Review of Models Used for Determining Consequences of UF₆ Release

Development of Model Evaluation Criteria

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ABSTRACT

The objective of this study is to examine the usefulness and effectiveness of currently existing models that simulate the release of uranium hexafluoride from UF_6 -handling facilities, subsequent reactions of UF_6 with atmospheric moisture, and the dispersion of UF_6 and reaction products in the atmosphere. The study evaluates screening-level and detailed public-domain models that were specifically developed for UF_6 and models that were originally developed for the treatment of dense gases but are applicable to UF_6 release, reaction, and dispersion. The model evaluation process is divided into three specific tasks: model-component evaluation; applicability evaluation; and user interface and quality assurance and quality control (QA/QC) evaluation. Within the model-component evaluation process, a model's treatments of source term, thermodynamics, and atmospheric dispersion are considered and model predictions are compared with actual observations. Within the applicability evaluation process, a model's applicability to Integrated Safety Analysis, Emergency Response Planning, and Post-Accident Analysis, and to site-specific considerations are assessed. Finally, within the user interface and QA/QC evaluation process, a model's user-friendliness, presence and clarity of documentation, ease of use, etc. are assessed, along with its handling of QA/QC. This document presents the complete methodology used in the evaluation process.

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EXECUTIVE SUMMARY

Accidental release of uranium hexafluoride (UF_6) from fuel cycle facilities continues to represent a potentially significant hazard at Nuclear Regulatory Commission-(NRC-) licensed fuel cycle facilities. Understanding the possible distribution of hazardous materials (uranium 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 to prevent such accidents and to mitigate their effects are adequate. Such an analysis of consequences is viewed as an essential part of an Integrated Safety Analysis (ISA). Also, emergency planning for responding to such accidents, i.e. Emergency Response Planning, (ERP) benefits from advance analysis of the likely paths of the released cloud or plume of these hazardous materials. In addition, in the event of an accidental release of UF_6 from an NRC-regulated facility, NRC may need to perform a Post-Accident Analysis (PAA). A PAA is conducted to evaluate both the severity of the accidental release and potential health impacts on the local population.

Each of these analyses requires the use of mathematical models. Mathematical models developed to evaluate impacts from an accidental release of UF_6 should be capable of adequately addressing both the source term and atmospheric dispersion components. Both source term and air dispersion analyses should take into account: (1) the physical and thermodynamic properties of UF_6 ; (2) the exothermic reactions that UF_6 undergoes with atmospheric moisture; (3) the physicochemical and transport properties of

the reaction products; and (4) the thermodynamic interactions of the plume containing UF_6 and its reaction products with the atmospheric boundary layer.

A number of source term and air dispersion models applicable to the ISA, Emergency Response Planning (ERP), and PAA are currently available, each with differing degrees of capabilities. This study examines the usefulness and effectiveness of currently existing models for the three different endpoints: ISA, ERP, and PAA. The study evaluates models that were specifically developed for UF_6 and those that were developed for the treatment of dense gases and are potentially applicable to UF_6 release, reaction, and dispersion. Both screening-level and detailed models are evaluated; however, only public-domain models are considered.

The model evaluation process is divided into three specific tasks: model-component evaluation; applicability evaluation; and user interface and quality assurance and quality control (QA/QC) evaluation. Within the component evaluation process, a model's treatment of source term, thermodynamics, and atmospheric dispersion is evaluated and model predictions are compared with actual observations. Within the applicability evaluation process, a model's applicability to ISA, ERP, and PAA, and a model's ability to accommodate certain site-specific considerations, are evaluated. Finally, within the user interface and QA/QC evaluation process, user-friendliness, presence and clarity of documentation, ease of use, etc., are evaluated, along with the handling of QA/QC issues (e.g., verification, validation, etc.).

This document presents the complete methodology used in the evaluation process, including both the characteristics and features evaluated, and the specific scoring and ranking techniques used to test the characteristics and features.

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1 STUDY OBJECTIVE

The accidental release of uranium hexafluoride (UF_6) represents a potentially significant hazard at Nuclear Regulatory Commission-(NRC-) licensed fuel cycle facilities. In fact, numerous releases of UF_6 have been reported from fuel cycle type facilities (NRC, 1988). The releases have caused at least three prompt fatalities and several injuries. The significant UF_6 releases have consistently been with UF_6 heated above its melting point ($65^\circ C$). The releases have been generally fairly rapid - lasting from a few minutes to about 45 minutes.

In January 1986, a UF_6 cylinder being heated in a steam chest at the Sequoyah Fuels Facility in Gore, Oklahoma, ruptured, leading to the release of about 14,240 kg (31,400 lbs) of UF_6 (NRC, 1986a; 1986b). The operator was killed in the incident.

It is important for NRC and its licensees to be well-prepared to assess the potential consequences arising from an accidental release of UF_6 .

The NRC request for proposal (RFP) to perform this study (NRC, 1995a), has identified three areas, within the NRC licensing process, that could benefit from the use of methods to assess the accidental release of UF_6 and the potential consequences to public health from such releases.

(1) Integrated Safety Analysis (ISA)

ISA is a systematic effort to identify process upsets or conditions at a facility that could lead to undesirable

consequences. According to draft NRC guidance for ISA (NRC, 1995b),

"... the ISA is expected to form the basis of a safety program that requires adequate controls and systems to be in place to ensure the safe operation of the facility. . ."

The draft guidance further indicates that

The results of an ISA consist of the identification of potential accidents, the consequences of the accidents, and the controls (i.e. the structure, system, equipment, components and personnel) relied on to prevent the accident from occurring or to reduce their consequences.

The use of analytical models is one versatile approach for predicting the characteristics of a release, the concentration resulting from a release, and a (possible) means to assess mitigation measures. It is versatile in the sense that one can vary the initiating events and the potential accident scenarios to perform "what-if" calculations.

(2) Emergency Response Planning (ERP)

As stated in the NRC RFP, (NRC, 1995a):

A model capable of predicting the concentration of UF_6 and its reaction products in the vicinity of the facility will be useful in recommending suitable actions in response to a chemical emergency.

For example, analytical models could be helpful in recommending whether employees or members of the general public should be evacuated or whether they should be sheltered in place. In developing plans for responding to emergency situations, before their actual occurrence, licensees will need to evaluate the consequences of various release scenarios using atmospheric dispersion models. The results of these model runs would then be available for use (i.e., for making decisions regarding protective actions) if an actual chemical release were to occur.

(3) Post-Accident Analysis (PAA)

The NRC RFP states:

Following an actual accident, NRC and its licensees have a responsibility to investigate the causes, propagation, mitigation, and consequences of the accident. This information is important to understand in order to prevent similar accidents from happening in the future or to mitigate their consequences. The consequences are also important to assess because the public has a right to know the impact of such accidents. To assure that accurate information is provided to the public and to responsible public officials, analytic models may be used to estimate the concentrations of hazardous materials that the public has been exposed to. This will help health officials respond to any

acute and chronic health needs that result from such exposure.

Models provide a means to reconstruct impacts from an accident based on different levels of data and information gathered before and after the accident.

The specific objective of the present study is to examine the usefulness of various analytical models, developed for source term characterization and atmospheric dispersion, for assessing the (potential) consequences of an accidental release of UF_6 , recognizing the complex physico-chemical properties of UF_6 and the exothermic nature of its reactions with atmospheric water vapor.

Evaluation criteria are needed to provide the basis for comparing potentially applicable methods.

The purpose of this document is to identify important process-level features that must be simulated by the model and to establish evaluation criteria that can be used to assess the potentially applicable models. These process-level features are briefly described in the next section; subsequent sections discuss evaluation criteria.

2 BACKGROUND CONSIDERATIONS

The assessments of UF₆ releases and subsequent atmospheric dispersion from such releases are complicated by the complex thermodynamics of the UF₆ water system. For example, liquid UF₆ cannot (normally) exist at normal atmospheric pressure. As a result, the release of a large quantity of liquid UF₆ can be expected to convert quickly after release to UF₆ vapor and UF₆ solid. The UF₆ vapor will disperse as a vapor cloud, with possibly complex thermodynamic behaviour, and a portion of the solid UF₆ will deposit on the ground forming a secondary source of UF₆ vapor that can persist for some time. Some portion of the liquid UF₆ will flash instantaneously to vapor on release to the atmosphere.

Once released to the atmosphere, UF₆ vapor reacts with the moisture in the air to produce a dense white cloud containing solid uranyl fluoride (UO₂F₂) and hydrofluoric acid (HF) (Bouziqes, *et al.*, 1978), viz:

The hydrolysis reaction produces 0.23 gram (g) of HF and 0.88 g of UO₂F₂ for each gram of hydrolyzed UF₆. The exothermic nature of the hydrolysis reaction is important since the UF₆ vapor cloud can be positively, neutrally, or negatively buoyant, depending on the various combinations of cloud temperatures and concentrations (Just, 1986).

In general terms, the release and dispersion of UF₆ can be considered in three phases:

- (1) the release;
- (2) transition phase; and
- (3) atmospheric dispersion.

Factors influencing the release include the following:

- Type of release;
- Conditions of release (e.g., temperature, pressure, and rate of release);
- Source geometry and geometry of adjoining buildings or surface features;
- Potential mitigating engineered features (e.g., water sprays); and
- Weather conditions at the time of release.

Factors of interest during the transition phase from source-dominated to atmospheric-dispersion-dominated behaviour include the following:

- Cloud thermodynamics arising from UF₆/water interaction;
- Energy and mass transfer processes between the UF₆ cloud, atmosphere, and ground; and
- Turbulent structure of the vapor cloud.

Factors of interest to the atmospheric dispersion phase include the following:

- Turbulent structure of the atmosphere;
- Wind speed;
- Effects of structures and orography; and
- Changes in mean wind direction (for long-lasting releases).

Many dense gas dispersion models have potential application to UF₆ (Touma, *et al.*,

1995; Hanna, *et al.*, 1993). However, the thermodynamics of UF_6 are relatively complex and few existing models appear to have the ability to adequately address UF_6 dispersion. In their 1992 review of existing atmospheric dispersion models, Sykes and Lewellen examined a wide variety of models and selected the following five models for detailed consideration:

- PLM89A, a Martin Marietta UF_6 model (a successor to Just's model);
- TRIAD, a National Oceanic and Atmospheric Administration UF_6 model;
- HG SYSTEM, a dense gas model (includes module for HF chemistry);
- ADAM, a U.S. Air Force dense gas model; and
- SLAB, a dense gas model developed by Lawrence Livermore National Laboratory.

Sykes and Lewellen (1992) concluded that none of the models examined (even the five selected ones) fully satisfied all the requirements of a safety analysis model and suggested that all the currently existing models be improved with respect to the following:

- Turbulent atmospheric dispersion;
- Building and terrain effects; and
- Effects of exothermic chemical reaction.

These authors also describe a number of model features that they consider desirable for the assessment of UF_6 dispersion. The desirable model characteristics identified by Sykes and Lewellen (1992) were also

adopted for this assessment, as noted in the following chapters. Although Sykes and Lewellen are correct in saying that models would benefit from improvements in the areas noted above as well as in other areas, it is not necessarily true that such improvements would be required for all possible applications. For example, relatively simple workbook calculations of the type set out in NRC's "RTM-93, Response Technical Manual" (NUREG/BR-0150, Rev. 3) or the Chlorine Institute's Pamphlet 74 titled "Estimating the Area Affected by a Chlorine Release," Edition 2, 1991, may well be adequate for some of the applications. Moreover, the relative simplicity of these models and their modest data requirements suggest that such simple models should be considered, albeit carefully, for many of the possible applications.

The discussions of the models presented above provide an appropriate basis for the identification of essential and desirable model characteristics as described in the following sections. These theoretical and technical requirements should however be moderated by consideration of the needs of the intended application and various practical issues including, for example, whether or not a particular model is proprietary, whether it is publicly available, and what its demands on input data are. For these reasons, the evaluation criteria must not exclude the simple and easy-to-use Gaussian plume and workbook models, whenever the application of such models is appropriate. In this study, only public-domain models are considered for evaluation.

3 TASK 1(A): COMPONENT EVALUATION CRITERIA DEVELOPMENT

This subtask addresses three important aspects of a model that are used to determine the consequences from a UF_6 release -- source term, chemistry and thermodynamics, and atmospheric dispersion. Since chemistry and thermodynamics play important roles in both source term and atmospheric dispersion modeling, they are addressed within the criteria being developed for the source term and atmospheric dispersion aspects. For the purposes of model comparisons, the evaluation criteria are set out in the form of criteria matrices.

3.1 Source Term

Source term is one of the most critical inputs to an atmospheric dispersion model. In most cases, the uncertainty in the estimation of source term dominates the uncertainties from all other input parameters. Therefore, estimation of source term requires proper identification, characterization, and modeling of all important factors leading to its quantification. Source terms in most models are represented in terms of the strength (e.g., mass release rate) and duration of a release.

Numerous releases of UF_6 have occurred in the past from UF_6 -conversion and -enrichment plants. Defining a generalized source term for UF_6 release is complicated because UF_6 may be released as a vapor, a liquid, or a mixture of the two, and the release could occur from one of several locations in a fuel manufacturing facility. A source term model must contain adequate and correct information on the release,

subsequent phase changes, and chemical reactions that UF_6 undergoes before being released to the atmosphere. Major considerations in evaluating the source term component of a model are as follows.

- (1) A source term expression in a model should contain information on the phase (gas, liquid, or solid), duration, time-dependent behavior, and quantity (or flow rate and duration) of the release for the specific accident scenario.

Records of past accidents indicate that a majority of accidents resulted from human errors arising out of repetitive working patterns and from equipment failures. Most of these releases occurred during the transfer of UF_6 from one container to another. These accidents may be classified into the following four categories:

- A. Failure of valve/pigtail (liquid UF_6);
- B. Failure of valve/pigtail (UF_6 vapor);
- C. Rupture of cylinder filled with liquid UF_6 ; and
- D. Rupture of cylinder filled with solid UF_6 .

Source terms for A and B types of release can be expressed in terms of the size of valve that failed, pressure gradient, duration of release, etc. Source terms for C and D types of release can be expressed in terms of fractions of cylinder contents along with the duration and time-dependent behavior of release.

Failure of piping in fuel cycle facilities is also a common accident. However, UF_6

leaks from such pipes are not immediately detected and cannot be easily quantified because of the insulation surrounding the pipes. These failures are usually caused by damage from outside or material defects (*e.g.*, welding defects). UF_6 releases from failure of these pipes are bounded in severity by the pigtail failure categories A and B. The potential for releases from pipe failures caused by heat and associated volume expansion is generally covered by design reviews. To summarize, the severity of the accident is bounded by the pigtail failure.

Categories C and D have been developed to address all possible modes of release from a cylinder. Actual releases from categories C and D could be in the form a mixture of a solid, liquid, and vapor. These categories are also designed to address the special case of a cylinder engulfed in fire. For a cylinder filled with solid UF_6 , one of the following situations can arise when the cylinder is heated, depending on the mass of UF_6 in the cylinder, rate of heating, and the volume of the cylinder.

- A portion of solid UF_6 changes into liquid and increases in volume. When the liquid fills up the entire volume of the cylinder within an initially overfilled cylinder, any further melting of solid UF_6 results in an hydraulic rupture of the cylinder due to hoop stress. When this happens, the liquid UF_6 is released from the cylinder. The liquid immediately flashes into solid and vapor forms of UF_6 .
- All of the solid UF_6 is converted into liquid in a cylinder that is initially filled with a specified quantity of UF_6 . Further heating of the cylinder leads to partial vaporization of liquid UF_6 , increasing its vapor pressure within the cylinder. Further heating and vaporization lead to increasing pressure within the cylinder, followed by a hydraulic rupture. In the case of a cylinder being engulfed by fire, catastrophic failure of the cylinder can occur. In the case of an explosion, the entire cylinder content is released to the atmosphere at once, whereas in the case of a hydraulic rupture, the release occurs over a larger time-period. In both cases, vapor and liquid UF_6 are released into the atmosphere, and the liquid UF_6 immediately flashes to solid and vapor forms.
- UF_6 leaks from a valve or crack on the cylinder surface. Releases will be in vapor form and will continue as long as the internal pressure is greater than the ambient pressure. In addition, the internal pressure continues to rise because of the fire. Because of lack of moisture around the fire, the cracks do not automatically seal by UO_2F_2 formation as they do in other situations.

From the amount of heat available, the mass of liquid UF_6 in the cylinder, and the cylinder volume, the forms and quantities of the UF_6 released can be estimated for a liquid-filled cylinder.

- (2) A source term model should have the ability to handle phase changes and/or chemical reactions associated with the initial phase of the release.

Since UF_6 exists only in the solid or vapor phases under ambient conditions, any UF_6 that is released as a liquid would be immediately flashed into solid and vapor phases. If the release is in liquid phase, the source term model should be able to estimate the relative rates and masses of solid and vapor forms generated.

Release of UF_6 from a processing plant is more complicated. Most processes associated with gaseous UF_6 are conducted under negative pressure, to minimize release. Hence, any opening created by a valve-failure, pigtail rupture, or pipe rupture will result in a rush of ambient air into the system and the formation of UO_2F_2 and HF.

Subsequently, when the internal pressure of the failed section equals the external ambient pressure, HF starts to escape. Size of opening, system pressure, and humidity of air are some of the factors that control the quantity of air that enters the failed section. Therefore, it is difficult to correctly determine the quantities of UF_6 , UO_2F_2 , and HF that are generated from a failed section.

However, the source term model should be capable of estimating such releases based on the knowledge of physical and operational conditions.

- (3) A source term model should be capable of quantifying a puff as well as a continuous release.

Many of the potential UF_6 releases during the material transfer processes represent puff (or short-duration) releases rather than continuous point or line sources. The duration of such releases depends on the nature of the accident and the emergency procedures used to contain the release. When a liquid-filled cylinder ruptures, the partial or entire content of the cylinder is released within a short duration, resulting in a large puff. A continuous release occurs, for example, when a cylinder is exposed to a fire with a leaky valve or a breach and the UF_6 in the cylinder escapes continuously for some time.

- (4) A source term model should be based on scenarios from past accidents as well as accidents that may occur in the future at fuel cycle facilities.

UF_6 is produced at fuel conversion plants. The uranium enrichment by gaseous diffusion process is accomplished by forcing gaseous UF_6 through a porous medium. Enriched UF_6 is sent to fuel fabrication plants to be converted into uranium dioxide. Most of the reported accidents have occurred during movement of cylinders within a site. A few accidents have occurred during transfer of UF_6 cylinders on site from one place to another. The reasons for these accidents during these transfer processes are not properly understood.

Cylinders moved between plants usually contain solid UF_6 in protective overpack. The major causes of cylinder failures outside the plants are related to carrier accidents such as automobile accident, ship collision, etc. The reason that

carrier accidents are not included specifically is that there is as yet no recorded case of one where any UF_6 has been lost.

Most of the accidents have occurred during movement of cylinders within a site. For example, accidents occur when liquid-filled cylinders are moved to cooling yards, when feed materials are moved to feed points, and when cylinders are moved to autoclave for sampling.

UF_6 releases from the nuclear fuel manufacturing processes are complicated for the following reasons:

- (a) The releases could occur in liquid, vapor, or solid phases; from pipe, valve, or cylinder; from inside a structure or outside.
- (b) Likely release scenarios could include (but not be limited to) valve/pigtail failure with liquid UF_6 ; valve/pigtail failure with vapor UF_6 ; liquid-filled cylinder failure; and solid-filled cylinder failure (from rust or exposure to fire).

The model should be capable of handling a good number of the above-mentioned releases and release scenarios. Also, the scenarios that are evaluated should be prioritized based on probability of occurrence and level of consequence. Models should be evaluated to ensure that they can handle scenarios that have reasonable probabilities of occurrence and have potentially significant consequences.

- (5) A source term model should be able to convert an internal release into an external source term.

Most of the releases connected with valve and pigtail failures occur inside buildings or in partially enclosed structures. If a release occurs inside a building, the source term model should be able to translate such an internal release into an external source term. This requires information on the building ventilation system along with release strength. Even though a source term can not define every possible building configuration, there should be a reasonable attempt to handle this with a few important parameters, such as building volume, ventilation rate, etc.

- (6) A source term model should be capable of handling at least a few of the most probable response measures affecting the release rate.

The application of emergency response measures may affect the source term because phase changes could occur and chemical reaction rates may be altered (slowed or hastened) by certain emergency responses.

Based on the above considerations, the following six criteria were developed to assess the source term component of a model.

- (1) *How many accident categories can the source term handle?*
- (2) *Does the source term algorithm handle puff release as well as continuous release?*

- (3) *Do the source term cases listed in the model reflect past accidents?*
- (4) *Does the source term contain mechanisms to translate an internal release into an external source?*
- (5) *Does the source term algorithm have the capabilities to analyze failure modes and does it quantify the release amount with appropriate phase?*
- (6) *Does the source term contain UF_6 reaction relationship with air and does it quantify final products (HF , UO_2F_2 , heat, etc.)?*

Table 3.1 provides the evaluation criteria matrix and detailed scoring criteria for each of the issues addressed above for each model. Table 3.2 presents a means to compare and rank different models.

3.2 Atmospheric Dispersion

UF_6 can be released to the atmosphere as a liquid, a vapor, or a mixture of the two, depending on the release conditions (notably pressure and temperature). If UF_6 vapor is released, it will start to mix with air immediately, reacting with water vapor in the air to produce UO_2F_2 and HF . If a liquid is released, a portion of it will evaporate or flash to vapor, depending on the conditions of pressure and temperature. This could possibly result in a two-phase flow in which the vapor and solid particles are transported, and made airborne. Since the UF_6 -water reaction is strongly exothermic, UF_6 solid, vapor or liquid falling onto pooled water (as might exist, for example, after a summer thunder-shower) can be expected to react vigorously, causing any unreacted UF_6 to vaporize.

Plume behavior following a release depends strongly on the thermodynamics of the plume which, in turn, depend on plume composition, atmospheric humidity, and temperature, all of which change as the UF_6 -(H_2O) reaction and dilution continue. In fact, a UF_6 plume can be negatively, positively, or neutrally buoyant.

Initial source geometry and building wake effects can also be important considerations in determining downwind concentrations, especially close to the source. For example, if a release is trapped in the wake of a nearby building, the initial dimensions of the source (i.e., apparent dimensions to a downwind receptor) could be very different from those in the absence of such an effect.

A previous review of UF_6 dispersion models by Sykes and Lewellen (1992) evaluated a wide variety of atmospheric dispersion models with potential applicability to UF_6 dispersion. This (screening) study identified five models for detailed consideration. Of the five models, only two had been developed specifically for UF_6 , whereas three were developed for dense gases. The study concluded that all the models would benefit from the following: (1) "improved treatment" of turbulent atmospheric dispersion (i.e., beyond the empirical stability classifications of Pasquill-Gifford-Turner and others); (2) building and terrain effects (e.g., initial source configuration and taking surface roughness into account as might be done for turbulence-based modeling); and (3) chemical reactions (UF_6 - H_2O reactions) and the associated plume thermodynamics in the atmospheric boundary layer.

The 1992 review considered the following atmospheric dispersion features:

- (1) *Ability to deal with transient releases.*
Releases may be continuous, of short duration, or nearly instantaneous (puff).

- (2) *Ability to deal with buoyant dynamics.*
Depending on atmospheric conditions and other physical/chemical reaction mechanisms associated with the source term, the plume may be positively, negatively, or neutrally buoyant.

- (3) *Representation of transient dynamics.*
Buoyancy should be handled separately for continuous and instantaneous puff releases.

- (4) *Representation of turbulent dispersion.*
The model may or may not handle windspeed fluctuations (turbulence). Handling of this feature depends on the treatment of atmospheric stability.

- (5) *Ability to consider building wake effects.*
The presence of a building in close proximity to or downwind from the release can substantially affect the initial plume dimensions and mixing and hence concentrations, especially at nearby receptors.

- (6) *Ability to incorporate terrain effects.*
Terrain effects can be important if major topographical features are present.

- (7) *Incorporation of plume chemistry.*
Consideration of plume chemistry can be important to the modeling, depending on the speed with which the reaction is completed, which, in turn, is driven by release rate and atmospheric conditions.

- (8) *Representation of statistical fluctuations (i.e., peak and mean concentrations, a factor important for toxicity assessment).*

Both mean and short-term maximum or peak concentrations are important in analyzing chronic and acute effects of UO_2F_2 and HF.

- (9) *Separate models for source representation and atmospheric dispersion.* The modular aspects of the model permitting the separation of source term from the dispersion term are important to enable the model to handle a variety of accident scenarios.

- (10) *Representation of aerosol dynamics.*
Issues of interest here include aerosol formation, transport, depletion by deposition to ground, and accumulation of UF_6 and reaction products on ground surface.

- (11) *Interaction with fog.* Interactions with fog water can affect buoyancy and deposition processes.

- (12) *Interaction with ground.* The plume may interact with the ground surface by exchanging heat and momentum.

Factors 1-12, identified in Sykes and Lewellen (1992), are all potentially relevant and should be considered. The 1993 report of SAIC to NRC (SAIC, 1993) also comments on the desirable features of a UF_6 dispersion model, including some not mentioned by Sykes and Lewellen. For the comparisons in our study, it would be useful to know whether the models can address the following additional factors.

(13)*Removal (deposition) of UF₆ and reaction products to the ground.* (This is not the same as criterion 12 of Sykes and Lewellen (1992) which deals mostly with heat transfer to the plume). A model should have the capabilities to model the wet and dry deposition processes for the various gaseous and particulate species during the transport of UF₆ and its reaction products in the atmosphere.

(14)*Effects of emergency response measures.* A model should have the capability to account for the effects of emergency response measures on the source term. Typically, as a result of the mitigative measures the source term would be reduced.

(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. Alternately, part of the plume containing primarily the lighter products of the reaction can become positively buoyant and can separate from the original plume. A model should have the capability to handle plume separation processes.

(16)*Aerosol formation and the droplet size of reactive airborne aerosol.* In the criterion, the focus is on a model's treatment of droplets of various sizes. Larger-sized UF₆ aerosols may undergo gravitational settling whereas smaller UO₂F₂ may undergo dry deposition.

(17)*Multiple sources and types of releases.* To model an accident that results in releases from several locations within a

plant, a model should have the capabilities to treat multiple sources in a single run. In addition, a model should be able to treat different types of sources in a single run.

Table 3.3 provides an evaluation criteria matrix for each of the issues addressed above for each model. Maximum potential scores have been assigned to each criterion. Actual scores will be assigned on the basis of whether the model addresses the issues raised in each criterion. Table 3.4 presents a means to compare and rank different models.

In addition to the evaluation of whether specific model features are present or absent and how the features have been modeled, it is important to evaluate how a model predicts a given observation. Even though the source term and dispersion components are evaluated separately, the evaluation of a model's capability to predict a given observation will be performed at the end of the evaluation for the dispersion component. Usually field experiments are conducted after an accident to measure downwind concentrations of a contaminant either in the air or in the soil after deposition and, typically, very little actual data are available that completely describe a source.

When data sets representing field measurements are available, predicted and observed ground-level concentrations of UF₆, UO₂F₂, and/or HF will be used to conduct model comparisons. Most models currently being used for the source term and dispersion analyses do not propagate uncertainties. Consequently, they produce single estimates of downwind ground-level concentrations. Using the predictions of point estimates and observed concentrations,

the following methods are among those being considered for the evaluation of models.

- *Graphical methods.* Plotting predicted and observed point estimates in different ways usually provides the most practical means of evaluating a model. Even though this method of evaluation is subjective, the results are usually clear and easy to understand.
- *Analytical methods.* The differences between predicted and observed pairs of values, also known as residuals, can be analyzed to determine the model bias. Model bias represents an overall tendency for over- or underprediction. Measures of bias are average residual, median residual, and the ratio of over- to under-predictions.

If time dependent observed data as well as the corresponding model simulation results are available, model predictions will be compared with observed values for transient or steady-state releases. This comparison will provide estimates of the agreement between observed data and the simulation results of a given model. Measures of agreement are the Pearson correlation coefficient and the fraction of observed-predicted pairs. These measures provide estimates of the levels of agreement between observed and predicted values within a given factor (*e.g.*, 2 or 4).

- *Other Statistical Analyses.* A student t-test will be used to compare average residual value to an expected value of zero. Wilcoxon test will be used to compare the magnitudes of positive and negative residuals. A number of other

tests will be evaluated and used, if necessary.

Other existing studies for evaluating models (*e.g.*, U.S. Environmental Protection Agency, 1992; Browne, *et al.*, 1985) will also be reviewed to include other applicable measures of model performance. When model predictions are accompanied by confidence bounds that express a range of values that should encompass the observed value, the same set of tests as described above will be conducted. For conducting the evaluation of model bias and reproducibility and other statistical analyses, the best estimate, 95th percentile, or another appropriate statistic will be calculated from the range of values predicted by the model for comparisons with observations.

Ranking different models on the basis of performance depends on the specific application. For ISA and ERP applications, a model that consistently overpredicts would be more appropriate than one that consistently underpredicts. For a PAA, a model that consistently produces an unbiased estimate is more appropriate. For each separate application, different models will be directly ranked on the basis of the results of graphical, analytical, and statistical tests presented earlier, keeping in mind the specific applications. Caution and judgment will be exercised to ensure that models which severely over, or underpredict are not ranked as superior to models that are generally more accurate. Rankings will be compiled in a single table (*e.g.*, Table 3.5). The table will be accompanied by (a) the results of the graphical, analytical, and statistical tests, and (b) the rationale for the assignment of ranks.

Table 3.1 Source term evaluation (Model name: _____)

Criteria*	Maximum score	Evaluation criteria	Points awarded
(1) How many accident categories can the source term handle?	10	10 points maximum for five or more cases. 5 points minimum for one case.	
(2) Does the source term algorithm handle puff release as well as continuous release?	15	15 points maximum for source term to handle both cases. 10 points minimum for a continuous source only.	
(3) Do the source term cases listed in the model reflect past accidents?	15	15 points maximum for a source that contains five or more accident cases relevant to future potential accidents. 5 points minimum for a source term containing one accident scenario. Points between them will be determined by combination of the number of cases and importance of those cases.	
(4) Does the source term contain mechanisms to translate an internal release into an external source?	15	15 points maximum for a source term containing mechanism to translate an internal leak to an external source. 5-point minimum for a source term with an external source only.	
(5) Does the source term algorithm have the capabilities to analyze failure modes and does it quantify the release amount with appropriate phase?	30	30 points for ability to handle all three initial phases at failure. 20 points for ability to handle two initial phases at failure. 10 points for ability to handle one initial phase at failure. Points in between can be given for quantifying methods.	
(6) Does the source term contain UF ₆ reaction relationship with air and does it quantify final products (HF, UO ₂ F ₂ , heat, etc.)?	25	25 points maximum for a source term containing detailed reaction steps to define product and quantity for five or more accident cases. 5 points minimum for a source term specifying UF ₆ or HF release rate without any analysis. Points between them will be determined by a combination of the number of cases and extent of analysis.	
Total score			

* Complete descriptions of the criteria are found in Section 3.1.

Table 3.2 Source term evaluation

Model name	Total score	Rank

Table 3.3 Atmospheric dispersion evaluation (Model name: _____)

Criteria*	Maximum score	Evaluation criteria	Points awarded
(1) Ability to deal with transient releases	25	Present or absent; score based on formulation	
(2) Ability to deal with buoyant dynamics	25	Present or absent; score based on formulation	
(3) Representation of transient dynamics	15	Present or absent; score based on formulation	
(4) Representation of turbulent dispersion	15	Present or absent; score based on formulation	
(5) Ability to consider building wake effects	25	Present or absent; score based on formulation	
(6) Ability to incorporate terrain effects	10	Present or absent	
(7) Incorporation of plume chemistry	25	Present or absent; score based on formulation	
(8) Representation of statistical fluctuations	15	Present or absent; score based on formulation	
(9) Separate models for source representation and atmospheric dispersion	15	Present or absent; score based on modularity	
(10) Representation of aerosol dynamics	5	Present or absent; score based on formulation	
(11) Interaction with fog	5	Present or absent; score based on formulation	
(12) Interaction with ground	5	Present or absent; score based on formulation	
(13) Removal (deposition) of UF_6 and reaction products to the ground	15	Present or absent; score based on formulation; (most important for post-accident analysis; not necessarily important for other applications).	
(14) Effects of emergency response measures	15	Present or absent; score based on formulation	
(15) Possibility of plume separation	5	Present or absent; score based on formulation	
(16) Aerosol formation and droplet size of reactive airborne aerosol	5	Present or absent; score based on formulation	
(17) Multiple sources and types of releases	10	Present or absent; score based on number of sources and source types that a model can handle in one run.	
Total score			

* Complete descriptions of the criteria are found in Section 3.2 of the report.

Table 3.4 Atmospheric dispersion evaluation

[illegible]

Table 3.5 Ranking of models based on comparisons of model predictions with field measurements

Model	Graphical test	Analytical tests		Other statistical tests	
		Bias	Reproducibility	Student t	Wilcoxon
(1) ISA Application					
Model 1 Model 2 . . . Model n					
(2) ERP Application					
Model 1 Model 2 . . . Model n					
(3) PAA Application					
Model 1 Model 2 . . . Model n					

4 TASK 1(B): APPLICABILITY EVALUATION CRITERIA DEVELOPMENT

The available models will be first grouped into screening-level and complex models. To determine applicability, a further distinction that focuses on the intended model application (ISA, ERP, and/or PAA) is required.

Evaluation criteria questions that will allow the screening-level or complex models to be categorized as suitable for ISA, ERP, and/or PAA are presented below.

4.1 ISA

- (1) *Does the model have an output that can be compared to the NRC accident criteria?*
- (2) *Does the model account for variable room ventilation rates to translate an internal release into an external release?*
- (3) *Can the model handle each of the failure modes and scenarios identified in source term evaluation criteria development so that a priori safety analyses can be conducted?*
- (4) *Can the model handle each of the evaluation components identified in atmospheric dispersion modeling so that a priori safety analyses can be conducted?*
- (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 ISA?*
- (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 ISA?*
- (7) *Can the model be simulated to include similar degrees of bias in both source term and dispersion so that their combined use leads to defensible and expected bias in the estimates of the output?*
- (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?*
- (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?*

4.2 ERP

- (1) *Does the model have an output that can be compared with the NRC accident criteria?*
- (2) *Can the model handle short-term meteorology (e.g., 15-minute or hourly meteorology) so that it can be simulated under various realistic atmospheric conditions for various lengths of time to evaluate concentrations affecting dense population groups around the release facility under various conditions of release?*
- (3) *Can the model be simulated under a transient mode? (Related to Question 2)*
- (4) *Can the model outputs be easily converted to concentration isopleths for UF₆ and its reaction products that can be superimposed on a population map of the region surrounding the facility?*
- (5) *Does the model have the capability to provide concentration predictions of UF₆ and its reaction products in the vicinity of the accident to allow planning for worker safety?*
- (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?*
- (7) *Does the model account for variable room ventilation rates to translate an internal release into an external release?*
- (8) *Can the model handle each of the failure modes and scenarios identified in source term evaluation criteria development so that a a priori response planning for a potential accident can be conducted?*
- (9) *Can the model handle each of the evaluation components identified in atmospheric dispersion modeling so that a a priori response planning for a potential accident can be conducted?*
- (10) *Does the model provide realistic estimates of the concentrations to ensure that the planned emergency response is appropriate?*
- (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? (Related to Question 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? Or, in other words, is the model modular in structure?*
- (13) *Can the model be used to calculate concentrations of UF₆ and reaction products in the control room from releases in a UF₆-handling facility?*

4.3 PAA

- (1) *Does the model allow the input of measured and realistic values so that the location of areas of maximum or critical impacts can be determined?*

- (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?*
- (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 estimated for the accident in question?*
- (4) *Can the model be simulated under transient conditions?*
- (5) *Can the model be simulated under an uncertainty analysis framework to obtain a range of possible concentration distribution of UF₆ and its reaction products?*
- (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 structure?*
- (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.)*
- (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?*

4.4 Site-Specific Factors

Some additional factors for evaluation pertaining to site- or event-specific considerations include the following.

- (1) *Ability to include environmental pathway analysis to evaluate health impacts on humans.*
- (2) *Ability to handle the presence of snow or rain either actively falling or already on the ground.*
- (3) *Ability to model complex terrain.*
- (4) *Ability to simulate long-term effects of deposition on agricultural areas.*
- (5) *Ability to model population effects (e.g., for densely populated urban areas).*
- (6) *Ability to conduct a human or an ecological impact assessment.*

In Table 4.1, the criteria questions identified above are classified as suitable for either a qualitative or for a quantitative evaluation. Table 4.2 provides a scoring methodology for the evaluation of all of the qualitative criteria questions (from Table 4.1) addressed under Task 1(b). Table 4.3 presents a means to compare and rank different models for these issues. Tables 4.4 and 4.5 present the same for criteria questions undergoing quantitative evaluations.

Table 4.1 Categorization of applicability issues in terms of qualitative and quantitative evaluation

Criterion*	Evaluation quantitative/qualitative
ISA	
(1) Does the model have an output that can be compared to the NRC accident criteria?	Qualitative
(2) Does the model account for variable room ventilation rates to translate an internal release into an external release?	Quantitative
(3) Can the model handle each of the failure modes and scenarios identified in source term evaluation criteria development so that <i>a priori</i> safety analyses can be conducted?	Quantitative
(4) Can the model handle each of the evaluation components identified in atmospheric dispersion modeling so that <i>a priori</i> safety analyses can be conducted?	Quantitative
(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 ISA?	Qualitative
(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 ISA?	Qualitative
(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?	Qualitative
(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?)	Qualitative
(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?	Qualitative
ERP	
(1) Does the model have an output that can be compared with the NRC accident criteria?	Qualitative

* Complete descriptions of the criteria are found in Section 4.1, 4.2, 4.3, and 4.4 of the report.

Table 4.1 (continued)

Criterion*	Evaluation quantitative/qualitative
(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 affecting dense population groups around the release facility under various conditions of release?	Qualitative
(3) Can the model be simulated under a transient mode? (Related to Question 2)	Qualitative
(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?	Quantitative
(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?	Quantitative
(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?	Quantitative
(7) Does the model account for variable room ventilation rates to translate an internal instantaneous release into a continuous external release?	Quantitative
(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?	Quantitative
(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?	Quantitative
(10) Does the model provide realistic estimates of the concentrations to ensure that the planned emergency response is appropriate?	Qualitative
(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? (Related to Question 10)	Qualitative
(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?)	Qualitative
(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?	Qualitative

* Complete descriptions of the criteria are found in Section 4.1, 4.2, 4.3, and 4.4 of the report.

Table 4.1 (continued)

Criterion*	Evaluation quantitative/qualitative
PAA	
(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?	Qualitative
(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?	Quantitative
(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?	Quantitative
(4) Can the model be simulated under transient conditions?	Qualitative
(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?	Qualitative
(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?)	Qualitative
(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.)	Qualitative
(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?	Qualitative
Site-Specific Factors	
(1) Ability to include environmental pathway analyses to evaluate health impacts on humans.	Qualitative
(2) Ability to handle the presence of snow or rain either on the ground or actively falling.	Qualitative
(3) Ability to model complex terrain.	Qualitative
(4) Ability to simulate long-term effects of deposition on agricultural areas.	Qualitative
(5) Ability to model population effects (e.g., for densely populated urban areas).	Qualitative
(6) Ability to conduct a human or an ecological impact assessment.	Qualitative

* Complete descriptions of the criteria are found in Section 4.1, 4.2, 4.3, and 4.4 of the report.

Table 4.2 Qualitatively evaluated applicability issues (Model name: _____)

Criterion	Does the model have the feature? Yes/No	Maximum score & evaluation criteria	Score
ISA*			
(1) Does the model have an output that can be compared to the NRC accident criteria?		20 points for yes and 10 for an output not related to NRC criteria.	
(2) Can the model be simulated under a worst-case, acute release model 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 ISA?		10 to 20 points depending on details.	
(3) 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 ISA?		10 to 20 points depending on details.	
(4) 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 or 0 points for yes or no.	
(5) 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?		10 or 0 points for yes or no.	
(6) Can the model be used to calculate concentrations of UF ₆ and reaction products in a control room from releases in a UF ₆ -handling facility?		5 or 0 points for yes or no.	

* From Table 6, only those criteria that are qualitatively evaluated are included in this table; the remaining are included in Table 9.

Table 4.2 (continued)

Criterion	Does the model have the feature? Yes/No	Maximum score & evaluation criteria	Score
ERP*			
(1) Does the model have an output that can be compared with the NRC accident criteria?		20 points for yes and 10 for output not related to NRC criteria.	
(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 affecting dense population groups around the release facility under various conditions of release?		10 to 20 points depending on capability.	
(3) Can the model be simulated under a transient mode? (Related to Question 2)		10 to 20 points variable depending on capability; 10 or 0 for yes or no.	
(4) Does the model provide realistic estimates of the concentrations to ensure that the planned emergency response is appropriate?		10 to 20 points depending on details.	
(5) 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? (Related to Question 10)		10 to 20 points depending on details.	
(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?		10 or 0 points for yes or no.	
(7) 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 or 0 points for yes or no.	

* From Table 6, only those criteria that are qualitatively evaluated are included in this table; the remaining are included in Table 9.

Table 4.2 (continued)

Criterion	Does the model have the feature? Yes/No	Maximum score & evaluation criteria	Score
PAA*			
(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 or 10 points for yes or no and details.	
(2) Can the model be simulated under transient conditions?		10 or 0 points for yes or no.	
(3) 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?		10 to 20 points depending on details.	
(4) 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?		10 or 0 points for yes or no.	
(5) 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.)		0 to 10 points depending on capability.	
(6) Can the model be used to calculate concentrations of UF ₆ and reaction products in a control room from releases in a UF ₆ -handling facility?		5 or 0 points for yes or no.	

* From Table 6, only those criteria that are qualitatively evaluated are included in this table; the remaining are included in Table 9.

Table 4.2 (continued)

Criterion	Does the model have the feature? Yes/No	Maximum score & evaluation criteria	Score
Site-Specific Factors*			
(1) Ability to include environmental pathways analysis to evaluate health impacts on humans.		10 to 30 points depending on details and accuracy.	
(2) Ability to compare environmental or other monitoring data for a PAA.		10 or 0 points for yes or no.	
(3) Ability to handle the presence of snow or rain either on the ground or actively falling.		10 or 0 points for yes or no.	
(4) Ability to model complex terrain.		10 to 20 points depending on details.	
(5) Ability to simulate long-term effects of deposition on agricultural areas.		10 to 20 points depending on details.	
(6) Ability to model population effects (e.g., for densely populated urban areas).		0 to 10 points depending on logic.	
(7) Ability to conduct a human or an ecological impact assessment.		0 to 10 points depending on methods and details.	
Total score			

* From Table 6, only those criteria that are qualitatively evaluated are included in this table; the remaining are included in Table 9.

Table 4.3 Qualitatively evaluated applicability issues

Model name	Total score	Rank

Table 4.4 Quantitatively evaluated applicability issues (Model name: _____)

Criterion	Maximum score	Score
ISA*		
(1) Does the model account for variable room ventilation rates to translate an internal release into an external release?	20 points for yes and 10 for individual (int. and ext.) treatment.	
(2) 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 analyses can be conducted?	10 to 30 points depending on the number of cases handled.	
(3) 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?	10 to 30 points depending on the number of components handled.	
ERP*		
(1) 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 or 0 points for yes or no.	
(2) 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?	10 to 30 points depending on details.	
(3) 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 or 0 points for yes or no.	
(4) Does the model account for variable room ventilation rates to translate an internal instantaneous release into a continuous external release?	20 points for yes and 10 for individual.	

* From Table 4.1, only those criteria that are quantitatively evaluated are included in this table; the remaining are included in Table 4.2

Table 4.4 (continued)

Criterion	Maximum score	Score
(5) 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?	10 to 30 points depending on numbers and details.	
(6) 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?	10 to 30 points depending on number and details.	
PAA*		
(1) 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?	10 to 30 points depending on number of modes handled.	
(2) 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?	10 to 30 points depending on number of components handled.	
Total score		

* From Table 4.1, only those criteria that are quantitatively evaluated are included in this table; the remaining are included in Table 4.2

5 TASK 1(C): USER INTERFACE AND MODEL QA/QC EVALUATION CRITERIA DEVELOPMENT

The purpose of conducting a user interface and model QA/QC evaluation is not to discard a model. On the contrary, if a model is found to be superior in terms of applicability and technical capabilities, the user interface and model QA/QC evaluation results can be used to make the model more user-friendly, and/or to provide improved documentation to assure the quality, consistency, and reproducibility of its results. Therefore, this step of evaluation does not eliminate any models as inapplicable or inadequate.

5.1 User Interface

The following factors have been identified for evaluation of a model's user interface.

- (1) *Clear documentation*
- (2) *Complete documentation*
- (3) *Correctness of documentation*
- (4) *Computer use*
- (5) *Model input scheme and input-stream preparation*
- (6) *Model simulation*
- (7) *Model output scheme*

Each of these factors is discussed below in detail. For each factor, a set of components that can be scored are identified. If a model is found to lack satisfactory user interface, but is otherwise evaluated as a useful code (by Tasks 3 and 4), specific

recommendations will be made for the improvement of the user interface characteristics of the model.

(1) *Clear documentation.*

Clarity of presentation in the documents that accompany a model is essential for a number of reasons as presented below.

- (a) It helps a user to understand and use the model in a relatively short time.
- (b) It ensures that the user is not running a model with little or no idea about what it does; this can lead to severe problems if a model is used for a purpose other than the one for which it was developed.
- (c) It allows the user to be satisfied that his/her use of the model is correct.
- (d) With clear presentation, the user will be able to contact appropriate experts (as identified in the document) for preparation of input values for certain key input parameters.

Evaluation of the clarity of documentation is subjective in nature. To maintain objectivity across models that are being evaluated, the document will be read by a senior as well as a junior user. The senior user is assumed to know the theoretical basis for the model and can run the model without detailed instructions. The junior user is assumed to be a novice who needs clear guidance. The models under evaluation will be ranked in decreasing order of clarity with 20 being the best score.

(2) Complete Documentation

Completeness of documentation will be checked with respect to the presence of the following items.

- (a) Statement of the model objective
- (b) Theoretical bases 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
- (j) Presentation of validation study

Each model documentation will be checked for the presence of the items listed above.

(3) Correct documentation

Usually errors in the documentation come to light when a model is actually being used by a person other than the model developer. These errors will be tabulated for each model. This can be supplied to each user as an addendum to the model documentation. This may not affect model evaluation process unless the errors are serious enough to affect the outcome of the model. If a serious error is identified, the model developer will be contacted for a quick resolution, if possible.

(4) Computer use

Computational speeds of IBM-PC computers have increased tremendously over the last few years. Use of these computers has also become ubiquitous. Therefore, it would be most advantageous to be able to make model simulations on an IBM-PC or a compatible. However, some earlier models may have been developed on platforms that were faster at the time (e.g., a SUN work station). Feasibility of converting these programs to PC versions will be investigated. If feasible, it will be done. If not, they will be simulated on a work station.

(5) Model input scheme and input stream preparation

Many models provide preprocessors to enable the user to prepare input files in a simplified manner. Presence or absence of preprocessors will be tabulated with 'yes' or 'no' responses. Input schemes from various models will be ranked by a junior as well as a senior user. The ranking will be done after using all models to prepare the input files for a given problem, and evaluating the ease with which they could be prepared. Some factors that might influence the input file preparation are as follows:

- (a) Adequate documentation for the choice of parameter values, recommended values in absence of site-specific data, etc.
- (b) Acquisition/preparation of certain types of data (e.g., the meteorological data set for a short- or long-term simulation).

(c) Manipulation of a data set obtained from a standard source (e.g., modification of the STAR data set obtained from the National Climatic Data Center, Asheville, NC, to the format required by the model).

(d) Proper documentation of the formats and units.

(e) Overall time taken for the input file preparation.

(6) Model simulation

Some of the simulation characteristics from different models that will be compared and ranked include the following:

- (a) Simulation time
- (b) Unexpected terminations
- (c) Unexpected errors

(7) Model output scheme

Output files from different models will be compared and ranked on the basis of the following features:

- (a) Clarity of output
- (b) Need for further analysis
- (c) Presence of post-processors for graphical outputs.

Table 5.1 provides an evaluation criteria matrix for each of the issues addressed above for each model. Table 5.2 presents a means to compare and rank different models.

5.2 Model QA/QC

Each model will be checked for the presence of the following documents.

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

The responses will be tabulated for all models. For QA/QC purposes, each of the listed documentation attributes will be evaluated for adequacy, correctness, and applicability. If a model does not have adequate QA/QC documentation, but is otherwise evaluated as a useful model, specific recommendations will be made to enhance the model's QA/QC documentation.

Table 5.3 provides an evaluation criteria matrix for each of the issues addressed above for each model. Table 5.4 provides a means to compare and rank different models.

Table 5.1 User interface (Model name: _____)

Criterion*	Maximum score & evaluation criteria	Score
(1) Clear documentation	Maximum score 20 points, subjective evaluation as presented in Section 5.0.	
(2) Complete documentation	Maximum score 20 points for all of the 10 (a to j) items presented in Section 5.0, and reduce 2 points for each item being absent.	
(3) Correctness of documentation	Maximum score of 10 points, subjective scoring	
(4) Computer use	Maximum score of 10 points if computer to be used is clearly identified and is a PC and 7.5 points, if it is a work station.	
(5) Model input scheme and input-stream preparation	Maximum score 50 points, subjective evaluation as presented in Section 5.0.	
(6) Model simulation	Maximum score 20 points, subjective and also comparative evaluations with respect to other models, as presented in Section 5.0.	
(7) Model output scheme	Maximum score 20 points, subjective and also comparative evaluations with respect to other models, as presented in Section 5.0.	
Total score		

* Complete descriptions of the criteria are found in Section 5.1 of the report.

Table 5.2 User interface

Model name	Total score	Rank

Table 5.3 Model QA/QC (Model name: _____)

Criterion	Maximum score & evaluation criteria	Score
(1) Theoretical manual	10 points for yes, 0 for no.	
(2) User's manual	10 points for yes, 0 for no.	
(3) Example problem	10 points for yes, 0 for no.	
(4) Documentation of model verification	10 points for yes, 0 for no.	
(5) Documentation of model testing using field data (validation)	10 points for yes, 0 for no.	
Total score		

* Complete descriptions of the criteria are found in Section 5.2 of the report.

Table 5.4 Model QA/QC

[illegible]

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