIC system provided outputs primarily for total uranium (see Section 3.2.1 for a full explanation of how the output concentration of UF₆ by the SAIC model is a surrogate for total uranium concentration). Although the outputs were clear, the concentrations of individual species (UF₆, HF, and UO₂F₂) were not provided. However, the model does calculate those concentrations internally. The output stream of the SAIC model should be modified to present the concentrations of all individual species in air. It also provided an estimate of the area within which the health impacts to individuals or populations could exceed certain regulatory standards. The post-processors provided with SAIC were not tested. The SAIC model was awarded 15 points.

The RTM-96 model was awarded 12 points (close to the minimum of 10 points) because no post-processing software existed. It is also cumbersome and time-consuming to generate a sufficient amount of output data from the model by hand-calculation, to prepare maps representing contours of air concentrations.

Because no simulations were conducted with the DEGADIS, SLAB, and AFTOX models and the Chlorine Institute methodology, and as they were not suitable for UF₆-specific

application as determined in the evaluations conducted in the previous sections, they were all awarded the minimum 10 points each.

5.2 Model Quality Assurance and Quality Control**Criterion 1. Presence of**

1. *Theoretical manual,*
2. *User's manual,*
3. *Example problem,*
4. *Documentation of model verification, and*
5. *Documentation of model testing using field data (validation).*

The HGSYSTEM/UF₆ was awarded 10 points each for items 1 and 2. It was awarded 5 points for item 3 for providing partial documentation of example problems as discussed in Section 2.3.1 under Criterion 2. It was awarded 0 points for item 4 for not providing model verification documentation. It was awarded 5 points for item 5 for providing incomplete documentation of model validation studies.

The SAIC model was awarded 10 points each for items 1 and 2. It was awarded 7.5 points for item 3 for providing more detailed representation of sample problems than the HGSYSTEM/UF₆ model. It was awarded 0 points for item 4 and 5 points for item 5 for incomplete documentation of the model validation studies.

The RTM-96 model was awarded 0 points for item 1 and 10 points for item 2. Because the instructions for model usage were extremely clear for the hand-calculation procedure, the model was awarded 5 points for item 3 even though an explicit example

problem was not provided. It was awarded 0 points for items 4 and 5.

The DEGADIS, SLAB, and AFTOX models were awarded 10 points each for items 1, 2, and 3, and 0 points for item 4 and 5. The Chlorine Institute methodology was awarded 7.5 points for item 1 for incomplete description of the theoretical approach. It was awarded 10 points each for items 2 and 3, and 0 points for items 4 and 5.

5.3 Results of the User Interface and Quality Assurance and Quality Control Evaluations

Tables 5.1 and 5.3 summarize the scores awarded for each criterion to each model for the evaluations of the user interface and quality assurance and quality control aspects of each model, respectively. Tables 5.2 and 5.4 summarize the total scores awarded to each model for the two aspects.

Table 5.1 Scores awarded to models on their user interfaces

Criterion	Maximum score	HGSYSTEM/UF ₆	SAIC	RTM-96	DEGADIS	SLAB	AFTOX	CIM*
(1) Clear documentation	20	15	19	15	12	10	12	7
(2) Complete documentation	20	18	19	13	16	16	12	2
(3) Correctness of documentation	10	9	5	8	7	7	10	5
(4) Computer use	10	10	10	10	10	10	10	10
(5) Model input scheme and input-stream preparation	50	40	45	45	25	30	35	25
(6) Model simulation	20	15	10	15	10	10	10	10
(7) Model output scheme	20	18	15	12	10	10	10	10
Total score	150	125	123	118	90	93	99	69

* Chlorine Institute methodology.

Table 5.2 Summary of the evaluation of model user interfaces

Model name	Total score	Rank
HGSYSTEM/UF ₆	125	1
SAIC	123	2
RTM-96	118	3
AFTOX	99	4
SLAB	93	5
DEGADIS	90	6
Chlorine Institute methodology	69	7

Table 5.3 Scores awarded to models on their quality assurance and quality control documentation

Criterion	Maximum score	HGSYSTEM/UF ₆	SAIC	RTM-96	DEGADIS	SLAB	AFTOX	CIM*
(1) Theoretical manual	10	10	10	0	10	10	10	7.5
(2) User's manual	10	10	10	10	10	10	10	10
(3) Example problem	10	5	7.5	5	10	10	10	10
(4) Documentation of model verification	10	0	0	0	0	0	0	0
(5) Documentation of model testing using field data (validation)	10	5	5	0	0	0	0	0
Total score	50	30	32.5	15	30	30	30	27.5

* Chlorine Institute methodology.

Table 5.4 **Summary of the evaluation of
model quality assurance and
quality control documentation**

Model name	Total score	Rank
SAIC	32.5	1
HGSYSTEM/UF ₆	30	2
DEGADIS	30	2
SLAB	30	2
AFTOX	30	2
Chlorine Institute methodology	27.5	6
RTM-96	15	7

6 RESULTS, RECOMMENDATIONS, AND CONCLUSIONS

6.1 Summary of Results

Table 6.1 presents a summary of the results from all of the evaluations conducted in the previous sections. Overall the HGSYSTEM/UF₆ model scored the highest, followed by the SAIC and RTM-96 models. The HGSYSTEM/UF₆ and SAIC models possess the maximum process-level details among the models tested for evaluating impacts from a UF₆ release. Relevant sections of this document identify specific actions that could be taken to improve each model. The developers of any model evaluated in this study can also use Table 6.1 to find areas in which potential improvements were identified in the course of this study.

Table 6.1 does not include the results of the performance evaluation of models presented in Section 3. In Section 6.2, a few recommendations are made for improvement of the HGSYSTEM/UF₆, SAIC, and RTM-96 models. In Section 6.3, overall conclusions from this study are summarized.

6.2 Recommendations

Major recommendations for future model improvements and use at fuel-cycle facilities are made only for the HGSYSTEM/UF₆, SAIC, and RTM-96 models because these are the only models that specifically address UF₆-specific issues.

The scoring tables and explanations of awarded scores presented in Sections 2

through 5 can be used by the developers of the HGSYSTEM/UF₆, SAIC, and RTM-96 models to identify areas in which the models can be improved. Some key areas of model improvement are discussed below.

- (1) *Treatment of Source Term.* The major emphasis of the models reviewed is on the dispersion computation, which minimizes the importance of the source-term computation. The treatment of source term could be improved in all of the models. Currently, the user cannot run the models without estimating the release rates externally. The HGSYSTEM/UF₆ model provides source-term estimation capabilities for the case of a pressurized release from a liquid-filled UF₆ cylinder. However, none of the three models evaluated performs the source-term calculations internally for all of the release types identified in Nair, *et al.* (1997). A primary reason for this deficiency could be that the models were developed primarily for the simulation of dispersion for different types of releases. However, if this additional capability is provided in the HGSYSTEM/UF₆ and SAIC models, or alternatively if proper guidance is provided with adequate documentation in the user's manuals, a model user at a fuel-cycle facility can easily perform the simulations using both HGSYSTEM/UF₆ and SAIC models. Since RTM-96 is a screening-level methodology developed on the basis of total quantity and duration of uranium release, only relatively simple guidance on source description is required.

Addition or improvement of source-term capabilities is particularly critical for integrated safety analysis and emergency response planning. For both these situations, *a priori* knowledge of the release rates and durations of release is not readily available. A variety of source terms can be developed for a postulated scenario by varying the operating conditions within the plant or storage conditions within a cylinder. Nair, *et al.* (1997) present a list of possible release scenarios. If source-term modules are developed for each of these scenarios and if default recommendations are made with respect to choice of parameter values in the absence of specific information from the facility, a model user at a fuel-cycle facility can easily perform the source term and dispersion calculations, evaluate the safety of the facility, and adequately plan for an emergency. The models should also provide the estimated values of the source term as outputs from the source-term modules. This would allow independent verifications of the source term and dispersion modules.

- (2) *Uncertainty Analysis.* Capabilities for conducting uncertainty analysis should be incorporated as an essential feature within each model. This would allow the model user to express his or her state of knowledge (or lack thereof) regarding an input parameter in terms of a range of likely values, with the associated probabilities of the occurrences of the values within the range. The model can then propagate the uncertainties about the input

parameters through every segment of the model to the final predicted concentration in air at a desired location. This will allow the true but unknown concentration to be bounded within a 95 percent subjective confidence interval of the predicted concentration. Results of the uncertainty analysis conducted in a Monte Carlo framework could also be used to meet the requirements of a sensitivity analysis.

The HGSYSTEM/UF₆ and SAIC models are already fairly complex, and it is recognized that embedding these models in a Monte Carlo framework of uncertainty analysis is not a trivial exercise. Nonetheless, further consideration must be given to this aspect with a view to developing appropriate models or to developing appropriate alternatives for performing uncertainty analysis.

- (3) *Estimates of Exposure.* Current regulations of the radiological effects of exposure to uranium are given in terms of the doses to the exposed individual. Toxic effects from chemical exposures to uranium are given in terms of the intake of uranium. It would be useful, therefore, for the HGSYSTEM/UF₆ and SAIC models to include the capabilities of estimating doses and intakes that can be directly compared with regulatory criteria. The RTM-96 model provides this capability.
- (4) *Justification for Conservatism Claimed in the Model Documentation for the RTM-96 Model.* Model documentation for the RTM-96 model (NRC, 1996)

and NRC (1988) do not provide any justification or rationale that can support the position that the RTM-96 model provides a conservative estimate of the desired endpoint. Results of the model testing exercise conducted in this study support the position that the RTM-96 model provides a conservative estimate of the desired endpoint, particularly at greater distances from the source. However, at distances less than 400 m, the model provided nonconservative estimates for the three Bordeaux releases, and conservative estimate for the Gore, Oklahoma, release.

Based on the conversations that the *SENES* team had with staff, it was learned the RTM-96 model was intended only for distances greater than a quarter mile or outside the site boundary. Currently, there is no cautionary note provided in the model documentation (NRC, 1996) that the methodology is not suitable for distances less than 400 m. Furthermore, the documentation provides specific reasons as to why, because of certain factors such as presence of buildings, certain specific values have been recommended for the dilution factor. If the methodology is not recommended for distances less than 400 m, it should be clearly stated in the model documentation, and the documentation should recommend that the methodology be only used for health estimates beyond 400 m.

The dispersion calculation in the RTM-96 model are based on a Gaussian plume approach. As a result

of an earlier review of dense-gas models for possible application to UF_6 (Lewellen and Sykes, 1992), the HGSYSTEM model was modified to include UF_6 -specific physical and chemical mechanisms, release scenarios, and user interfaces. If the chemistry and thermodynamics were not important during the transport of UF_6 in the atmosphere, a Gaussian plume model would have been sufficient. A Gaussian dispersion model can also be adequate if one were to start the model application at a downwind location where the plume has just become passive or where all reactions have been completed.

A reactive UF_6 plume can hover on the ground during the initial phase of the transport after release. It converts to a passive plume only after some time, depending on the quantity of UF_6 in the plume and the prevailing atmospheric conditions. It is not clear how a vertically and laterally expanding Gaussian plume can conservatively mimic a ground-hovering plume with vertical contraction and lateral expansion. Authors of the RTM-96 model need to clarify this issue using the dynamics of plume development and the chemistry and thermodynamics of UF_6 .

As stated earlier, the results of model tests conducted in this study with the RTM-96 model clearly indicate that the model consistently provides conservative estimates at distances greater than 400 m from the source. Because of the reservations expressed in the preceding paragraphs, however,

a generalized statement that the RTM-96 model will consistently provide conservative estimates at greater distances from the source cannot be made. However, the model does offer a useful screening-level tool for the estimation of total uranium and HF concentrations at greater than 400 m from the source.

- (5) *Outputs from the SAIC Model.* The SAIC model predicts only the total uranium concentrations in air. (It outputs UF_6 concentrations as if the UF_6 has not undergone any chemical reaction.) The concentrations of individual species (UF_6 , HF, and UO_2F_2) are important if a complete health impact assessment is to be carried out. For the assessment of HF toxicity, the required HF concentration cannot be calculated from the output concentration of total uranium, except when the UF_6 reaction is complete (see Section 3.2.1 for a full discussion of SAIC model outputs). The SAIC model should be modified so that concentrations of all relevant constituents of the plume are output by the model.

The SAIC model internally calculates the concentrations of all species associated with the UF_6 release during every stage of the plume development by accounting for the relevant reactions and thermodynamics, and a relatively simple modification to the code can ensure that these concentrations are printed to the output file. Therefore, the SAIC model was not severely penalized in this study for not

providing the concentrations of individual species in its output file. It is strongly recommended that the SAIC model should be modified as suggested here.

- (6) *Building Effects and Wet and Dry Deposition in the SAIC Model.* Effects of the presence of buildings on the concentrations of UF_6 and its reaction as, for example, done by the HGSYSTEM/ UF_6 model, should also be included in the SAIC model. These effects include concentration patterns on building faces because of vent releases, lateral confinement in building canyons, and downwash into building wakes, as presented in response to Criterion 5 of the dispersion component evaluation in Section 2.2. Effects of dry and wet deposition should also be included in the SAIC model.
- (7) *Plume Depletion from Deposition.* The HGSYSTEM/ UF_6 model provides the capabilities to calculate wet- and dry-deposition rates. However, it does not account for the depletion of UF_6 and the products of its reactions from the plume because of deposition processes. For a ground-hugging or slumping plume, plume depletion could significantly reduce the severity of accidents at increasing distances from the source. Even though the approach in the HGSYSTEM/ UF_6 model is conservative, the degree of conservatism could be too severe, resulting in a severe overestimation of the potential hazard from an accident. Proper justification must be provided

in the model documentation if plume depletion is not accounted for in the calculation of air concentrations.

(8) *Unexpected Termination of Model Run.*

When certain air-to-UF₆ mixing ratios were used for the definition of the initial plume in the SAIC model, the model simulations terminated without explanation. Such terminations should be systematically identified and eliminated from both HGSYSTEM/UF₆ and SAIC models. Any constraints on input values should be explained in the model documentations.

(9) *UF₆-Specific Models.* The models are applicable to many contaminants (other than just UF₆), which make the model documentation cumbersome and difficult to use. It may be worthwhile to make these models UF₆-specific. Source term modules specific to UF₆ can then be more easily incorporated into the models.

(10) *Total Uranium Concentration from the RTM-96 Model.* The RTM-96 model estimates the intake of total uranium by the inhalation pathway. The total uranium concentration in air can be back-calculated using the duration of release and the breathing rate. It would be useful to include this step as part of the model so that the user can directly obtain the total uranium concentration in air.

6.3 Conclusions

A model selected to support integrated safety analysis, post-accident analysis, and emergency response planning must be able to provide reliable estimates of total uranium and HF concentrations that do not substantially over- or underestimate the actual concentrations resulting from an accidental release of UF₆ at a nuclear fuel-cycle facility. Results of the qualitative and quantitative analyses conducted in this study indicate that three models, HGSYSTEM/UF₆, SAIC, and RTM-96 have the capabilities and potential to be used to support these analyses at a nuclear fuel-cycle facility. Performances of these models with respect to the requirements of the analyses can be summarized as follows, based on the quantitative analysis conducted in this study:

- The HGSYSTEM/UF₆ model is capable of providing predictions, of total uranium, that underestimate the measured concentrations by a factor of 2, and overestimate them by, at the most, an order of magnitude.
- The SAIC model is capable of providing predictions of total uranium concentrations that over- and underestimate the measured concentrations by an order of magnitude.
- The RTM-96 model is capable of providing predictions of total uranium concentrations beyond 400 m that do not underestimate the measured concentrations. Within 400 m, the model provides predictions that underestimate

the measured concentrations by over an order of magnitude.

Documentation for the RTM-96 model does not present the theoretical bases for the approach and assumptions used in the model. Therefore, more tests with data from field experiments or accidents should be conducted with the model to ensure that it will continue to provide conservative estimates at distances of over 400 m.

It should be noted that the applications of these models at another site may not produce similar performances because of a variety of reasons, including differences in modelers' capabilities and experience affecting the choices of input parameters and availability of accurate meteorological data. Depending on the maximum levels of over- and underpredictions of the downwind concentrations of total uranium or HF that are determined to be acceptable, a user can use the above-mentioned performance characteristics to select an appropriate model to support an integrated safety

analysis, a post-accident analysis, or an emergency planning at a nuclear fuel-cycle facility.

A full-scale uncertainty analysis in a Monte Carlo framework should be conducted on the models to evaluate the sensitivity of the output concentration of total uranium to simultaneous variations of all input parameters. To conduct this multi-parameter sensitivity analysis, each module from the HGSYSTEM/UF₆ and SAIC models must be modified to include uncertainty analysis capabilities. Efforts in support of such modifications could include development of an uncertainty analysis driver code for each module, development of probability density functions for all uncertain variables, identification of important dependencies among model variables, and development of post-processing codes to permit statistical analysis of the results. This will allow for a more robust analysis to be performed on the models, to identify the model components and parameters that dominate the overall expression of uncertainty in the model predictions.

Table 6.1 Summary of the model evaluation results ^a

Model	Component evaluation		Applicability evaluation				User interface & QA/QC		Total score	Rank
	Source term	Dispersion	ISA ^b	ERP ^c	PAA ^d	SSF ^e	UI ^f	QA/QC		
HGSYSTEM/UF ₆	93.5	185	140	202	132	46	125	30	953.5	1
SAIC	88	155	133	178.5	119	65	123	32.5	894	2
RTM-96	73	73	94.5	145.5	94.5	53	118	15	666.5	3
DEGADIS	68	68.5	86	124	87	30	90	30	583.5	4
SLAB	67	67.5	86	114	87	30	93	30	574.5	5
AFTOX	67	40	75	102	77	30	99	30	520	6
CIM ^g	65	48.5	67	102	74	34	69	27.5	487	7
Maximum score	110	235	165	255	135	130	150	50	1230	

^a Note that these results do not include the results of the model testing simulations presented in Section 3. Section 6.1 provides a brief discussion on the implications of the results presented in this table.

^b Integrated safety analysis.

^c Emergency response planning.

^d Post-accident analysis.

^e Site-specific factors.

^f User interface.

^g Chlorine Institute methodology.

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APPENDIX A**Modeling Hints to Estimate Certain Input Parameters for UF₆ Releases****A.1 Introduction**

During the course of model testing, it became apparent that the modeler requires considerable judgment to set up an input file for every new application. To alleviate some of the difficulties in preparing the input streams, a discussion of three related features -- initial dilution (air entrainment); building wake effects; and distance to completion of uranium hexafluoride (UF₆) reaction with water, are provided in this appendix.

A.2 Air Entrainment

For the simulations conducted in this study with the HGSYSTEM/UF₆ and the SAIC models, most of the input parameters were taken from the Modelers Data Archive (MDA) (Hanna, *et al.*, 1991). A key important parameter is the initial vapor (pure-phase UF₆) to air-mixing ratio. This parameter is calculated internally in the HGSYSTEM/UF₆ model, and is required as an input for the SAIC model. However, guidance for estimating the amount of air initially entrained into the plume or the mixing ratio is not provided in the documentation for the SAIC model. Using Equation (2-16) from the model documentation for the SACRUNCH module of the SAIC model and other assumptions on cloud velocity, cloud dimension, cloud density, and Richardson number, the vapor-to-air-mixing ratio can be estimated to be

between 1:5 and 1:10 for continuous releases. Based on prior modeling experience and that gained during this study, a mixing ratio of 1:10 for continuous releases has provided reasonable agreement between model predictions and measurements. Therefore, a mixing ratio of 1:10 would appear to be reasonable in the absence of other site-specific information. However, derivation of this parameter from site-specific information would be the most preferred method to use.

For instantaneous releases, based on Equation (2-3) from the documentation for the SADENZ module of the SAIC model and assumptions on cloud velocity, cloud dimension, cloud density, and Richardson number, the vapor-to-air-mixing ratio can be estimated to be between 0.5 and 2. Based on prior modeling experience and that gained during this study, a mixing ratio of 1:2 for instantaneous releases has provided reasonable agreement between model predictions and observations. Therefore, a mixing ratio of 1:2 is recommended for any future modeling in the absence of other site-specific information. However, derivation of this parameter from site-specific information would be the most preferred method to use.

A.3 Building Wake

Another important parameter, not completely addressed in the documentation for the HGSYSTEM/UF₆ model (see Chapter 9.5 in HGSYSTEM Technical Reference Manual; Hanna, *et al.*, 1994), and not addressed in the documentation for the SAIC model, is the influence of building wake on initial dispersion. For releases influenced by large structures, building wake effects can be important. This parameter

can be addressed by modifying the source size to reflect building dimensions for obtaining predictions at receptor locations closer than 10 building dimensions. Based on the results of Gore Oklahoma modeling, presented in Section 3.2.3.2, for farther distances, the normal source size should be used. The HGSYSTEM Technical Reference Manual (Hanna, *et al.*, 1994) suggests replacement of the existing building wake algorithm with the Environmental Protection Agency's (EPA) downwash algorithm for the far wake as implemented in the Industrial Source Complex (ISC) model (U.S. EPA, 1995). For details, the reader is referred to the ISC documentation.

A.4 Distance to Complete UF_6 Reaction

A.4.1 Introduction

On release to the atmosphere, UF_6 reacts vigorously with water that may be present in the atmosphere (or on the ground). This hydrolysis reaction is strongly exothermic, and can exert a strong influence on the behavior of the UF_6 cloud or plume. Moreover, the degree of completion of this reaction is an important factor in determining the transition from special air-dispersion models (*e.g.*, dense-gas models with chemistry) to more conventional models of atmospheric dispersion (*e.g.*, Gaussian puff or Gaussian plume).

These notes outline a simple analytical (approximation) approach to assess the downwind distance from the point of release that is required for the complete conversion of UF_6 to the hydrolysis products uranyl fluoride (UO_2F_2) and hydrogen fluoride (HF)

for both short-term (puff) and continuous releases. The distance to complete conversion can be converted to travel time by dividing the distance by the average windspeed. Two approaches are considered for puff releases. A simple analysis for a continuous release of UF_6 is also provided. Nomograms for estimating the downwind distance for complete conversion, dependent on atmospheric temperature and relative humidity, are provided.

A.4.2 Approximate Approaches for Puff Release

Basic Assumptions:

- Release occurs near ground level.
- Release occurs as a puff.
- Dispersion coefficients are based on Schulze (1991) and Slade (1968).
- Heat generation by the UF_6 hydrolysis reaction is neglected.
- Volume change caused by the UF_6 hydrolysis reaction is neglected.
- $\sigma_y(x)$ relationships are used for extrapolating dispersion parameter data to short distances ($x < 100$ m).
- $\sigma_x(x) = \sigma_y(x)$ (x = distance in the wind direction).

Approach 1

This approach is based on following UF_6 concentration at the center of the puff as a function of distance; (*i.e.*, the puff is followed until even the maximum

concentration inside the puff is fully converted to HF by the air humidity). Thus, the approach assumes that the UF_6 at the periphery of the puff is more likely to be consumed by water vapor than UF_6 in the center, where the UF_6 concentration is relatively higher. An approach that assumes that the UF_6 is uniformly dispersed within the puff is discussed in Approach 2.

The calculation of the UF_6 reaction distance is performed by calculating the distance at which the maximum puff concentrations become equal to the water concentration (in air) that is required for a full conversion (Slade, 1968):

$$C(x=ut, y=0, z=0) = 2Q / \{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z\} = \{RH \times AH_s / 0.1023\} = f \quad (2.1)$$

where:

Q	=	total amount of UF_6 released (kg);
RH	=	relative humidity (fraction);
AH_s	=	absolute humidity at saturation (kg water/ m^3 air) from the Antoine equation (Himmelbleu, 1984);
f	=	number of kg of UF_6 that will react with 1 m^3 of air, with given RH and AH_s , $(2\pi)^{3/2} = 15.75$;
σ	=	dispersion coefficient (m),
u	=	wind velocity (m s^{-1}), and
t	=	time (s).

Approach 2

This approach is simpler and perhaps less realistic. It assumes that there is a uniform concentration of UF_6 in the puff. For a puff

release, it can be shown that 96.7 percent of the released UF_6 will be contained within a volume V where:

$$V = \text{volume of puff} = 4.3 \sigma_x \times 4.3 \sigma_y \times 2.15 \sigma_z \quad (2.2)$$

where:

Q	=	total amount of UF_6 released (kg),
f	=	number of kg of UF_6 that will react with 1 m^3 of air, with given RH and AH_s ,
RH	=	relative humidity (fraction), and
AH_s	=	absolute humidity at saturation (kg water/ m^3 air).

For this model, the volume of air needed for complete reaction is given by:

$$\{(4.3)^3 \sigma_x \sigma_y \sigma_z / 2\} = (Q/f) \quad (2.3)$$

and therefore

$$\{2Q / (4.3)^3 \sigma_x \sigma_y \sigma_z\} = f \quad (2.4)$$

A.4.3 Estimate of Dispersion Parameters

As mentioned above, the σ -values were based on $\sigma(x)$ data from Schulze (1991) as follows.

$$\begin{aligned} \sigma &= \sigma_x = \sigma_y = \sigma_z \\ \sigma &= ax^b \\ \log \sigma &= \log a + b \log x \end{aligned}$$

The values of fitted parameters a and b are presented in Table A.1.

Table A.1 Fitted parameters for the estimation of dispersion coefficients

Meteorological conditions	σ_z		σ_r	
	a	b	a	b
Unstable	85.6	0.74	80.0	0.89
Neutral	18.6	0.70	36.5*	0.89
Very stable	3.3	0.61	9.5	0.89

* These approximately fitted parameters are similar to the ones cited in Slade (1968), except for $a = 36.5$ for neutral conditions. For present purposes, these values are used; however, if a more accurate derivation is required, the accuracy of the dispersion coefficients will also have to be enhanced.

A.4.4 Sample Results for Puff Release

The two approaches described in Section A.4.2 were used to calculate approximate distance (m) to complete the hydrolysis reaction. Tables A.2, A.3, and A.4 present approximate values of the distance (m) to complete reaction for several typical sets of conditions.

Example (1)

$$\begin{aligned} T &= 10^\circ\text{C} \\ RH &= 50\% \\ AH_s &= 9.2 \times 10^{-3} \\ f &= 0.045 \text{ kg/m}^3 \end{aligned}$$

$$AH_s \times RH = 4.6 \times 10^{-3} \text{ kg/m}^3.$$

Table A.2 Distance (m) to complete reaction for Example 1

Q (kg)	Approach 1 (assume maximum concentration)			Approach 2 (assume uniform concentration)		
	Unstable	Neutral	Very stable	Unstable	Neutral	Very stable
1	<10	25	140	<10	15	70
10	20	60	370	10	35	190
100	50	165	1000	25	85	500
1000	120	420	2600	65	220	1300

Example (2)

$$\begin{aligned} T &= 20^\circ\text{C} \\ RH &= 60\% \\ AH_s &= 1.7 \times 10^{-2} \text{ kg/m}^3 \\ f &= 0.1 \text{ kg/m}^3 \end{aligned}$$

$$AH_s \times RH = 1.02 \times 10^{-2} \text{ kg/m}^3.$$

Table A.3 Distance (m) to complete reaction for Example 2

Q(kg)	Approach 1 (follow maximum concentration)			Approach 2 (assume uniform concentration)		
	Unstable	Neutral	Very stable	Unstable	Neutral	Very stable
1	<10	20	100	<10	<10	50
10	15	50	270	<10	25	140
100	35	120	700	20	60	360
1000	90	300	1800	50	160	950

Example (3)

T	=	30°C
RH	=	100%
AH _s	=	3 x 10 ⁻²
f	=	0.29 kg/m ³

$$RH \times AH_s = 3 \times 10^{-2} \text{ kg/m}^3.$$

Table A.4 Distance (m) to complete reaction for Example 3

Q (kg)	Approach 1 (follow maximum concentrations)			Approach 2 (assume uniform concentration)		
	Unstable	Neutral	Very stable	Unstable	Neutral	Very stable
1	<10	15	65	<10	<10	35
10	10	30	170	<10	15	90
100	25	80	440	15	40	230
1000	60	190	1150	30	100	600

The results of these sample calculations were extrapolated to other conditions (based on Approach 1), and the results are presented in a nomogram form in Figure A.1. For comparison purposes, these rather crude estimates can be compared to distances, to complete reaction calculated by the HGSYSTEM/UF₆ model. For example, considering a temperature of 20 °C, relative humidity of 60 percent, release of 1000 kg of UF₆, D stability, 5 m radius of the source,

and a wind speed of 5 m/s, the HEGADAS-T module estimates 300 to 400 m for UF₆ reaction to be completed. From Figure A.1, the required distance is 300 m.

A.4.5 Temperature Dependence

To relate the humidity scale to a temperature scale, the vapor pressure above water (i.e., absolute humidity) was derived as a function of temperature. The derivation is based on

the following thermodynamic equations:

$$H_2O(l) = H_2O(g), \quad \Delta G = \Delta H - T\Delta S$$

$$\Delta H(298) = -241.818 + 285.830 \text{ kJ/mol} = 44.012 \text{ kJ/mol}$$

$$\Delta S(298) = 188.825 - 69.91 \text{ J/K/mol} = 118.915 \text{ J/K/mol}$$

$$\Delta C_p(298) = 33.577 - 75.291 \text{ J/K/mol} = -41.71 \text{ J/K/mol} \quad (2.5)$$

$$P(\text{bar}) = \exp(-\Delta G/RT)$$

$$\ln P(\text{bar}) = -\Delta H/RT + \Delta S/R \sim -\Delta H(298)/RT + \Delta S(298)/R$$

The absolute humidity at saturation, AH_s (kg/m^3), can therefore be calculated (approximately) from Equation (2.5) using the ideal gas law,

$$PV = nRT \quad (2.7)$$

with

$AH_s = Mn/V = PM/RT$ = concentration of water vapor at saturation and
 M = molecular weight of water.

This approximation is valid for a small ΔT range (i.e., if $\Delta C_p = 0$).

Therefore:

$$\ln P(\text{bar}) = -5293.46/T + 14.302 \quad (2.6)$$

where T is the absolute temperature in degree Kelvin. This equation was tested against an engineering table (CRC Handbook, 1981). The results are in good agreement for the temperature-range of interest, as shown in Table A.5.

The resulting relationship of AH_s versus T is shown in Figure A.2. It is an almost (but not quite) linear function within the range of interest. The results of Figure A.2 were used to add a temperature axis to Figure A.1.

Table A.5 Comparison of the vapor pressure of water against values tabulated in CRC Handbook (1981)

T (°C)	ln(P(bar))	P(atm)	P(mm of water)	CRC Value P(mm of water)	Deviation, %
5	-4.7290	0.00872	6.627	6.543	1.29
10	-4.3929	0.01220	9.274	9.209	0.71
15	-4.0685	0.01688	12.828	12.788	0.32
20	-3.7552	0.02309	17.549	17.535	0.08
25	-3.4524	0.03126	23.755	23.756	-0.00
30	-3.1595	0.04189	31.837	31.824	0.04
35	-2.8762	0.05561	42.265	42.175	0.21

The temperature scale in Figure A.1 is for AH_8 (i.e., RH = 100 percent). Results for other RH values can be obtained by using the RH x AH_8 scale in the same figure.

A.4.6 Conclusions for Puff Release

(i) The UF_6 persistence distance is larger for:

- Larger releases
- Stable, lower for neutral, and still lower, for unstable meteorological conditions
- Lower humidity

as expected. The distance to complete reaction is "short" except for dry desert conditions and stable atmospheric conditions. Estimates derived by the approximations outlined in this appendix compare favorably with the more detailed results obtained with the HGSYSTEM/ UF_6 model.

(ii) The relationship log (distance) vs. log (water content) is approximately linear (see Figure A.1). This can

perhaps be used to derive "rules of thumb" for UF_6 modeling.

(iii) The distance calculated by Approach 2 (i.e., uniform mixing) is about half of the distance calculated by Approach 1. Comparisons with detailed models can be used to determine the validity of the approximations. Approach 1 is expected to provide more realistic estimates of the distance to completion. For a "rule-of-thumb" estimation, the curves in Figure A.1 can be used.

A.4.7 Continuous Release

Similar calculations can be performed for continuous releases. However, guidance can also be obtained from the HGSYSTEM/ UF_6 model. Table A.6 presents results from the HGSYSTEM/ UF_6 model. The model is run for four different releases and the same meteorological conditions: $T = 20^\circ\text{C}$, relative humidity 50 percent, stability D, and wind speed of 5 m/s. Based on Table A.6, the distance to complete UF_6 reaction can be determined for different releases as a first estimate.

Table A.6 Results of the HGSYSTEM/ UF_6 model for distance to complete UF_6 reaction^{a,b}

Release, kg/s	Distance, m
1	360-500
2.5	500-690
10	810-1100
100	1350-2500

^a $u = 5$ m/s; $T = 20^\circ\text{C}$; RH = 50 percent; and D = stability.

^b Corresponds to the Gore, Oklahoma, release.

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Figure A.1 Nomogram for distance to complete UF_6 hydrolysis for "Puff" release.

Figure A.2 Absolute humidity at saturation versus temperature.