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**U.S. Nuclear Regulatory Commission  
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# RASCAL 3.0: Description of Models and Methods

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Prepared by

A. L. Sjoreen<sup>a</sup>

J. V. Ramsdell, Jr.<sup>b</sup>

T. J. McKenna<sup>c</sup>

S. A. McGuire<sup>d</sup>

C. Fosmire<sup>e</sup>

G. F. Athey<sup>f</sup>

<sup>a</sup>Oak Ridge National Laboratory

P.O. Box 2008

Oak Ridge, TN 37831

<sup>b</sup>Pacific Northwest National Laboratories

P.O. Box 999

Richland, WA 99352

<sup>c</sup>International Atomic Energy Agency

Wagramerstrasse 5

P.O. Box 100

A-1400, Vienna, Austria

<sup>d</sup>Incident Response Operations

U.S. Nuclear Regulatory Commission

Washington, DC 20555-0001

<sup>e</sup>Innovative Emergency Management

8555 United Plaza Boulevard

Baton Rouge, LA 70809

<sup>f</sup>Athey Consulting

P.O. Box 178

Charlestown, WV 25414

S. A. McGuire, NRC Project Manager

**Prepared for**

**Incident Response Operations**

**U.S. Nuclear Regulatory Commission**

**Washington, DC 20555-0001**



## ABSTRACT

The Radiologic Assessment System for Consequence AnaLysis (RASCAL) 3.0 is the latest version of the RASCAL series of codes. RASCAL was developed for use by U.S. Nuclear Regulatory Commission personnel who conduct an independent assessment of radiological accidents to prepare dose projections. It includes three sets of tools for use in consequence analysis STDose, FMDose, and DecayCalc. STDose estimates (1) source terms for radiological accidents, (2) atmospheric transport, diffusion, and deposition of effluents from the accidents, and (3) doses from exposure to the effluents. FMDose calculates doses from environmental measurements of activity in the air and on the ground. DecayCalc calculates activity of radionuclides present at a future time following decay and ingrowth. The current version of RASCAL includes computational techniques that are substantially modified from those used in the prior versions of RASCAL and significantly expands the capabilities of STDose. The major changes to STDose are (1) the inclusion of time-dependent source terms and source terms for fuel cycle and materials accidents, (2) the inclusion of radiological decay during atmospheric transport, (3) the addition of a  $\text{UF}_6$  atmospheric transport model, and (4) the ability to include meteorological data from multiple stations and the effects of terrain. The major changes to FMDose are the addition of emergency-worker guidance and derived intervention-level calculations.

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## LIST OF ABBREVIATIONS

ANSI/ANS	American National Standard Institute/American Nuclear Society
ARF	activity release fractions
BWR	boiling water reactor
CEDE	committed effective dose equivalent
CDS	core damage state
DIL	derived intervention levels
FRMAC	Federal Radiological Monitoring and Assessment Center
IF	inhalation fractions
LRF	leakage rate fraction
MFR	mass flow rate
NRC	Nuclear Regulatory Commission
PAG	protective action guide
PWR	pressurized water reactor
RDF	reduction factors
STCP	Source Term Code Package
TEDE	total effective dose equivalent

# 1 INTRODUCTION

The Radiological Assessment System for Consequence AnaLysis (RASCAL) 3.0 is the latest version of RASCAL (Athey, Sjoreen, and McKenna 1989; Athey et al. 1993, Sjoreen et al. 1994, Athey, Sjoreen, and Ramsdell 1997). RASCAL was developed for use by U.S. Nuclear Regulatory Commission (NRC) personnel who conduct an independent assessment of radiological accidents to prepare dose projections. RASCAL includes three sets of tools for use in consequence analysis STDose, FMDose, and DecayCalc. STDose estimates (1) source terms for radiological accidents, (2) atmospheric transport, diffusion, and deposition of effluents from the accidents, and (3) doses from exposure to the effluents. FMDose calculates doses from environmental measurements of activity in the air and on the ground at a single location. DecayCalc calculates activity of radionuclides present at a future time following radiological decay and ingrowth.

Documentation for the earlier versions of RASCAL has generally been limited to user's guides (Athey, Sjoreen, and McKenna 1989, Athey et al. 1993, Sjoreen et al. 1994, Athey, Sjoreen, and Ramsdell 1997) and workbooks (Athey, Sjoreen, and McKenna 1993, Athey and McKenna 1994). The user's guides have contained brief technical descriptions of the computational models implemented in the consequence assessment tools and have referred readers to other documents for details. The current version of RASCAL includes computational techniques that are substantially modified from those used in the prior versions of RASCAL and significantly expands the capabilities of STDose. Therefore we are publishing this compilation of the technical bases for the RASCAL 3.0 tools.

## 1.1 STDose

STDose is the primary tool for consequence analysis. It includes five computational modules — STCALC, TADPLUME, TADPUFF, UF6PLUME, and METPROC. The technical bases for these modules are presented in this document. The sixth STDose module, VIEWMET, is used by STDose to display meteorological data and does not perform any computations. VIEWMET is not discussed further in this document.

STCALC estimates the amount of radioactive (or hazardous) material released from a wide variety of potential radiological accident scenarios. The source term calculations performed can be generally categorized as (1) nuclear power plant accidents, (2) spent reactor fuel accidents, (3) fuel cycle facility/UF<sub>6</sub> accidents, (4) uranium fires and explosions, (5) criticality accidents, and (6) isotopic releases (e.g., transportation, materials). The source terms estimated are time dependent and are intended to be somewhat conservative but in general to be "best guess" estimates. The technical bases for STCALC estimates for reactor and spent fuel accidents are presented in Section 2. The technical bases for STCALC estimates for fuel cycle and materials accidents are presented in Section 3.

TADPLUME and TADPUFF perform atmospheric transport, diffusion, and dose calculations for releases in which the activity released can be treated as a passive atmospheric constituent. For RASCAL 3.0 these codes have been modified to permit temporal variation of release rates by radionuclide and to track deposition by radionuclide. TADPUFF has been modified to accept spatial as well as temporal variation of winds, atmospheric stability, precipitation, and mixing-layer thickness. The codes now

report  $^{131}\text{I}$  air concentrations and open- and closed-window dose rates in addition to the doses reported in earlier versions of RASCAL. All results are reported at 15-min intervals. The technical bases for TADPLUME and TADPUFF are presented in Section 4.

TADPLUME and TADPUFF do not adequately model the processes that are important when  $\text{UF}_6$  is released to the atmosphere.  $\text{UF}_6$  is initially a dense gas, and it reacts chemically with the water in the atmosphere to give HF and  $\text{UO}_2\text{F}_2$ . UF6PLUME is a version of TADPLUME that has been modified to treat the dense gas dispersion and chemical reactions associated with  $\text{UF}_6$ . The technical bases for UF6PLUME are presented in Section 5.

As indicated above, one of the areas in which RASCAL 3.0 has expanded capabilities is in the treatment of the meteorological conditions. In earlier versions of RASCAL, variation in meteorological conditions was limited; data could be entered only four times at a single location. Therefore, TADPLUME and TADPUFF could run using the same meteorological data. TADPUFF now has the capability to use spatially and temporally varying meteorological conditions. To support this increased capability, the meteorological data entry component of earlier versions of RASCAL has been moved to a separate module, METPROC, that can be run either from STDose or as a stand-alone program. This module includes meteorological data entry, conversion of the data to engineering units used by TADPLUME and TADPUFF, and preparation of input files for TADPLUME and TADPUFF. The TADPUFF files contain fields that describe the spatial variation of meteorological conditions. Meteorological data may be entered for as many as 36 locations, and the number of observations is not limited. METPROC has options that, if selected, evaluate stability data for consistency with season and time of day, estimate mixing-layer height from meteorological data or climatology, substitute climatological estimates for missing data, and modify the wind field for topographic effects. The technical bases for METPROC are presented in Section 6.

## **1.2 FMDOSE**

FMDose is a stand-alone program that calculates doses, derived intervention levels (DILs), and emergency-worker turn-back guidance at a single field measurement location. It calculates doses and DILs for both the early phase and the intermediate phase of the accident. Calculational methods are based on the Federal Radiological Monitoring and Assessment Center (FRMAC) Assessment Manual (DOE 1995). All calculations require the user to enter at least one air or ground concentration and a meter reading. For emergency worker guidance and early-phase doses based on air concentrations, FMDose assumes that all radionuclide concentrations are constant over the exposure period. All other dose and DIL calculations include decay and decay-product ingrowth. The calculation of the decay of ground concentrations includes weathering. The technical bases for FMDose are presented in Section 7.

## **1.3 DECAY CALCULATIONS**

Almost all modules in RASCAL 3 require some kind of decay calculation. All use the same data and basic method of calculation. DecayCalc is a stand-alone program that only calculates radiological decay and daughter ingrowth. The technical bases for the decay calculations are presented in Section 8.

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## 2 REACTOR AND SPENT FUEL SOURCE TERM CALCULATIONS IN STDose

The source term calculations in STDose estimate the amount of radioactive (or hazardous) material released based on a wide variety of potential radiological accident scenarios. The source term calculations performed that pertain to reactor sites generally can be categorized as (1) nuclear power plant accidents, (2) spent reactor fuel accidents, and (3) effluent releases that can be characterized by an isotopic mix. These calculations are performed using an extension of the method of estimating source terms from reactor accident conditions described in NUREG-1228 (McKenna and Giitter 1988).

STDose divides the source term calculation into three parts: first, it calculates the amount of activity available for release based on the source term type; second, this activity is reduced, based on the reduction mechanisms that the user has selected for the release pathway; and third, the activity is released according to the release rate selected. This can be shown as

$$S_{ij} = I_i \times ARF_{ij} \times \prod_k RDF_{ik} \times LF_j \quad (2.1)$$

where

$S_{ij}$  = total amount of radionuclide  $i$  released under accident conditions  $j$ ,

$I_i$  = inventory of radionuclide  $i$ ,

$ARF_{ij}$  = airborne release fraction of radionuclide  $i$  under accident conditions  $j$ ,

$RDF_{ik}$  = reduction factor that applies to radionuclide  $i$  for reduction mechanism  $k$ ,

$LF_j$  = leakage fraction selected under accident conditions  $j$ .

In RASCAL 3.0, nuclear power plant accidents and effluent source terms may change with time. Source terms are recomputed at intervals of varying length, called time steps. A new time step starts whenever the user changes any of the time-dependent data or every 15 min, whichever is less. At the end of each time step, the inventory of activity is decremented for the amount of activity released or removed by reduction and the effects of radiological decay, so that no more than the total inventory can be released. Time steps may be no less than 1 min and must be an integral number of minutes. Before passing the source term to the atmospheric transport model, STDose converts the user-selected time steps to the 15-min time steps used by the atmospheric transport models. Note that neither the type of source term calculation nor release pathway may change with time. The minimum amount of activity of any one nuclide that will be passed to atmospheric transport models in one time-step is  $10^{-15}$  Ci.

STDose includes six release pathways for nuclear power plant accidents. Only those pathways that are appropriate to the accident type, location, and method of source calculation are available to the user in any assessment. Data specific to each reactor site are shown in Appendix A. Spent fuel accidents have a single release pathway available. All release pathways only allow those reduction mechanisms that are possible for that type of accident. Table 2.1 shows the relationships among the types of source terms and release pathways.



**Table 2.1 Relationship of Reactor and Spent Fuel Source Terms to Release Pathways**

<b>Event type</b>	<b>Source term</b>	<b>Release pathways available</b>
Nuclear power plant	Coolant sample	Steam generator tube rupture Containment bypass
Nuclear power plant	Containment air sample Containment radiation monitor	Containment leakage or failure
Nuclear power plant	Effluent gross concentrations release rate	Direct
Nuclear power plant Pressurized water reactor (PWR) only	Core cooling status User-defined core damage estimate	Containment leakage or failure Steam generator tube rupture Containment bypass
Nuclear power plant Boiling water reactor (BWR) only	Core cooling status User-defined core damage estimate	Wet well Dry well Containment bypass
Reactor spent fuel	Pool storage - uncovered fuel Pool storage - damaged assembly under water Dry storage cask event	Spent fuel release
Effluent	Effluent Release Rates Effluent Concentrations	Direct

The following discussion of the STDose calculations is divided into three parts. First, all the source term calculations are presented. These are followed by discussions of the reductions possible according to the release pathway. Finally, the calculation of leakage factor is presented.

## **2.1 CALCULATION OF THE AMOUNT OF ACTIVITY AVAILABLE FOR RELEASE IN NUCLEAR POWER PLANT ACCIDENTS**

Seven types of source term data can be used to estimate the source term for a nuclear power plant accident: (1) core cooling status, (2) containment radiation monitor, (3) coolant sample, (4) containment air sample, (5) user-defined core damage estimate, (6) effluent releases measured directly, and (7) effluent gross concentrations release rates. In the core cooling status and containment radiation monitor, the user enters data that are used to estimate the core damage state or the activity in the coolant. In all other source term types, the user enters a direct estimate of activity available for release. The calculations performed for each of these types of data are discussed in the following sections.

Nuclear power plant nuclide inventory data are used in computing nuclear power plant and spent fuel accidents. The inventories used for pressurized water reactors (PWRs) and boiling water reactors (BWRs) are from NUREG-1150 (NRC 1990). Normal coolant concentrations are from (ANSI 1999). Due to limitations in the number of nuclides that can be transported in the atmosphere, only those nuclides that are expected to be significant contributors to dose are included in the coolant inventory. These data are shown in Table 2.2. Default inventories assume a burn-up of 18,000 MWD/MTU. In all calculations, the inventories are adjusted for the actual burnup. All radionuclides in the initial inventory that have a half-life of more than one year are computed as

$$INV_B = INV_I \times \frac{BURNUP_{ACTUAL}}{BURNUP_{ASSUMED}} \quad (2.2)$$

where the assumed burnup is 18,000 MWD/MTU.

In all cases, if the reactor is shut down prior to the start of the release, the inventory or coolant activity is decayed over the shutdown period prior to any other calculations being performed.

### 2.1.1 Core Cooling Status

STDose can use data on the core cooling status to estimate the core damage state or coolant activity. The core damage state is based on the amount of time the core is uncovered. The resulting amount of core activity available in containment or coolant are based on the core release fractions in Tables 3-12 and 3-13 in NUREG-1465 (Soffer et al. 1992). The core release fractions are shown in the following Tables 2.3 and 2.4. Note that the fractions shown in these tables are cumulative; that is, the fraction released in a vessel melt-through is the sum of the cladding failure, core melt, and vessel melt-through fractions. The fractions are listed according to Source Term Code Package (STCP) categories as revised in NUREG-1465 (Soffer et al. 1992). The chemical elements in each of the STCP categories are listed in Table 2.5. The isotopes of all elements not listed in this table are not included in the initial source term calculations. When a daughter grows in during the scenario, its release fraction is that of its STCP category, not that of its parent.

STDose recomputes the core-damage state every time step or 15 min, whichever is less. First it computes the core uncover duration, based on the core uncover time entered by the user and the current time in the scenario calculations. The core-damage state selected is the one into which the current core uncover duration falls. For example, when a BWR core has been uncovered for 1 h and 45 min, it has a core-damage state of "core melt"; that is 1.75 h is greater than the total cladding failure duration (0.5 h) and less than the total cladding failure plus core melt durations (0.5 h + 1.5 h). The fraction of that core-damage state,  $F_{CDS}$  that has been released from the core at any time is determined as

$$F_{CDS} = \frac{DU - D_{CDS-1}}{D_{CDS}} \quad (2.3)$$

**Table 2.2 Nuclear Power Plant Core Inventory and Coolant Concentrations**

	Inventory <sup>a</sup>	PWR coolant <sup>b</sup>	BWR coolant <sup>b</sup>		Inventory <sup>a</sup>	PWR coolant <sup>b</sup>	BWR coolant <sup>b</sup>
Nuclide	Ci/MW(t)	Ci/g	Ci/g	Nuclide	Ci/MW(t)	Ci/MW(t)	Ci/MW(t)
Ba-140	5.30e+04	1.30e-08	4.00e-10	Mo-99	5.30e+04	6.40e-09	2.00e-09
Ce-144	2.80e+04	4.00e-09	3.00e-12	Np-239	5.50e+05	2.20e-09	8.00e-09
Co-58	0	4.60e-09	1.00e-10	Ru-103	3.70e+04	7.50e-09	2.00e-11
Co-60	0	5.30e-10	2.00e-10	Ru-106	8.00e+03	9.00e-08	3.00e-12
Cs-134	2.50e+03	3.70e-11	3.00e-11	Sb-127	2.00e+03	0	0
Cs-136	1.00e+03	8.70e-10	2.00e-11	Sb-129	1.10e+04	0	0
Cs-137	1.60e+03	5.30e-11	8.00e-11	Sr-89	3.10e+04	1.40e-10	1.00e-10
H-3	0	1.00e-06	1.00e-08	Sr-90	1.20e+03	1.20e-11	7.00e-12
I-131	2.80e+04	2.00e-09	2.20e-09	Sr-91	3.70e+04	9.60e-10	4.00e-09
I-132	4.00e+04	6.00e-08	2.20e-08	Tc-99m	0	4.70e-09	2.00e-09
I-133	5.70e+04	2.60e-08	1.50e-08	Te-129m	1.80e+03	1.90e-10	4.00e-11
I-134	6.30e+04	1.00e-06	4.30e-08	Te-131m	4.00e+03	1.50e-09	1.00e-10
I-135	5.00e+04	5.50e-08	2.20e-08	Te-132	4.00e+04	1.70e-09	1.00e-11
Kr-85	1.90e+02	4.30e-07	0	Xe-131m	3.30e+02	7.30e-07	0
Kr-85m	8.00e+03	1.60e-07	0	Xe-133	5.70e+04	2.90e-08	0
Kr-87	1.60e+04	1.70e-08	0	Xe-133m	2.00e+03	7.00e-08	0
Kr-88	2.30e+04	1.80e-08	0	Xe-135	1.10e+04	6.70e-08	0
La-140	5.30e+04	2.50e-08	4.00e-10	Xe-138	5.70e+04	6.10e-08	0.00e+00
Mn-54	0	1.60e-09	3.50e-11	Y-91	4.00e+04	5.20e-12	4.00e-11

<sup>a</sup>The inventories are from NUREG-1228, Table 2.2 (McKenna and Gitter 1988).

<sup>b</sup>Coolant concentrations are from ANSI 1999.

where

$D_U$  = the current core uncover duration (h),

$D_{CDS-1}$  = the core uncover duration (h) at the beginning of core damage state CDS,

$D_{CDS}$  = the total duration that core damage state CDS is expected to occur.

In the example given above,  $D_U$  is 1.75 h,  $D_{CDS-1}$  is 0.5 h and  $D_{CDS}$  is 1.5 h. So  $F_{CDS}$  is  $(1.75-0.5)/1.5$  or 0.833 h.

If the user has entered a time at which the core is recovered, then core damage and release of material from the core stops, and the core-damage state remains the same.

If the reactor core has never been uncovered, only coolant activity may be released. Note that rapid increases in the iodine and other fission-product concentrations in the coolant as high as 3 orders of

magnitude may be seen following reactor shutdown, startup, rapid power change, and reactor coolant system depressurization. Such increases are referred to as iodine spikes. The user may select a spiking factor from 1 to 1000. The activity of all radionuclides in the coolant except noble gases are multiplied by this spiking factor.

**Table 2.3 BWR Core Activity Release Fractions**

	<b>Cladding failure</b>	<b>Core melt</b>	<b>Vessel melt-through</b>
Duration of core damage state (h)	0.5	1.5	3.0
Core uncover duration at which this core damage state begins (h)	0.0	0.5	2.0
Noble gases	0.05	0.95	0
Halogens	0.05	0.25	0.30
Alkali metals	0.05	0.20	0.35
Tellurium group	0	0.05	0.25
Barium, strontium	0	0.02	0.1
Noble metals	0	0.0025	0.0025
Cerium group	0	0.0005	0.005
Lanthanides	0	0.0002	0.005

*Source:* Table 3-12 from NUREG-1465 (Soffer et al. 1992)

### 2.1.2 Containment Radiation Monitor

STDose can use a containment radiation monitor reading to estimate the core damage state or the amount of activity in the coolant. The user can enter changes in the monitor readings with time, so this calculation can result in a time-varying source term. The fractional core-damage state or coolant condition is determined based on the data in Figs. A.5 — A.12 in RTM-96 (McKenna, et al. 1996), that are shown as Figures 2.1—2.8 below. The bars in these figures represent the range from 1 to 100% of the labeled core-damage state. The data in these figures were calculated assuming a reactor power of 3000 MW(t). Note that these figures use the older terminology “gap” and “in-vessel melt” to refer to cladding failure and core melt, respectively. In this section only, the older terms are used for ease of comparison with the figures.

To estimate the core-damage state, STDose first determines which set of data in the figures should be used. It selects the figure to use, based on the containment type and whether or not containment sprays are operating and, for BWRs, whether the monitor is in the wet well or dry well. Since the figures

**Table 2.4 PWR Core Activity Release Fractions**

	<b>Cladding failure</b>	<b>Core melt</b>	<b>Vessel melt through</b>
Duration of core damage state (h)	0.5	1.3	2.0
Core uncover duration at which this core damage state begins (h)	0.0	0.5	1.8
Noble gases	0.05	0.95	0
Halogens	0.05	0.35	0.25
Alkali metals	0.05	0.25	0.35
Tellurium group	0	0.05	0.25
Barium, strontium	0	0.02	0.1
Noble metals	0	0.0025	0.0025
Cerium group	0	0.0005	0.005
Lanthanides	0	0.0002	0.005

*Source:* Table 3-13 from NUREG-1465 (Soffer et al. 1992)

**Table 2.5 Elements in Revised STCP Categories**

<b>STCP Category</b>	<b>Category name</b>	<b>Elements</b>
1	Noble gases	Xe, Kr
2	Halogens	I, Br
3	Alkali metals	Cs, Rb
4	Tellurium group	Te, Sb, Se
5	Barium, strontium	Ba, Sr
6	Noble metals	Ru, Rh, Pd, Mo, Tc, Co
7	Cerium group	La, Zr, Nd, Eu, Nb, Pm, Pr, Sm, Y, Cm, Am
8	Lanthanides	Ce, Pu, Np

*Source:* Table 3-8 from NUREG-1465 (Soffer et al. 1992)

include data for 1 h and 24 h of hold-up in the containment, STDose adjusts these data for the actual hold-up time entered by the user. If the hold-up time entered is less than 1 h or greater than 24 h, the data for the respective time is used as shown. If the holdup time is between 1 h and 24 h, then STDose does a linear interpolation to determine the data to use at the time selected.

After the correct data are selected, STDose scales the monitor reading entered by the user to account for the difference in the reactor power used to produce the figure and the reactor power entered by the user in the accident scenario. This scaled monitor reading,  $R$ , is calculated by

$$R = \frac{3000 \times MR}{\text{Power}} , \quad (2.4)$$

where

MR = the containment monitor reading entered,

Power = the reactor power [MW(t)].

STDose then determines which of the core-damage states or coolant conditions fall between the 1 and 100% level. Containment monitor readings can represent either (1) in-vessel melt or gap core-damage states, or (2) normal or spiked coolant conditions. If no other data are available, STDose assumes that any reading that falls between 100% of spiked coolant and 1% of vessel melt represents gap activity. A reading greater than 1% vessel melt is assumed to be vessel melt. A reading representing between 1% and 100% spiked coolant is assumed to be spiked coolant. A reading of less than 1% spiked coolant is assumed to be normal coolant. If the user enters a core uncover time, it can be used to distinguish between the overlapping scales of the gap and in-vessel core-damage states. For example, if the core of a PWR has been uncovered less than 30 min, the reading must represent gap activity.

When STDose determines that the estimated core-damage state is gap or in-vessel melt, it then computes the fraction of either state that the reading represents. This percentage cannot be more than 100%. The percentage,  $P$ , of the damage state selected is calculated by

$$P = 100 \times \frac{R}{P_{1D}} , \quad (2.5)$$

where

$P_{1D}$  = the meter reading assumed for 1% of the core-damage state for a 3000 MW(t) reactor.

If the monitor reading represents spiked coolant, STDose uses a spiking factor of 100. This factor is used because it is the factor used in determining the monitor responses to spiked coolant shown in Figures 2.1-2.8.

The calculations based on monitor readings should provide the maximum reading expected under the conditions stated. The calculations assume (1) a prompt release to containment of all the fission products

in the coolant, spiked coolant, gap, or in-vessel melt; (2) uniform mixing in the containment; and (3) an unshielded monitor that can see a large fraction of the containment volume. Because the mix is most likely different from that assumed in the calibration of the monitor, the actual reading at the upper end of the scale could differ by a factor of 10–100 if a shielded detector is used for the higher radiation measurements.

The levels of damage indicated in the figures should be considered minimum levels unless there are inconsistent monitor readings. Inconsistent readings may be caused by uneven mixing in containment [e.g., steam rising to top of dome or not enough time for uniform mixing to occur (it may take hours)].

### 2.1.3 Coolant Sample

When the user enters the activity in a coolant sample, it completely defines the activity available for release. No further calculations are performed. It cannot be used to estimate the core-damage state. The activity can be released only through a steam generator tube rupture or containment bypass.

### 2.1.4 Containment Air Sample

When the user enters the activity in a containment air sample, it completely defines the activity available for release. No further calculations are performed. It cannot be used to estimate the core-damage state. A containment air sample cannot be used to define the activity released in a steam generator tube rupture or containment bypass.

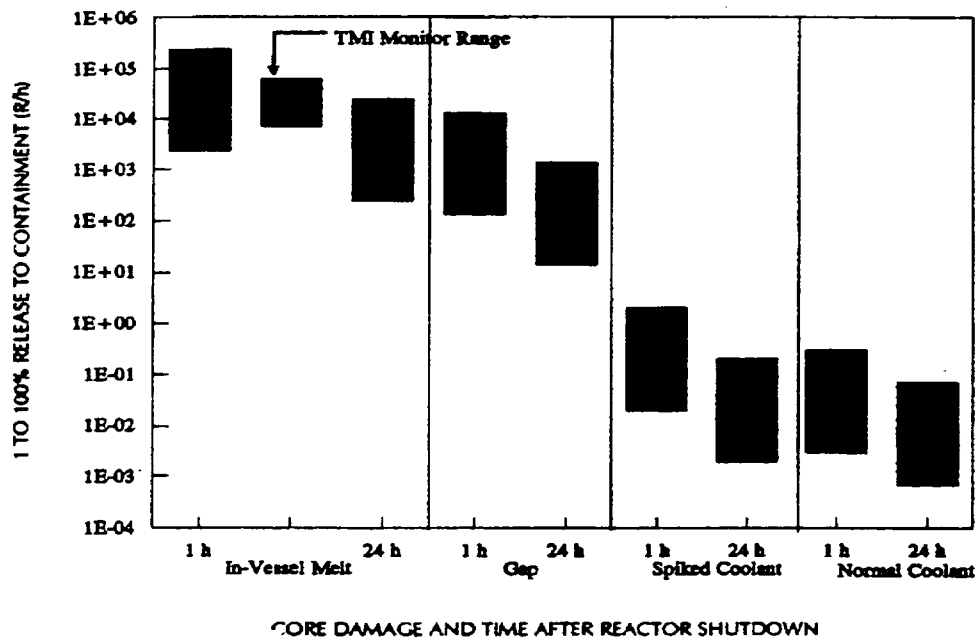


Figure 2.1 PWR Containment Monitor Response (sprays on).

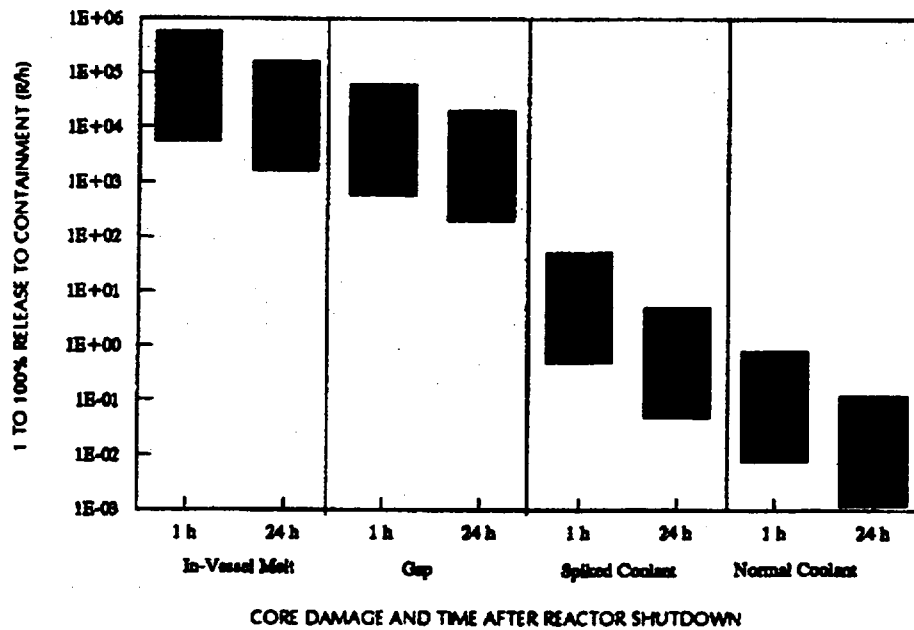


Figure 2.2 PWR Containment Monitor Response (sprays off).

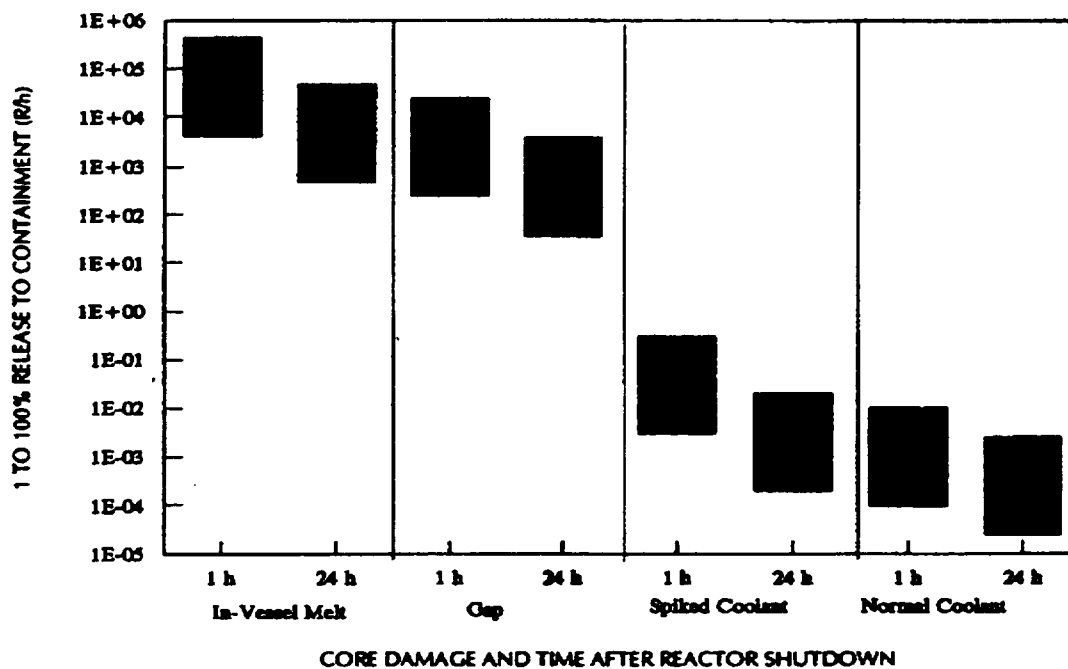


Figure 2.3 BWR Mark I & II Dry Well Containment Monitor Response (sprays on).



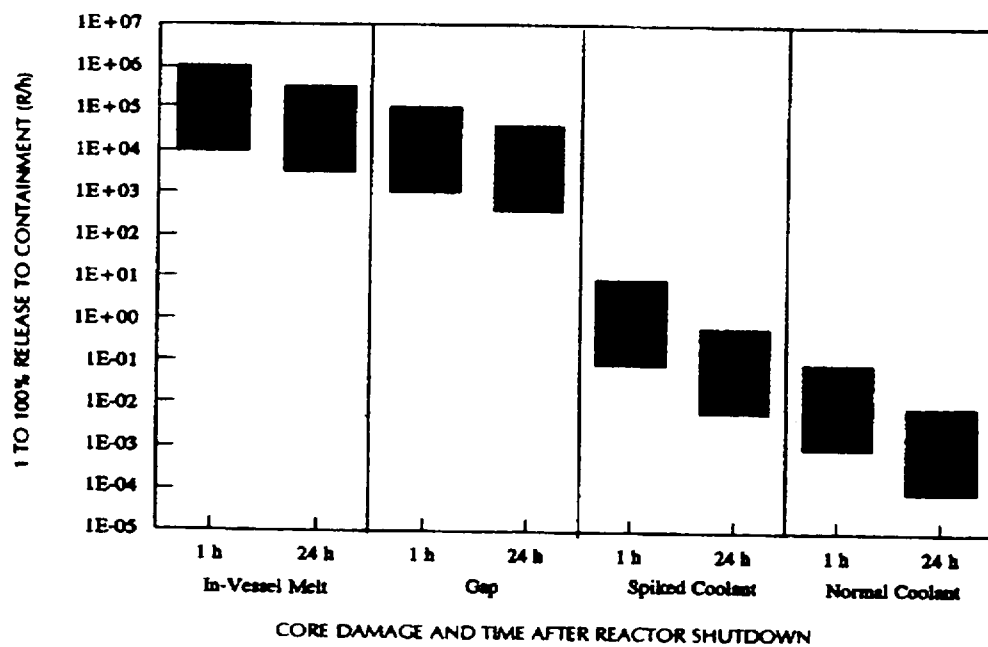


Figure 2.4 BWR Mark I & II Dry Well Containment Monitor Response (sprays off).

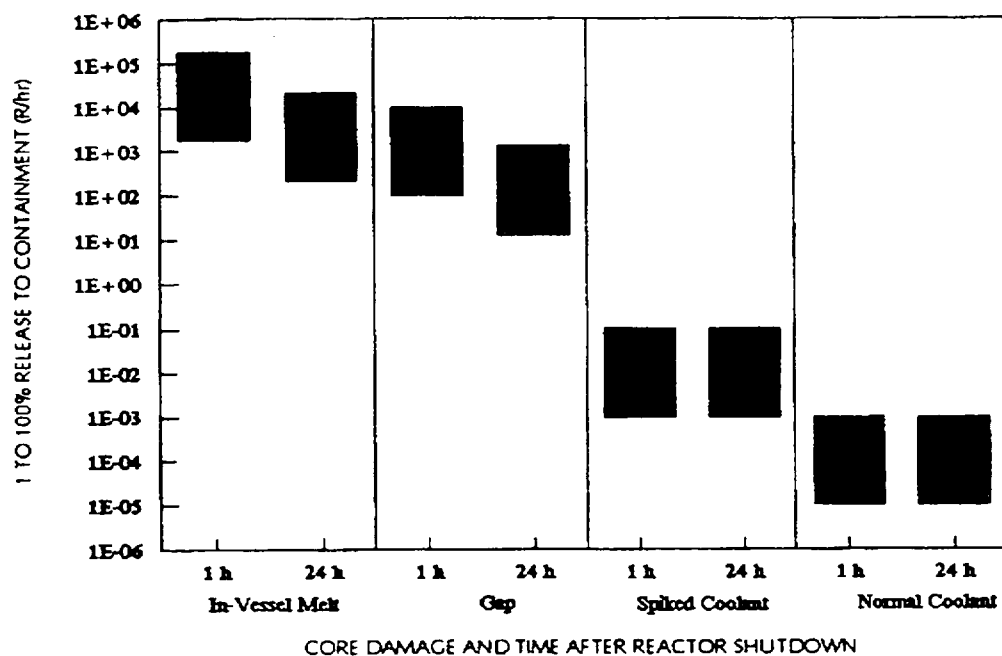


Figure 2.5 BWR Mark I & II Wet Well Containment Monitor Response (sprays on).

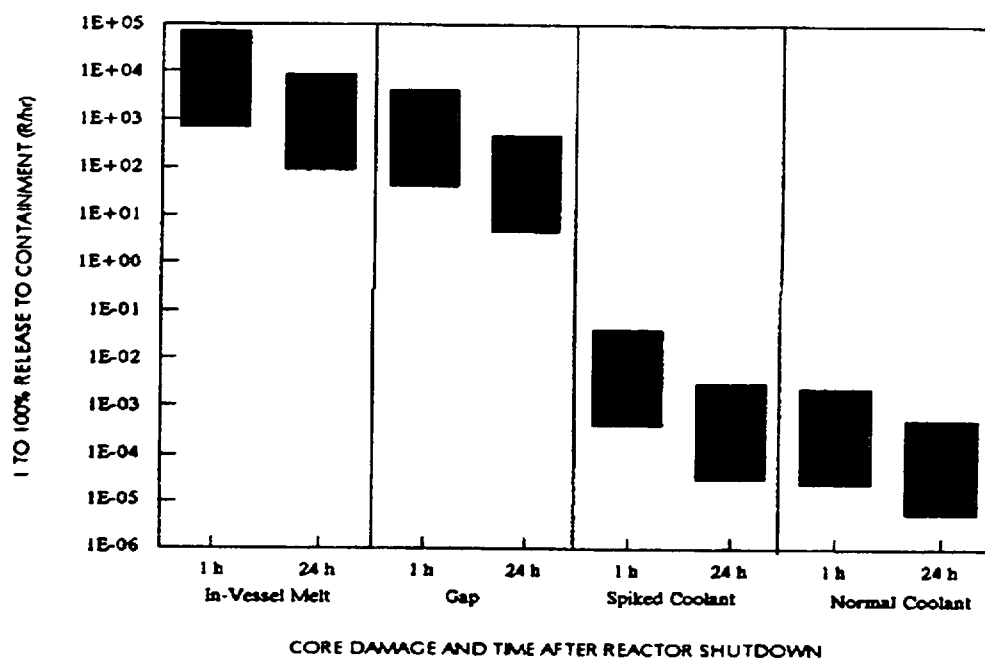


Figure 2.6 BWR Mark III Dry Well Containment Monitor Response (sprays on).

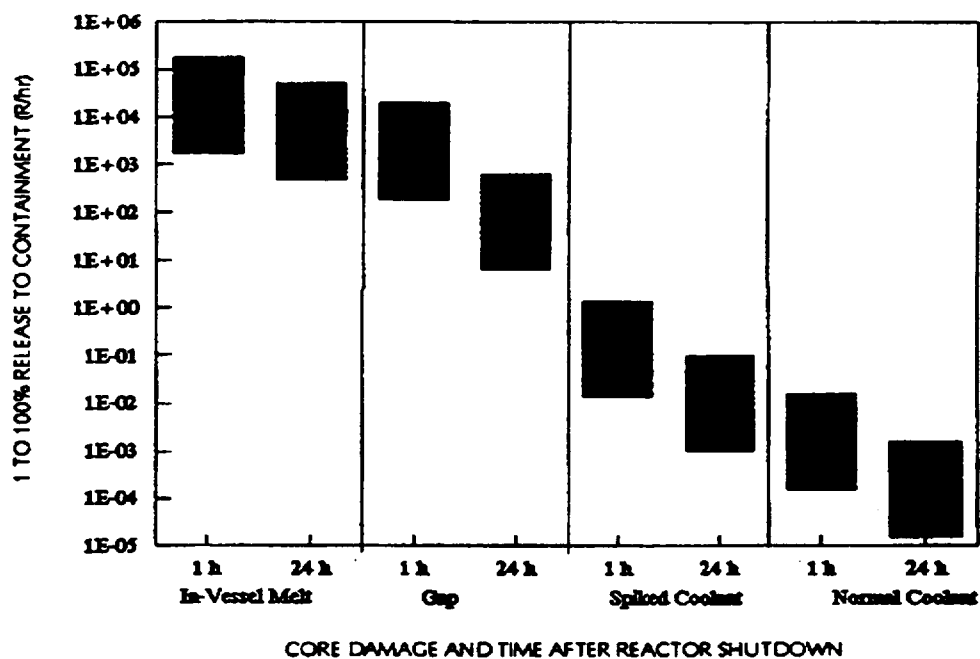


Figure 2.7 BWR Mark III Dry Well Containment Monitor Response (sprays off).

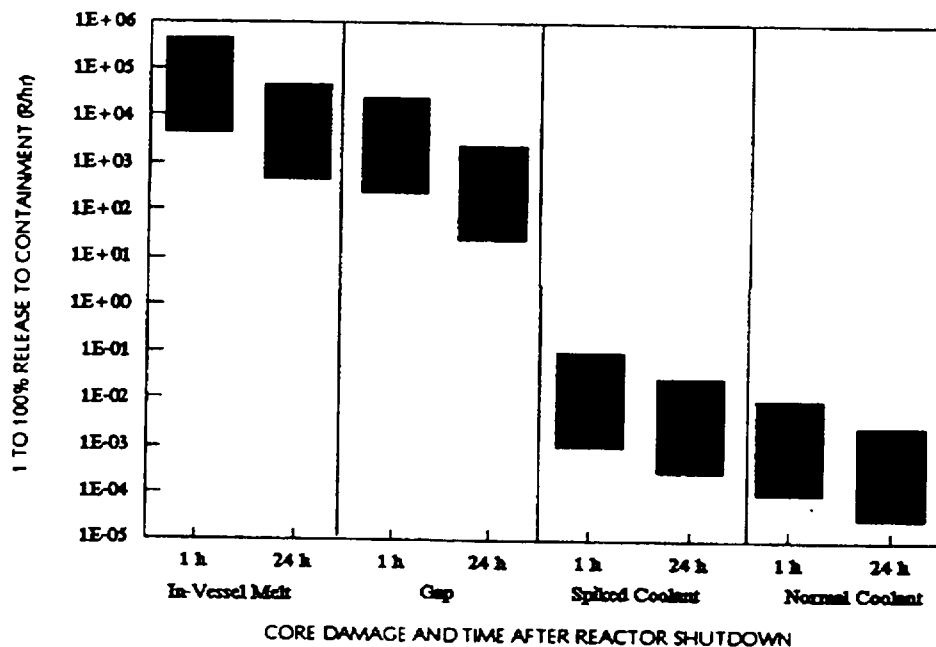


Figure 2.8 BWR Mark III Wet Well Containment Monitor Response.

### 2.1.5 User-Defined Core Damage Estimate

The user can select a core-damage state directly. The state selected may be “none,” increased fuel pin leakage, 1 to 100% of cladding failure, 1 to 100% of core melt, or 100% vessel melt through. If the user selects “none,” there is no source term and no calculations are performed. Increased fuel pin leakage results in a coolant release. The user may enter a coolant spiking factor from 1 to 1000. The core damage activity release fractions (ARFs) used for each of the other states are shown in Tables 2.3 and 2.4 (Soffer et al. 1992). The source term,  $S_{ij}$ , is then computed as

$$S_{ij} = I_i \times ARF_{ij} \quad (2.6)$$

where  $I_i$  is the inventory of radionuclide  $i$ .

### 2.1.6 Monitored Release – Mixtures

The effluent gross concentrations release rate source term calculation is intended for assessments when the user can enter an activity release rate (i.e., a stack monitor reading) and a release duration and can estimate the radionuclide mix. The user can enter the estimated mix either of two ways: (1) as a core damage state or (2) as the percentages of the release that are represented by each of the eight STCP categories. When the user has selected the mix as a core-damage state, then the mix can be modified by the effects of filters, sprays, retention in a pool, or 2 h of holdup. These factors will change the mix because they affect only the non-noble gases.

When the sample is taken at a time that is later than the start of the release, the nuclide concentrations are first computed at the sample time. Then they are adjusted back to the values they would have had at the start of release time, due to the effects of radiological decay. Daughter ingrowth is not considered here.

STDose computes the source term using Eq. (2.1) without the leakage fraction. First STDose determines the source term that would result for a reactor with a power of 1 MW(t) using the selected radionuclide mix. If the core-damage state is entered, the fractions from Tables 2.3. or 2.4 for that state are used. STDose then scales all activities in the computed mix up (or down) so that they sum to the total amount of activity released. The activity released is determined by the product of the release rate and duration that were entered by the user.

### **2.1.7 Effluent Source Terms**

Two other types of effluent source terms are available: effluent release rates and effluent concentrations. Effluent release rates are simply used as entered. The user is not given the opportunity to enter reduction factors since this option assumes that the user knows what is being released. Up to three sets of rates may be entered along with their start and end times. No decay is calculated in the source term calculation. When effluent concentrations are entered, the user also enters an overall release rate. The amount of activity released is computed as the concentration times the rate times the release duration. Up to three sets of concentrations and rates may be entered. The effluent concentrations may be decayed over a selected time period prior to release to the environment, and decay is calculated over the duration of the release.

## **2.2 ACTIVITY RELEASED IN SPENT FUEL STORAGE ACCIDENTS**

RASCAL calculates releases for three types of spent fuel storage accidents: (1) releases when the fuel stored in a pool is uncovered, the fuel overheats, and the cladding is damaged, (2) releases when the fuel stored in a pool is damaged under water, and (3) releases when an accident causes damage to the cladding of the fuel stored in a dry storage cask and causes the integrity of the dry storage cask to be lost.

For each accident, the activity in the damaged fuel elements is calculated as follows. The activity in the fuel involved at the time of reactor shutdown is first computed. This activity is computed as the number of batches (or assemblies) involved times the fraction of a reactor core that one batch (or assembly) represents times the activity in a full reactor core. By definition, a batch is defined as one-third of the fuel in any core. The number of assemblies per core is specific to the plant selected and is included in the facility database and may be adjusted by the user. The activity in a full reactor core is computed as the reactor power in MW(t) from the database or entered by the user times the core inventory per MW(t) listed in Table 2.2 (McKenna and Giitter 1988) adjusted for the actual burn-up of the fuel as described in Eq. (2.2). Note that the burn-up of the spent fuel may be different than the burn-up of the reactor core. Finally, the activity is reduced to account for radiological decay during the storage period.

### **2.2.1 Spent Fuel Pool**

The spent fuel pool release is based on information from NUREG/CR-6451 (Travis, Davis, and Grove 1997). RASCAL assumes that the fuel in a pool must be uncovered for more than 2 h in order for the fuel to reach 1200°F, the temperature at which cladding failures are expected. This assumption is based on the heat-up rate of 30-day-old fuel. Because it does not give credit for heat removal by steam cooling, this assumption is conservative. No cladding failure or releases are projected if the fuel is uncovered for less than 2 h. After 2 h the fuel is projected to rupture due to internal pressure releasing the “hot gap” fraction of the fission products in the fuel. Only fuel that has been irradiated within the past year for a PWR or 180 days for a BWR is assumed to be able to reach 1200°F after it is uncovered. This is based on the observation that one-year-old fuel required 10 hr or more to reach 1200°F. With steam cooling this fuel is not expected to reach this temperature.

The user enters the number of fuel batches or assemblies that are one, two, and three years old. (No other fuel ages are allowed.) If the reactor is a PWR, the user enters whether the density of the fuel pool racking is high or low. The accident conditions that the user enters are the length of time the fuel is uncovered, if and when the fuel was recovered, and if and when the pool was drained. Because it is assumed that the fuel is uncovered, there is no fission product reduction due to scrubbing in the pool.

Fuel release fractions are shown in Table 2.6 (Travis, Davis, and Grove 1997) by STCP category. RASCAL determines which fuel release fractions to use based on conditions in the pool, the fuel racking, and the fuel age. If the pool is never totally drained, only fuel that has been in storage for one year or less is considered to be damaged and the release fractions used are those for a hot-gap release. In a PWR with high-density pool racking or in a BWR, if the pool is totally drained for at least 2 h all fuel is damaged and the release fractions used are for a fire release. In a PWR with low-density pool racking if the pool is totally drained for at least 2 h a fire release occurs in all fuel that has been in storage for one year or less. Fuel that has been stored for more than one year is involved in a fire release only if there is at least one batch of fuel that has been in storage for one year or less. If all fuel is older than one year, then hot-gap release fractions are used for all the fuel.

A reduction factor of 0.01 is applied to non-noble gas fission products if the user specifies that the release from the building will occur through a filtered vent. The user also specifies the duration of the release and the percentage release rate.

### **2.2.2 Fuel Damaged Under Water**

The spent fuel damaged under water scenario is based on NUREG/CR-6451 (Travis, Davis, and Grove 1997). Fuel that is mechanically damaged under water is assumed to remain cold but experiences cladding failure. This results in a cold gap release. All damaged fuel is assumed to have been stored for the same length of time. A reduction factor of 0.01 is always applied to non-noble gas fission products released from fuel under water to account for scrubbing in the pool. In addition, a reduction factor of 0.01 is applied

**Table 2.6 Fuel Release Fractions Used in Spent Fuel Accidents<sup>a</sup>**

STCP category	Fire <sup>b</sup>	Hot gap	Cold gap
Noble gases	1	0.4	0.4
Halogens	0.7	$3 \times 10^{-2}$	$3 \times 10^{-3}$
Alkali metals	0.3	$3 \times 10^{-2}$	$3 \times 10^{-3}$
Tellurium group	$6 \times 10^{-3}$	$1 \times 10^{-3}$	$1 \times 10^{-4}$
Barium, strontium	$6 \times 10^{-4}$	$6 \times 10^{-6}$	$6 \times 10^{-7}$
Noble metals	$6 \times 10^{-6}$	$6 \times 10^{-6}$	$6 \times 10^{-7}$
Cerium group	$2 \times 10^{-6}$	$6 \times 10^{-6}$	$6 \times 10^{-7}$
Lanthanides	$2 \times 10^{-6}$	$6 \times 10^{-6}$	$6 \times 10^{-7}$

<sup>a</sup>Source: First three columns from Table 3.2 in NUREG/CR-6451 (Travis, Davis, and Grove 1997).

<sup>b</sup>The fire release from a spent fuel pool values are the geometric mean of the high and low fractions presented in the referenced NUREG/CR-6451.

to non-noble gas fission products if the user specifies that the release will be through a filtered vent. The user specifies the duration of the release and the percentage release rate.

### **2.2.3 Release from a Dry Storage Cask**

A release is assumed to occur if an accident causes damage to the cladding of the fuel stored in the cask and causes the integrity of the fuel cask to be lost. It is assumed that only one cask is involved in the accident. The user can define the number of assemblies involved in the accident by selecting the type of fuel cask or by directly entering the number of assemblies. Activity can be released from the cask if there is either major damage to the cask and the fuel elements inside of it or if there is a loss of cooling for more than the thermal limit (24 h). If assemblies are damaged without heating cold gap release fractions in Table 2.6 are used. Loss of cooling results in a hot gap release. The hot gap spent fuel pool release fractions in Table 2.6 are used. In calculating the activities, all fuel in the cask is assumed to have been in storage for the same amount of time. There are no reduction mechanisms to reduce the amount of activity released. The user specifies the duration of the release and the percentage release rate.

No release is assumed to occur if cooling is lost for less than the thermal limit or the cask is engulfed in a fire because the casks are designed to maintain their integrity in those situations.

## 2.3 CALCULATION OF RELEASE REDUCTION FOR REACTOR RELEASE PATHWAYS

Reactor accident release pathways allow consideration of the reduction due to the physical systems that are present. The release pathway selected limits the available reduction mechanisms and the way in which the leak rate can be defined. In nuclear power plant releases, the reduction mechanisms available are dependent on the source term calculation type and the release pathway chosen. Each of the release pathways and reduction mechanisms, and the data used for them, are discussed in more detail below. Six types of release pathways have been defined. Table 2.7 shows which reduction mechanisms are available for each pathway.

Reduction factors (RDF in Eq. 2.1) are applied as scaling factors, as described in NUREG-1228 (McKenna and Giitter 1988). All reduction factors, except fire reduction, are defined for three categories: noble gases (STCP category 1), halogens (STCP category 2), and other particles. Noble gas factors all default to one. RASCAL 3.0 assumes that halogens and other particles have the same reduction. The default values for all reduction factors and their references are included in Table 2.8. In some cases the user can turn reduction mechanisms on and off as the accident progresses. Also, the reduction factors themselves may be modified for filters.

STDose reactor source term calculations include a maximum effectiveness for sprays and a maximum effectiveness for all reduction, excluding filters. See Table 2.8. For each, the appropriate reduction factor or product of reduction factors computed at each time step is compared to the maximum and is not allowed to surpass it.

Steam generator condition does not affect the total amount of activity present; it only reduces the amount of activity released. Activity removed by all other mechanisms is made permanently unavailable for release. Sprays and holdup in containment will not be applied simultaneously, and holdup applies only in large containment or auxiliary buildings. Plate-out apply only to bypass accidents and will not be combined with any other reduction mechanism.

All reduction mechanisms are be characterized by a constant factor except sprays and hold-up. The RDFs for sprays and holdup are computed at each time step as an exponential function of time. Two factors each are used, an "initial"  $\lambda_i$  that is applied only for the initial time interval listed in Table 2.7 and a "continuing"  $\lambda_c$  that is applied thereafter. The reduction factors used for sprays and hold-up are dependent on the total amount of time that each mechanism has been acting. So initially the RDF for sprays or hold-up is

$$RDF = e^{-\lambda T} \quad (2.7)$$

where

T = the total amount of time (h) the sprays or holdup have been acting.

**Table 2.7 Reduction Factors Available in Each Reactor  
Release Pathway**

Pathway Reduction mechanism	Containment leakage	Containment bypass	Wet well leakage	Dry well leakage	Steam generator tube rupture
Fire					
Filters		X <sup>a</sup>	X	X	
Sprays	X	X <sup>a</sup>		X	
Containment holdup	X		X	X	
Plate out (bypass only)		X <sup>b</sup>			
Sub-cooled or saturated pool			X		
Ice condenser	X <sup>c</sup>				
Steam generator—partitioned or not partitioned					X <sup>d</sup>
Steam jet air ejector release					X <sup>d</sup>

<sup>a</sup>Only when through a building

<sup>b</sup>Only if no other reduction is active

<sup>c</sup>PWR with ice condenser only

<sup>d</sup>PWR only

After the amount of time that the reduction mechanism is active has passed the initial time interval,  $T_1$ , the RDF is

$$RDF = e^{-\lambda_1 T_1} \times e^{-\lambda_c (T - T_1)} \quad (2.8)$$

Since the user can enter release and reduction data that changes with time, it is possible to turn the sprays on and off several times. The initial spray,  $\lambda_1$ , applies to (1) all the activity in containment the first time the sprays are turned on, and (2) all the activity that enters the containment the first time that sprays are active. If the sprays are turned off and then turned back on, only the continuing  $\lambda_c$  is used. The initial  $\lambda_1$  for holdup applies only if the sprays were never turned on. Otherwise the continuing  $\lambda_c$  is used.



**Table 2.8 Reactor Reduction Factors**

<b>Reduction</b>	<b>Noble gas</b>	<b>Halogen or Other</b>	<b>Ref. NUREG</b>
Filters	1	0.01	1228
Sub-cooled pool	1	0.01	1228
Saturated pool	1	0.05	1228
Sprays (exponential time dependence)	1	$\begin{matrix} \text{h factor} \\ < 0.25 & e^{-1.2 t} \\ \geq 0.25 & e^{-0.2 t} \end{matrix}$	/CR-4722 (Figure 5)
Containment hold-up (exponential time dependence)	1	$\begin{matrix} \text{h factor} \\ < 2 & e^{-1.2 t} \\ \geq 2 & e^{-0.15 t} \end{matrix}$	1150 App. B
Plate out (containment bypass only)	1	0.4	1228
Ice condenser—no fans or recirculation	1	0.5	1228
Ice condenser - 1 h or more recirculation	1	0.25	1228
Steam generator tube rupture—to secondary	1	0.02	1228
Steam generator tube rupture—not partitioned or solid	1	0.5	1228
Steam generator tube rupture—steam jet air ejector release	1	0.05	1228
Minimum reduction, except for filters	0	0.001	1228
Minimum reduction, sprays only	0	0.03	/CR-4722 (Figure 5)

## 2.4 CALCULATION OF LEAKAGE FACTORS FOR REACTOR ACCIDENTS

Four types of reactor leak rates are used in RASCAL 3.0: (1) percent of total amount per unit time, (2) based on containment pressure and hole size, (3) flow rate (volume or mass per unit time), and (4) a “direct” release, with all activity released during the selected release duration. The types of flow rates available in each type of release pathway are shown in Table 2.9. Because the atmospheric transport models expect the source term to be in terms of a rate, rather than a total amount, the leakage data that the user enters is always converted to a leakage rate fraction (LRF) by STDose.

**Table 2.9 Leak Rate Types Available in each Reactor Release Pathway**

Pathway	%/h	Containment pressure and hole size	cfm, kg/s, gal/m	Direct
Bypass	X		X	X
Containment leakage	X	X		
Wet well	X	X	X	
Dry well	X	X		
Steam generator tube rupture			X	
Reactor Effluent				X

### 2.4.1 Percent per Hour

The %/h release rate releases a fixed fraction of the source term per unit time. The actual leakage rate fraction used is computed based on the length of the time step entered by the user. This release rate results in the source term being released at a constant rate over time.

### 2.4.2 Containment Pressure and Hole Size

The containment pressure and hole size option is available only for a facility with a design pressure and containment volume. In this case, the equation (Blevins 1984) for the mass flow rate, MFR, is

$$MFR = C \left( \frac{\pi D^2}{4} \right) \sqrt{2\rho (P_1 - P_2)g} \quad , \quad (2.9)$$

where

C = 0.63,

D = hole diam,

$\rho$  = density of containment atmosphere,

$P_1$  = pressure in containment,

$P_2$  = atmospheric pressure,

g = acceleration of gravity.

The leakage rate fraction, LRF, of the containment volume atmosphere released, then is

$$LRF = \frac{MFR \times D_R}{\rho V_C} , \quad (2.10)$$

where

$D_R$  = the release duration,

$V_C$  = the containment volume.

When the user enters a containment pressure that is less than atmospheric pressure, STDose sets LRF to zero. STDose does not compute the change in containment pressure. The user may enter changing containment pressures as the assessment proceeds.

### 2.4.3 Flow Rate

When a flow rate is entered by the user, the leakage rate fraction is computed as the flow rate divided by the total volume that contains the source term. This volume may be the containment volume, a building volume, or the coolant volume, depending on the source term type.

### 2.4.4 Direct

In a “direct” release, the leakage rate fraction is computed differently, depending on the source term type. In a bypass release when the activity being released is coolant, the release duration is assumed to be 15 min. In a bypass release when core activity is being released, the release duration is assumed to be the amount of time needed to release all the activity in that core damage state, as listed in Table 2.3. The leakage fraction is set to allow for a release to occur only during the duration selected. For effluent releases the release rates are used as entered by the user. No leakage rate fraction is needed, so none is computed.

## 2.5 REFERENCES

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### 3 FUEL CYCLE AND MATERIALS SOURCE TERM CALCULATIONS IN STDose

The source term calculations in STDose estimate the amount of radioactive (or hazardous) material released based on a wide variety of potential radiological accident scenarios. The source term calculations performed that pertain to fuel-cycle facility and materials accidents can be generally categorized as (1) fuel-cycle facility/UF<sub>6</sub> accidents, (2) uranium fires and explosions, (3) criticality accidents, and (4) isotopic releases (e.g., transportation, materials).

STDose divides the source term calculation into three parts: first, it calculates the amount of activity available for release based on the source term type; second, this activity is reduced, based on the reduction mechanisms that the user has selected for the release pathway; and third, the activity is released according to the release rate selected. This can be shown as

$$S_{ij} = I_i \times ARF_{ij} \times \prod_k RDF_{ik} \times LF_j, \quad (3.1)$$

where

- $S_{ij}$  = is total amount of radionuclide  $i$  released under accident conditions  $j$ ,
- $I_i$  = is inventory of radionuclide  $i$ ,
- $ARF_{ij}$  = is airborne release fraction of radionuclide  $i$  under accident conditions  $j$ ,
- $RDF_{ik}$  = is reduction factor that applies to radionuclide  $i$  for reduction mechanism  $k$ ,
- $LF_j$  = is leakage fraction selected for accident conditions  $j$ .

In RASCAL 3.0, source terms may change with time. Source terms are recomputed at intervals of varying length, called time steps. A new time step starts whenever the user changes any of the time-dependent data or every 15 min, whichever is less. At the end of each time step, the inventory of activity is decremented for the amount of activity released or removed by reduction and the effects of radiological decay, so that no more than the total inventory can be released. Time steps may be no less than 1 min and must be an integral number of minutes. Before passing the source term to the atmospheric transport model, STDose converts the user-selected time steps to the 15-min time steps used by the atmospheric transport models. Note that the type of source term calculation may not change with time. The minimum amount of activity of any one nuclide that will be passed to atmospheric transport models in one time step is  $10^{-15}$  Ci.

STDose allows a single release pathway for each of the fuel-cycle and materials accident types. The release pathways only allow those reduction mechanisms that are possible for that type of accident.

The following discussion of the fuel-cycle and materials STDose calculations is divided into three parts. First all the source term calculations are presented. These are followed by discussions of the reductions possible according to the release pathway. Finally, the calculation of leakage factor is presented.

## 3.1 CALCULATION OF THE AMOUNT OF ACTIVITY AVAILABLE FOR RELEASE IN FUEL CYCLE AND MATERIALS SOURCE TERMS

### 3.1.1 UF<sub>6</sub> Releases from Cylinders and Cascade Systems

Two types of source term scenarios are available that release UF<sub>6</sub>: cascade releases and cylinder releases. Only gaseous diffusion plants have cascades. Cylinder releases can occur at any facility that stores UF<sub>6</sub>.

In the cascade scenario, the user enters the amount of UF<sub>6</sub> in the cascade. This amount may be entered (1) directly or (2) as a total mass, in the pounds of UF<sub>6</sub> per cell and the number of units or cells in the cascade that are involved in the release. STDose assumes that there are ten cells per unit. When the number of cells is entered, the amount of material available is the product of the number of cells times their inventory. When the number of units is entered, this result is divided by ten. The user also enters the maximum fraction of the mass of material in the cascade that is available for release and the rate at which the material escapes from the cascade to its building.

In the cylinder scenario, the user enters the amount of UF<sub>6</sub> in a cylinder release as the mass of the available inventory or as the number of 14-ton, 10-ton, and 2.5-ton cylinders involved. The 2.5-ton cylinder is assumed to contain 2277 kg UF<sub>6</sub>, the 10-ton cylinder is assumed to contain 9539 kg, and the 14-ton cylinder, 12,338 kg. The initial amount of material is the sum of the number of each type of cylinder times the amount of UF<sub>6</sub> in that type of cylinder. The user also enters the rate at which material is escaping from the cylinder. The user enters a maximum fraction of the cylinder that can be released, unless the UF<sub>6</sub> is liquid and the release is caused by a valve failure. In this case, the valve location is used to set the maximum release fraction. The relationship between valve position and release fraction is shown in Table 3.1. (All cylinders are assumed to have the same maximum release fraction and release rate.) All UF<sub>6</sub> releases through a building (or filters) are assumed to convert to UO<sub>2</sub>F<sub>2</sub> and HF prior to release to the atmosphere. All releases of UF<sub>6</sub> that are solid in their cylinders are converted to UO<sub>2</sub>F<sub>2</sub> and HF prior to release to the atmosphere, unless the cylinder is in a fire. UF<sub>6</sub> is converted as 1 kg of UF<sub>6</sub> = 0.88 kg UO<sub>2</sub>F<sub>2</sub> + 0.23 kg HF.

**Table 3.1 UF<sub>6</sub> Release Fractions Based  
on Valve Location**

Valve position	Maximum release fraction
360° — facing up	1.00
270° — facing the side	0.50
180° — facing down	0.25

In both cases, the user enters the uranium enrichment level. STDose converts the mass of  $\text{UF}_6$  to activity using the enrichment level and the specific activity. This conversion is done by interpolation using a spline fit to the data in Table E-4 of NUREG/BR-0150 (McKenna, et. al 1996).

No radiological decay is computed in  $\text{UF}_6$  accident scenarios.

### **3.1.2 Fires and Explosions Involving Uranium Oxide**

In STDose, accidents involving uranium oxide can be modeled as either fires or as explosions. The scenarios available in STDose were selected to span a wide range of possible accidents. Uranium oxide fires may occur in several different types of facilities. In the milling of uranium ore, a fire can occur in a drum of milled ore or during the process of extracting solvent. After the ore is milled, the production of reactor fuel begins with creating a powder from the  $\text{UO}_2$ . Both wet and dry processes are used to produce this powder. Uranium-oxide-contaminated waste can be stored in several forms, and any of these can be involved in a fire. Uranium oxide explosions are characterized as (1) those caused by the detonation of high explosives in contact with the material, (2) those caused by a fire (deflagration), and (3) those caused by a sudden pressure change in the material container (venting). The  $\text{UO}_2$  in the explosion may be in liquid, solid, or powder form, or it simply may be surface contamination.

For all cases, the user enters the amount of material ( $\text{UO}_2$ ) at risk and its enrichment level. For all cases, the user chooses among a variety of accident conditions. These accident conditions are listed in Tables 3.2 and 3.3 (DOE 1994). Each set of accident conditions is associated with a default set of airborne release fractions (ARFs) and inhalation fractions (IFs). The ARFs and IFs are considered to be conservative. The IF is the fraction of the material released that is expected to be inhaled. The material is defined as all vapors and any particulate material that has a diameter of  $< 10 \mu\text{m}$ . (Note that the IFs are not used in the source term calculation. They are used in the calculation of inhalation dose to reduce the amount of material inhaled.) The default values for the ARFs and IFs are shown in Tables 3.2 and 3.3 (DOE 1994).

STDose calculates the source term by first converting the mass of  $\text{UO}_2$  to U by multiplying by 0.88. Then the amount of material is converted from mass to activity as described in Section 3.1.1. The source term is the product of this activity times the ARF value.

### **3.1.3 Criticality Accidents**

A criticality accident results from the uncontrolled release of energy from an assemblage of fissile material. In RASCAL 3.0, a criticality accident may be modeled using the assumptions in NUREG/CR-6410 (SAIC 1998). In addition, the criticality data may be entered directly by the user. The physical systems modeled are listed in Table 3.4 (SAIC 1998). This table also presents the assumed number of fissions in the first burst of the criticality and the total yield. The assumed amounts of each radionuclide released per  $10^{19}$  fissions are listed in Table 3.5 (SAIC 1998). These values are based on ORIGEN calculations (ORNL 1989).

**Table 3.2 Airborne Release Fractions and Respiration Fractions  
Used in Uranium Oxide Fires<sup>a</sup>**

Type of fire	Condition	ARF	IF
Production process	Dry process	$1 \times 10^{-3}$	1
	Wet process	$3 \times 10^{-5}$	1
HEPA filter	At high temperature	$1 \times 10^{-4}$	1
	Failure	1	1
Incinerator exhaust		$4 \times 10^{-1}$	1
Waste fire	Solid packaged in drums	$5 \times 10^{-4}$	1
	Solid loosely packed	$5 \times 10^{-2}$	1
	Combustible liquid	$3 \times 10^{-2}$	1
	Non-combustible liquid	$2 \times 10^{-3}$	1
Uranium mill	Drum in a fire	$1 \times 10^{-3}$	1
	Solvent extraction	$3 \times 10^{-2}$	1

<sup>a</sup>Source: DOE 1994.

The activity released in a criticality occurs in discrete bursts. In the predefined scenarios, the bursts are assumed to be 10 min apart. The fission may not continue for more than 48 bursts. The number of fissions in all except the first burst is

$$FB = \frac{Y_T - Y_I}{(48 - 1)} \quad (3.2)$$

where

$Y_T$  = the total yield of the criticality (column 3 in Table 3.4),

$Y_I$  = the yield of the initial burst (column 2 in Table 3.4).

To calculate the source term, STDose first determines the initial activity of each radionuclide present as the product of the yield of the first burst (in  $10^{19}$  fissions) and the activity per  $10^{19}$  fissions listed in Table 3.5. For each following time step, STDose: (1) determines if the criticality is still occurring and if enough time has passed for one or more bursts to have occurred, and if so, adds the appropriate activity, (2) reduces the amount of activity for the amount released, and (3) applies radiological decay to the result. A criticality will end when either the total number of allowed bursts have been accounted for or when the “end of criticality” time entered by the user has been reached. Note that if the user selects a release duration that is not long enough to include all 48 bursts, the total activity released will be less than the total yield listed in Table 3.5.



**Table 3.3 Airborne Release Fractions and Respiration Fractions  
Used in Uranium Explosions<sup>a</sup>**

<b>Explosion characteristics</b>	<b>Material form</b>	<b>ARF</b>	<b>IF</b>
Detonation	Liquid	1	1
	Solid	1	$2 \times 10^{-1}$
	Powder	1	$2 \times 10^{-1}$
	Surface contamination	$1 \times 10^{-3}$	1
Deflagration	Liquid	$1 \times 10^{-6}$	1
	Solid	0	0
	Powder	$5 \times 10^{-3}$	$1 \times 10^{-3}$
	Surface contamination	$3 \times 10^{-1}$	
Venting	Liquid	$2 \times 10^{-3}$	1
	Solid	0	0
	Powder	$1 \times 10^{-1}$	$7 \times 10^{-1}$
	Surface contamination	$1 \times 10^{-3}$	1

<sup>a</sup> Source: DOE 1994.

For criticality accidents, the criticality-shine dose is computed with the source term. The shielding thicknesses entered by the user are used only in this calculation. The dose in rem,  $D_{crit}$ , at 10 ft is computed as (Hopper and Broadhead 1998)

$$D_{crit} = D_{gamma} + D_{neutron} \quad (3.3)$$

$$D_{gamma} = 1 \times 10^{-15} \times F \times e^{-(0.386 \times S + 0.147 \times C + 0.092 \times W)} \quad (3.4)$$

$$D_{neutron} = 1 \times 10^{-14} \times F \times e^{-(0.256 \times S + 0.240 \times C + 0.277 \times W)} \quad (3.5)$$

**Table 3.4 Fission Yields Used in Criticality Calculations<sup>a</sup>**

<b>System modeled in the scenario</b>	<b>Initial burst yield (fissions)</b>	<b>Total yield (fissions)</b>
Solution < 100 gal	$1 \times 10^{17}$	$3 \times 10^{18}$
Solution > 100 gal	$1 \times 10^{18}$	$3 \times 10^{19}$
Liquid/powder	$3 \times 10^{20}$	$3 \times 10^{20}$
Liquid/metal pieces	$3 \times 10^{18}$	$1 \times 10^{19}$
Solid uranium	$3 \times 10^{19}$	$3 \times 10^{19}$
Solid plutonium	$1 \times 10^{18}$	$1 \times 10^{18}$
Large storage arrays below prompt critical	None	$1 \times 10^{19}$
Large storage arrays above prompt critical	$3 \times 10^{22}$	$3 \times 10^{22}$

<sup>a</sup>Source: SAIC 1998.

where

- F = the total number of fissions,
- S = the thickness of steel shielding in inches,
- W = the thickness of water shielding in inches,
- C = the thickness of concrete shielding in inches.

Doses,  $D_{crit_i}$ , (rem) at other distances,  $D_i$  are computed as:

$$D_{crit_i} = \left( \frac{10}{D_i} \right)^2 \times D_{crit} \quad (3.6)$$

### 3.1.4 Isotopic Source Terms

Three types of isotopic source terms are available: (1) isotopic release rates, (2) isotopic concentrations, and (3) sources and materials in a fire. Uranium oxide fires were discussed in Section 3.1.2.

Isotopic release rates are simply used as entered. The user may not enter reduction factors, since this calculation assumes that the user knows exactly what is being released. Up to three sets of rates may be entered along with their start and end times. No decay is calculated in the source term calculation.

When isotopic concentrations are entered, the user also enters an overall release rate. The amount of activity released is computed as the concentration times the rate times the release duration. Up to three sets of concentrations and rates may be entered. The isotopic concentrations may be decayed over a selected time period prior to release, and decay is calculated over the duration of the release.

**Table 3.5 Activity (Ci) Released in Criticality  
of  $10^{19}$  Fissions<sup>a</sup>**

<b>Radionuclide</b>	<b>Activity (Ci)</b>	<b>Radionuclide</b>	<b>Activity (Ci)</b>
Kr-83m	1.5E2	I-131	7.3E0
Kr-85m	8.9E1	I-132	1.0E3
Kr-85	1.3E-5	I-133	1.7E2
Kr-87	1.1E3	I-134	4.2E3
Kr-88	6.6E2	I-135	5.0E2
Kr-89	4.6E4	Sr-91	3.2E2
Xe-133m	1.9E-2	Sr-92	1.2E3
Xe-133	2.7E-3	Ru-106	2.0E-2
Xe-135m	3.3E2	Cs-137	1.0E-2
Xe-135	5.2E0	Ba-139	2.4E3
Xe-137	2.4E4	Ba-140	1.1E1
Xe-138	1.0E4	Ce-143	1.0E2

<sup>a</sup>Source: SAIC 1998.

In a fire release, the user enters the amount of each radionuclide present. The amount of material released is reduced by the fire reduction factors. No other types of reduction are allowed. The default values for these fire reduction factors are from NUREG/BR-0150 (McKenna, et al. 1996). They are shown in Tables 3.6 and 3.7. The default fire release fractions are supplied for each element. The user can also enter these fractions directly.

For all types of isotopic releases, if the user selects release units in mass, rather than activity, the source term is converted to Curies using the specific activity of each radionuclide. The user may specify the enrichment level for enriched uranium. The enrichment level for natural uranium is assumed to be 0.7% (McKenna, et al. 1996, Table E-5). Specific activity is computed as described in Section 3.1.1. For natural and enriched uranium, radiological decay and dose are calculated assuming the properties of  $U^{238}$

and  $U^{234}$ , respectively.  $U^{234}$  is used rather than  $U^{235}$  because  $U^{234}$  has a specific activity about 3 orders of magnitude higher than that of  $U^{235}$ .

**Table 3.6 Fire Release Fractions by Compound Form<sup>a</sup>**

Form of compound <sup>b</sup>	Release fraction <sup>c</sup>
Noble gas	1.0
Very mobile form	1.0
Volatile or combustible compound	0.5
Carbon	0.01
Semivolatile compound	0.01
Nonvolatile compound	0.001
U and Pu metal	0.001
Nonvolatile in a flammable liquid	0.005
Nonvolatile in a non-flammable liquid	0.001
Nonvolatile solid	0.0001

Source: <sup>a</sup>Table F-2, McKenna et al. 1996.

<sup>b</sup>If the compound form is not known, the user enters the fire release fractions in Table 3.6.

<sup>c</sup>The fire release fraction is the fraction of the isotope released when the material is involved in a fire; it equals the total activity released (Ci) divided by the activity involved in fire (Ci).

### 3.2 CALCULATION OF RELEASE REDUCTION FOR EACH FUEL CYCLE AND MATERIALS RELEASE PATHWAY

Most fuel cycle and materials accident release pathways allow consideration of the reduction caused by the physical systems that are present. The release pathways limit the available reduction mechanisms and the way in which the leak rate can be defined. Each of the release pathways and reduction mechanisms and the data used for them are discussed in more detail below. Five types of release pathways have been defined. Table 3.8 shows which reduction mechanisms are available for each pathway.

Reduction factors (RDF in Eq. 3.1) are applied as scaling factors, as described in NUREG-1228 (McKenna and Giitter 1988). All reduction factors, except fire reduction, are defined for three categories: noble gases (STCP category 1), halogens (STCP category 2), and other particles. Noble gas factors all default to one. RASCAL 3.0 assumes that halogens and other particles have the same

reduction. Fire release fractions are element specific. The fire reduction factors are shown in Tables 3.6 and 3.7 and are from NUREG-1140 (McGuire 1998). The default values for all other reduction factors and their references are included in Table 3.8. The default reduction factors for filters and “other” reduction may be modified by the user.

The calculation of the total reduction factor includes a maximum effectiveness for sprays and a maximum effectiveness for all reduction, excluding filters (see Table 3.9). For each, the appropriate reduction factor or product of reduction factors computed at each time step is compared to the maximum and is not allowed to surpass it.

All reduction mechanisms are constant factors except for the reduction due to the action of sprays. The RDF for sprays is computed at each time step as an exponential function of time. Two factors each are used, an “initial”  $\lambda_i$ , which is only applied for the initial time interval listed in Table 3.9, and a “continuing”  $\lambda_c$ , which is applied thereafter. The reduction factor used for sprays is dependent on the total amount of time that the sprays have been acting. So initially the RDF for sprays is

$$\text{RDF} = e^{-\lambda T} \quad (3.7)$$

where T is the total amount of time (h) the sprays have been acting.

After the amount of time that the reduction mechanism is active has exceeded the initial time interval,  $T_i$ , the RDF is

$$\text{RDF} = e^{-\lambda T_i} \times e^{-\lambda_c (T - T_i)} \quad (3.8)$$

### 3.3 CALCULATION OF LEAKAGE FACTORS FOR FUEL CYCLE AND MATERIALS ACCIDENTS

Three types of leak rates are used in fuel-cycle and materials releases in RASCAL 3.0. They are (1) percent of total amount per unit time, (2) flow rate (volume or mass per unit time), and (3) a “direct” release, with all activity released during the selected release duration. The types of flow rates available in each type of release pathway are shown in Table 3.10. Because the atmospheric transport models expect the source term to be in terms of a rate, rather than a total amount, the leakage data that the user enters is always converted to a leakage rate fraction (LRF) by STDose.

#### 3.3.1 Percent per Hour

The percent per hour (%/h) release rate releases a fixed fraction of the source term per unit time. The actual leakage rate fraction used is computed based on the length of the time step entered by the user. This release rate results in the source term being released at a constant rate over time.

**Table 3.7 Fire Release Fractions by Element<sup>a</sup>**

<b>Element<sup>b</sup></b>	<b>Release fraction<sup>c</sup></b>	<b>Element</b>	<b>Release fraction</b>	<b>Element</b>	<b>Release fraction</b>	<b>Element</b>	<b>Release fraction</b>
H(gas)	0.5	Se	0.01	I	0.5	W	0.01
C	0.01	Kr	1.0	Xe	1.0	Ir	0.001
Na	0.01	Rb	0.01	Cs	0.01	Au	0.01
P	0.5	Sr	0.01	Ba	0.01	Hg	0.01
S	0.5	Y	0.01	La	0.01	Tl	0.01
Cl	0.5	Zr	0.01	Ce	0.01	Pb	0.01
K	0.01	Nb	0.01	Pr	0.01	Bi	0.01
Ca	0.01	Mo	0.01	Pm	0.01	Po	0.01
Sc	0.01	Tc	0.01	Sm	0.01	Ra	0.001
Ti	0.01	Ru	0.1	Eu	0.01	Ac	0.001
V	0.01	Rh	0.01	Gd	0.01	Th	0.001
Cr	0.01	Ag	0.01	Tb	0.01	Pa	0.001
Mn	0.01	Cd	0.01	Ho	0.01	U	0.001
Fe	0.01	In	0.01	Tm	0.01	Np	0.001
Co	0.001	Sn	0.01	Yb	0.01	Pu	0.001
Zn	0.01	Sb	0.01	Hf	0.01	Am	0.001
Ge	0.01	Te	0.01	Ta	0.001		

<sup>a</sup>Table F-3 from McKenna et al. 1996. The release fraction for ruthenium was changed from the value of 0.01 in NUREG-1140 to a value of 0.1. NUREG-1140 assumed that ruthenium was nonvolatile (McGuire 1998). However, research in NUREG/CR-6218 (Power, Kmetyk, and Schmidt 1994) indicates (in Table 5) that at high temperatures ruthenium starts to become volatile. The ruthenium release fraction of 0.1 is less than the value of 0.5 used in NUREG-1140 for volatile compounds because ruthenium is less volatile than other volatile compounds, becoming highly volatile only at temperatures not normally reached in building fires. The carbon release fraction is appropriate for carbon compounds other than CO<sub>2</sub>. Those compounds deliver most of the dose. The dose conversion factors used for carbon are for those carbon compounds.

<sup>b</sup>If the specific compound form of the isotope is known, Table 3.5 should be used.

<sup>c</sup>The fire release fraction is the fraction of the isotope released when the material is involved in a fire, and equals the total activity released (Ci), users should divide by the activity involved in fire (Ci).

**Table 3.8 Reduction Factors Available in Each  
Fuel Cycle and Materials Release Pathway**

Pathway Reduction mechanism	Isotopic	UF <sub>6</sub> cylinder	Cascade	Criticality	Fire or explosion
Fire	X <sup>a</sup>				
Filters		X <sup>b</sup>			X
Sprays					X
Building retention		X <sup>b</sup>	X <sup>b</sup>		X
Other				X	

<sup>a</sup>Isotopes and materials in a fire only

<sup>b</sup> Factors used may be modified by the user

**Table 3.9 Reduction Factors for Fuel Cycle and Materials**

Reduction	Noble gas	Halogen and Other	Ref. NUREG
Filters	1	0.01	1228
Sprays (exponential time dependence)	1	$\begin{matrix} h & \text{factor} \\ < 0.25 & e^{-12t} \\ \geq 0.25 & e^{-0.2t} \end{matrix}$	/CR-4722 (Fig. 5)
Containment holdup (exponential time dependence)	1	$\begin{matrix} h & \text{factor} \\ < 2 & e^{-1.2t} \\ \geq 2 & e^{-0.15t} \end{matrix}$	1150 App. B
Other reduction	1	1	N/A
Minimum reduction, except for filters	0	0.001	1228
Minimum reduction, sprays only	0	0.03	/CR-4722 (Fig. 5)

**Table 3.10 Leak Rate Types Available in Each Fuel Cycle  
and Materials Release Pathway**

Pathway	%/h	cfm, kg/s, gal/m	Direct
UF <sub>6</sub> cylinder	X	X	
UF <sub>6</sub> cascade		X	X
Criticality	X		
UO <sub>2</sub> fire or explosion			X
Isotopic		X	X

### 3.3.2 Flow Rate

When a flow rate is entered by the user, the leakage rate fraction is computed as the flow rate divided by the total building volume that contains the source term.

### 3.3.3 Direct

In a “direct” release, the user only enters the release duration. The leakage rate fraction is computed differently, depending on the source term type. For the UF<sub>6</sub> cascade and the UO<sub>2</sub> fire or explosion, the leakage rate fraction is set at 100% divided by the release duration. For isotopic releases, those rates are entered by the user. No leakage rate fraction is needed, so none is computed.

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## 4 TRANSPORT, DIFFUSION, AND DOSE CALCULATIONS

RASCAL 3.0 uses Gaussian models to describe the atmospheric dispersion of radioactive and chemical effluents from nuclear facilities. These models have frequently been used in licensing and emergency response calculations made by the NRC staff, [e.g., PAVAN (Bander 1982), XOQDOQ (Sagendorf, Goll, and Sandusky 1982), MESORAD (Scherpelz et al. 1986; Ramsdell et al. 1988), and RASCAL Version 2.0 (Athey et al. 1993)], because they quickly provide reasonable estimates of atmospheric concentrations, deposition, and doses given relatively limited information on topography and meteorology. A straight-line Gaussian plume model, TADPLUME, is used near the release point where travel times are short and plume depletion associated with dry deposition is small. A Lagrangian-trajectory Gaussian puff model, TADPUFF, is used at longer distances where temporal or spatial variations in meteorological conditions or depletion of the plume due to dry deposition may be significant.

This section describes TADPLUME and TADPUFF. It begins with a short theoretical derivation of Gaussian plume and puff models, and then describes the implementation of those models in TADPLUME and TADPUFF. The section concludes with a description of the dose calculations that are embedded in TADPLUME and TADPUFF. Section 5 describes UF6PLUME, a straight-line Gaussian plume model developed to handle the complexities associated with releases of UF<sub>6</sub>.

### 4.1 THEORETICAL BASES FOR GAUSSIAN MODELS

The derivation of the Gaussian models used to describe atmospheric dispersion is discussed in many texts. Various texts including Slade (1968), Csanady (1973), Randerson (1984), and Seinfeld (1986) provide the bases for the following discussion. They may be consulted where additional detail is desired.

Atmospheric dispersion is governed, in part, by a differential equation called the diffusion equation. With a set of assumptions that can reasonably be applied to atmospheric processes, the diffusion equation has a specific, closed-form algebraic solution that is Gaussian. In one dimension, the solution is

$$\chi(x) / Q = \frac{1}{(2\pi)^{1/2} \sigma} \exp \left[ -\frac{1}{2} \left( \frac{x - x_0}{\sigma} \right)^2 \right], \quad (4.1)$$

where

$\chi(x)$  = concentration at a distance  $x$  from the center,  $x_0$ , of the concentration distribution,  
 $Q$  = amount of material released,  
 $\sigma$  = dispersion parameter.

Atmospheric dispersion parameters are functions of either distance from the release point or time since release. They may also be functions of atmospheric stability and surface roughness. Numerous atmospheric dispersion experiments have been conducted to evaluate dispersion parameters and to develop methods to predict dispersion-parameter estimates from readily available data. A number of these experiments are described by Draxler (1984).

#### 4.1.1 Gaussian Puff Model

The one-dimensional solution of the diffusion equation can be expanded to three dimensions using the principle of superposition to get the basic Gaussian puff model. In a Cartesian coordinate system with  $x$  and  $y$  axes in a horizontal plane and  $z$  in the vertical, the normalized concentration in the vicinity of the puff is

$$\chi(x, y, z) / Q = \frac{1}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \exp\left[-\frac{1}{2}\left(\frac{x-x_0}{\sigma_x}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{y-y_0}{\sigma_y}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{z-z_0}{\sigma_z}\right)^2\right]. \quad (4.2)$$

This equation, when combined with a transport mechanism to move the center of the puff ( $x_0, y_0, z_0$ ), is a simplified version of TADPUFF, the puff model in RASCAL 3.0. The dispersion parameters are shown as functions of direction from the puff center. However, in most implementations of the puff model, the puff is assumed to be symmetrical in the  $x$  and  $y$  directions. Hence,  $x$  and  $y$  may be replaced by the horizontal distance  $r$  from the center of the puff.

As shown previously, the height of the center of the puff is sufficient for vertical dispersion to proceed unimpeded either by the ground or by an elevated layer of the atmosphere. Unimpeded vertical dispersion is generally not the case. Typically, the earth's surface and the top of the atmospheric mixing layer are assumed to be reflective surfaces. When these assumptions are made, the vertical exponential term

$$\exp\left[-\frac{1}{2}\left(\frac{z-z_0}{\sigma_z}\right)^2\right]$$

is replaced by a sum of exponential terms that account for reflection. This sum is

$$\sum_{n=-\infty}^{\infty} \left\{ \exp\left[-\frac{1}{2}\left(\frac{2nH - h - z}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{2nH + h - z}{\sigma_z}\right)^2\right] \right\},$$

where  $H$  is the height of the top of the mixing layer, and  $h$  is the release height. In practice, only a small number of terms need be considered. In RASCAL 3.0, as in MESORAD (Scherpelz et al. 1986; Ramsdell, et al. 1988) and earlier versions of RASCAL, the summation is carried out from  $n = -2$  to  $2$ . This term can be simplified if one or more of  $H$ ,  $h$ , or  $z$  equals zero. For example if  $H$  is large compared to  $\sigma_z$  and  $z$  is zero, the summation may be replaced by

$$2 \exp\left[-\frac{1}{2}\left(\frac{h}{\sigma_z}\right)^2\right].$$

At long down-wind distances where the vertical dispersion parameter is the same magnitude as the mixing layer thickness, the puff model can be further simplified by assuming that material is uniformly

distributed in the vertical. With this last assumption, the puff model becomes

$$\chi(r)/Q = \frac{1}{2\pi\sigma_r^2 H} \exp\left[-\frac{1}{2}\left(\frac{r}{\sigma_r}\right)^2\right], \quad (4.3)$$

where  $H$  is the mixing layer thickness. RASCAL switches to the uniformly mixed model when  $\sigma_z > 1.05H$ .

#### 4.1.2 Straight-Line Gaussian Plume Models

Puff models represent plumes as a series of puffs. Concentrations at a point in the plume are calculated by adding the concentrations at the point associated with all puffs in the vicinity of the point. In effect, the puff models perform a numerical time integration of concentration as puffs pass by the point. Near a release point, the meteorological conditions may be assumed to be constant as the puff moves from the source to the receptor. If the wind speed is assumed to be much greater than zero and the point for which the concentration is to be calculated is sufficiently far down wind that the change in dispersion parameters with distance as puffs pass the point can be neglected, then the puff model can be integrated analytically to give a plume model.

Assuming that the  $x$ -axis is aligned with the mean transport direction and that the mean wind speed is  $u$ , then the average concentration during plume passage is given by

$$\chi(x,y,z) = \int_{t=-\infty}^{t=\infty} \frac{Q'F_yF_z}{(2\pi)^{3/2}\sigma_x(x)\sigma_y(x)\sigma_z(x)} \exp\left[-\frac{1}{2}\left(\frac{x-ut}{\sigma_x(x)}\right)^2\right] dt, \quad (4.4)$$

where

$\chi$  = average concentration,  
 $Q'$  = release rate,  
 $F_y, F_z$  = lateral and vertical exponential terms, shown above,  
 $x$  = down-wind distance at which  $\sigma_x$ ,  $\sigma_y$  and  $\sigma_z$  are evaluated,  
 $u$  = wind speed,  
 $t$  = time.

On integration, the plume model becomes

$$\chi(x,y,z)/Q' = \frac{F_yF_z}{2\pi u\sigma_y\sigma_z}, \quad (4.5)$$

which is a simplified version of TADPLUME, the straight-line Gaussian model used in RASCAL. The straight-line Gaussian plume model for ground-level releases is frequently given as

$$\chi/Q' = \frac{1}{\pi u \sigma_y \sigma_z} \exp \left[ -\frac{1}{2} \left( \frac{y}{\sigma_y} \right)^2 \right], \quad (4.6)$$

where  $F_y$  in Eq. (4.5) is the exponential term in Eq. (4.6). When the release and receptor are at ground level and  $H$  is large, the sum of exponential terms that comprise  $F_z$  has a value of 2. Hence, the constant 2 in Eq. (4.5) does not appear in Eq. (4.6).

Another assumption that deserves comment is that the meteorological conditions are assumed to be horizontally homogeneous and stationary. This means that the wind direction and speed responsible for transporting the plume from the release point to the receptor and the turbulence responsible for diffusion are assumed not to change with location throughout the model domain. It also means that the meteorological conditions do not change as a function of time during the release and time required for transport. Together, these assumptions constrain the usefulness of the straight-line plume model to estimating concentrations and doses at receptors near the release point for short-duration releases; at longer distances another model is required.

#### 4.1.3 Treatment of Calm Winds

The Gaussian puff model behaves well in calm winds. If the dispersion parameters are a function of time, as they are in many models, the material in the puff continues to disperse even though it isn't moving. If, as in RASCAL 3.0, the dispersion parameters are calculated as the function of travel distance, dispersion ceases during calm winds, and the material distribution remains unchanged as long as the wind is calm. In either case, deposition, depletion, exposures, and doses are calculated just as they are during windy conditions.

The straight-line Gaussian plume model in Eq. (4.5) tends to over estimate concentrations and doses during low-wind speed conditions and becomes undefined for calm wind conditions because wind speed is in the denominator. This behavior is the result of the derivation of the straight-line Gaussian plume model assumes that the wind speed is significantly greater than zero thus eliminating a portion of the solution of the dispersion equation that deals with low-wind speed diffusion. To compensate for the missing part of the solution, many straight-line models assume a wind speed of 0.5 to 1 m/s when calm winds are encountered. However, this assumption does not address the other aspect of calm winds — the lack of a well-defined wind direction. No entirely satisfactory wind direction assumption exists for calm winds for a model such as RASCAL.

When the wind speed falls below 0.447 m/s (1 mph), TADPLUME switches from the standard Gaussian plume model previously described to a plume model derived by Frenkiel (1953). In this model, described by Csanady (1973) and Kao (1984), the dispersion parameters ( $\sigma_x$ ,  $\sigma_y$ ,  $\sigma_z$ ) are assumed to be functions of along wind, cross wind, and vertical turbulence levels ( $\sigma_u$ ,  $\sigma_v$ ,  $\sigma_w$ ) and travel time (e.g.,  $\sigma_y = \sigma_v t$ ). With this assumption,

$$\chi/Q' = \frac{\sigma_u \exp \left( -\frac{U^2}{2\sigma_u^2} \right)}{(2\pi)^{3/2} \sigma_v \sigma_w r^2} \left[ 1 + \left( \frac{\pi}{2} \right)^{1/2} \frac{Ux}{\sigma_u r} \exp \left( \frac{U^2 x^2}{2\sigma_u^2 r^2} \right) \operatorname{erfc} \left( -\frac{1}{2^{1/2}} \frac{Ux}{\sigma_u r} \right) \right], \quad (4.7)$$

where  $r$  is a pseudo-diagonal distance from a point directly above the release point to the intake.

The definition of  $r$  is

$$r^2 = x^2 + \left(\frac{\sigma_u}{\sigma_v}\right)^2 y^2 + \left(\frac{\sigma_u}{\sigma_w}\right)^2 z^2, \quad (4.8)$$

where

- $x$  = the downwind distance,
- $y$  = the cross wind distance from the plume center line,
- $z$  = the vertical distance from the plume center line.

For positions under the center line of a plume,  $y = 0.0$ , and  $z = h_s + \Delta h$ , thus

$$r^2 = x^2 + \left(\frac{\sigma_u}{\sigma_w}\right)^2 (h_s + \Delta h)^2. \quad (4.9)$$

TADPLUME assumes that  $\sigma_u = \sigma_v = 0.4$  m/s and that  $\sigma_w = 0.04$  m/s based on a cursory review of atmospheric turbulence data.

Equation (4.7) is well behaved in low-wind speed conditions and gives finite  $\chi/Q$  values for calm wind (mean wind velocity = 0). As wind speed increases,  $\chi/Q$  values increase to a maximum value for a wind speed in the 1 to 2 m/s range and then decrease as the wind speed continues to increase. The equation is used in TADPLUME for wind speeds between 0.1 and 0.4 m/s. The direction of the  $x$  axis (plume center line) is determined by the wind direction at the release point. During these periods this direction may be the last reported direction.

For calm winds, Eq. (4.7) has a simple form that is similar to the standard Gaussian puff model. It is

$$\chi/Q' = \frac{\sigma_u}{(2\pi)^{3/2} \sigma_v \sigma_w r^2}. \quad (4.10)$$

This equation is used for wind speeds  $< 0.1$  m/s. In this calculation,  $y$  is assumed to be zero, and the resulting  $\chi/Q'$  is a function only of  $x$  and  $z$ . The  $\chi/Q'$  calculated at each distance is applied in all directions.

In TADPLUME use of Eq. (4.9) and Eq. (4.10) is limited to receptors less than 16.1 km (10 mi) from the release point. Calculations are not made for greater distances.

#### 4.1.4 Model Domains

TADPLUME and TADPUFF use different model domains. The TADPLUME domain consists of a

polar grid with receptor nodes at 10° intervals on circles at eight radial distances that may be adjusted to suit the problem at hand. The TADPUFF domain consists of a square Cartesian grid with receptor nodes uniformly spaced throughout the domain. The polar grid has a higher node density near the release point than the Cartesian grid, and conversely, the Cartesian grid has a higher node density in the far field than the polar grid.

In general, the receptor nodes for the two grids do not coincide. This fact leads to apparent discrepancies in the doses reported in the maximum value tables in the model output for the two models for wind directions other than north, east, south, or west. The doses reported for TADPLUME are for the plume centerline at each distance. The doses reported for TADPUFF are the highest doses calculated at nodes at about the nominal distance -- for example, 5 miles. The node with the highest dose may or may not be on plume centerline, and may be nearer or farther from the release point than the nominal distance. When a direct comparison of doses calculated by the two models is desired, the wind direction for the period of calculations should be north, east, south, or west. For these wind directions, both TADPLUME and TADPUFF calculate plume centerline concentrations and doses.

## **4.2 TRANSPORT**

Atmospheric transport refers to the movement of material from the source to downwind receptors. The following two sections describe the treatment of atmospheric transport in RASCAL 3.0.

### **4.2.1 TADPLUME Transport**

TADPLUME is a straight-line Gaussian model. As this name implies, the model assumes straight-line transport based on the wind direction at the time and place of release. TADPLUME rounds the wind direction to the closest 10° as it calculates the transport direction to ensure that the axis of the plume passes directly over receptors. As is common in straight-line Gaussian models, transit time is not considered in determining when material arrives at receptors; material arrives at receptors at the time of release. As a result, dose rates calculated by TADPLUME cannot be used to estimate the time of arrival of a plume at a receptor and are not likely to correspond with dose rates measured in the field. Transit time, calculated using the wind speed at the release height, is used to calculate the decay of radionuclides between the source and the receptors. It is also used to calculate depletion of material in the plume due to wet deposition. Decay calculations are performed at 5-min intervals; depletion is calculated for the full transit time.

### **4.2.2 TADPUFF Transport**

Unlike TADPLUME, TADPUFF explicitly accounts for transit time in all calculations because the model tracks the movement of individual puffs and calculates concentrations and doses based on puff positions. As a result, dose rates calculated by TADPUFF may be used to estimate the time of arrival of a plume and may be compared with dose rates measured in the field. Decay and ingrowth of radionuclides and depletion of the puffs as a result of wet and dry deposition are calculated at 5-min intervals.

TADPUFF differs significantly from TADPLUME in that neither the wind data nor the wind fields are

modified to force the centers of puffs to pass directly over the receptor nodes. As a result, when the wind direction is constant, TADPUFF may not calculate centerline concentrations and doses. However, as time goes by and wind directions change, TADPUFF will give more realistic concentration and dose patterns than TADPLUME. In addition, TADPUFF may give more realistic concentration and dose patterns than TADPLUME when topography modifies the winds because the wind fields used by TADPUFF can be modified to account for topography. The wind data used by TADPLUME are not modified to account for topography.

The movement of puffs is controlled by the wind at the center of the puff as the puffs move through the model domain. The spatial variation of winds is represented in TADPUFF by two-dimensional fields of vectors that give the direction and speed of puff movement. These fields are prepared by the meteorological model discussed in Section 6 and are updated at 15-min intervals based on the available wind data.

Calculation of puff movement is a six-step process. In sequence, the steps are

1. Make an initial estimate of the direction and speed of the puff movement given the current puff position and height above ground using bilinear interpolation (Press, et al. 1986) of the vectors at the nearest nodes of the field;
2. Make an initial estimate of the puff position at the end of the period using the the initial estimates of direction and speed;
3. Make a second estimate of the direction and speed of puff movement using the estimated puff position at the end of the period;
4. Make a second estimate of the puff position at the end of the period using the estimate of direction and speed from step 3;
5. Average the end points calculated in steps 2 and 4;
6. Calculate the final estimate of direction and speed of puff movement using the puff's initial position and the average end point calculated in step 5.

The actual puff movement for the period may take place in one or several steps. The step size is adjusted to ensure adequate accuracy in the integration of concentrations that takes place at receptors. Errors in the integration should be less than 5% at common wind speeds. Larger errors may occur near the release point and in high wind speed conditions, because the minimum step size is 30 s. These larger errors should not be a problem because the plume model output should be used for receptors near the release point.

The vector fields prepared by the meteorological program are for a height of 10 m above ground. These vectors are used for puffs that represent ground-level releases. If the release height is greater than 12 m, a wind-speed profile is used to adjust the transport speed from 10 m to the puff transport height. The profile used to adjust the wind speed considers both surface friction and atmospheric stability (see Section 6.4.2 or Panofsky and Dutton 1984, Sections 6.4-6.6).



### 4.3 DISPERSION PARAMETERS

The horizontal dispersion parameters ( $\sigma_y$  and  $\sigma_z$ ) used in TADPLUME and TADPUFF are based on the results of a large number of dispersion experiments conducted in the 1950s and 1960s. The experiments, which were conducted over relatively flat terrain, typically involved tracer releases ranging from about 10 min to 1 h in duration with ground-level concentration measurements at distances ranging from 100 m to several kilometers. Only a few direct measurements of vertical dispersion parameters ( $\sigma_z$ ) were made. Consequently, vertical dispersion parameters have been estimated with dispersion models using measured values of the horizontal dispersion parameter and measured concentrations. Dispersion parameters have been summarized in many forms. Perhaps the best known summary is the set of dispersion parameter curves called the Pasquill-Gifford curves (Gifford 1976).

Regulatory guidance published by the NRC includes graphic depiction of these curves, and numerical approximations to the curves are included in many computer codes used by the NRC. In RASCAL 3.0, dispersion parameters are estimated using the same basic algorithms that were used in earlier RASCAL versions and are used in other NRC codes including PAVAN (Bander 1982) and XOQDOQ (Sagendorf, Goll, and Sandusky 1982). These parameterizations have generally been attributed to Eimutis and Konicek (1972). However, the  $\sigma_y$  parameterization is properly attributed to Tadmor and Gur (1969), and the  $\sigma_z$  parameterization is properly attributed to Martin and Tikvart (1968).

The basic dispersion parameter relationships used in the NRC codes are

$$\sigma_y = a_y x^{0.9031} \quad (4.11)$$

and

$$\sigma_z = a_z(x) \cdot x^{b_z(x)} + c_z(x) \quad (4.12)$$

where

$x$  = the distance from the release point, in meters,

$a_y$  = a function of stability class,

$a_z$ ,  $b_z$ , and  $c_z$  = functions of stability class and distance.

Table 4.1 gives values for  $a_y$ ,  $a_z$ ,  $b_z$ , and  $c_z$ . Note that 0.9031,  $a_y$ ,  $a_z$ ,  $b_z$  and  $c_z$  are empirical constants evaluated by fitting curves. Of these constants, 0.9031 and  $b_z$  are dimensionless;  $c_z$  has dimensions of meters; and  $a_y$  and  $a_z$  have dimensions of  $m^{(1-0.9031)}$  and  $m^{(1-b_z)}$ , respectively.

**Table 4.1 Constant Values for Calculation of Atmospheric Dispersion Parameters**

		Stability Class						
Distance Range (m)		A	B	C	D	E	F	G
$a_y$	all x	0.3658	0.2751	0.2089	0.1471	0.1046	0.0722	0.0481
$a_z$	x < 100 m	0.192	0.156	0.116	0.079	0.063	0.053	0.032
	100 m < x < 1000 m	0.00066	0.0382	0.113	0.222	0.211	0.086	0.052
	1000 m < x	0.00024	0.055	0.113	1.26	6.73	18.05	10.83
$b_z$	x < 100 m	0.936	0.922	0.905	0.881	0.871	0.814	0.814
	100 m < x < 1000 m	1.941	1.149	0.911	0.725	0.678	0.74	0.74
	1000 m < x	2.094	1.098	0.911	0.516	0.305	0.18	0.18
$c_z$	x < 100 m	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	100 m < x < 1000 m	9.27	3.3	0.0	-1.7	-1.3	-0.35	-0.21
	1000 m < x	-9.6	2.0	0.0	-13.0	-34.0	-48.6	-29.2

Atmospheric dispersion experiments did not stop after development of the Pasquill-Gifford curves. However, the emphasis of the experiments did shift. For example, there have been experiments that examined dispersion in the vicinity of buildings and other experiments that examined dispersion under low wind-speed conditions. Ramsdell (1990) describes corrections to the basic dispersion parameter relationships in Eq. (4.11) and (4.12) that improve the dispersion parameter estimates in the vicinity of buildings. These corrections are included in RASCAL 3.0 as an option for ground-level releases.

Enhanced dispersion parameters,  $\Sigma_y$  and  $\Sigma_z$ , are defined as

$$\Sigma_y = (\sigma_y^2 + \Delta\sigma_y^2)^{1/2} \quad (4.13)$$

and

$$\Sigma_z = (\sigma_z^2 + \Delta\sigma_z^2)^{1/2}, \quad (4.14)$$

where the enhancement terms,  $\Delta\sigma_y^2$  and  $\Delta\sigma_z^2$  have the form

$$\Delta\sigma^2(t) = A [1 - (1 + t/T) \exp(-t/T)], \quad (4.15)$$

where

$t$  = transport time (distance divided by the wind speed in TADPLUME and time since release in TADPUFF),

$A_y = 0.5T^2$  ( $T$  is the horizontal time scale for wake turbulence),

$$A_z = 0.5T^2/(2+z/L) ,$$

$$T = B^{1/2}/u^* ,$$

B = projected building area,

u\* = scaling wind speed (friction velocity) calculated from the wind speed, stability, and surface roughness using the wind-profile relationships discussed in Section 6.4.2 ,

z = release height (all releases are assumed to be  $\geq 10$  m),

L = Monin-Obukov length which is a function of stability. Evaluation of L is described in Section 6.4.1

Near the release point, the enhancement terms are primarily functions of wind speed and distance; they are weakly dependent on stability; and they are independent of building dimensions. The enhancement terms increase with increasing distance from the release point until they reach an asymptotic limit that is a function of the building area. The terms are large for low wind speeds and decrease as the wind speed increases. They are negligible for wind speeds above about 4 m/s. This behavior is supported by a recent analysis of dispersion and turbulence data (Ramsdell and Foscire 1998). The results of that analysis also suggests that the enhanced dispersion noted in the vicinity of buildings at low wind speeds in wake dispersion experiments may be as much an artifact caused by underestimation of dispersion by the basic dispersion algorithms (Eqs. 4.11 and 4.12) as it is due to increased turbulence in the vicinity of buildings. Consequently, use of the building wake correction option is recommended for all releases other than isolated stacks.

#### 4.3.1 TADPLUME Dispersion Parameters

The computational algorithms used in TADPLUME calculate dispersion parameters directly from Eqs. (4.11) through (4.15) as the parameters are needed. Equations (4.11) and (4.12) are used for plume releases from isolated stacks and for other releases if the building wake correction is not selected. If the building wake options is selected, all five equations are used.

#### 4.3.2 TADPUFF Dispersion Parameters

In TADPUFF, the wind direction, wind speed, and stability are permitted to change as a function of time and position. As a result, puffs may follow curved trajectories and even return to the release point, and stability may change along the puff's trajectory. If dispersion parameters were calculated directly, as in TADPLUME, discontinuities in the dispersion parameters and possible reduction in plume dimensions with increasing time could occur. Neither condition is consistent with the known characteristics of atmospheric dispersion. Consequently, dispersion parameters for TADPUFF cannot be directly calculated from Eqs. (4.11) through (4.15) as is done in TADPLUME.

In TADPUFF, dispersion parameters are calculated in a four-step process as the puffs move through the model domain.

1. Calculate virtual distances from the puff center to the release point based on the current puff dimensions and the meteorological conditions at the position of the puff. The virtual distances are imaginary distance that, if used in Eq. (4.11) ( $x_{vy}$ ) and Eq. (4.12) ( $x_{vz}$ ) with the meteorological conditions at the puff position, would give the current dispersion parameters;
2. Add the distance to be moved during the next time step to the virtual distances;

3. Calculate the new dispersion parameters using the sums calculated in step 2; and
4. Add the enhancement term, if appropriate.

Separate virtual distances are required for the horizontal and vertical dispersion parameters because the dispersion parameters increase at different rates. The equations for the virtual distances are

$$x_{vy} = \left( \frac{\sigma_y}{a_y} \right)^{1/0.9031} \quad (4.16)$$

and

$$x_{vz} = \left[ \frac{\sigma_z - c_z(x)}{a_z(x)} \right]^{1/b_z(x)} \quad (4.17)$$

Note that these equations are the same as Eqs. (4.11) and (4.12) solved for  $x$  rather than  $\sigma$ .

#### 4.4 MIXING LAYER THICKNESS

The mixing layer thickness is included in all RASCAL 3.0 dispersion calculations. The thickness is passed to the atmospheric dispersion programs in the meteorological data files that are created by the meteorological data processing program. The meteorological data processing program has three options for determining the mixing layer thickness for each station. The thickness may be estimated from meteorological data and surface roughness; it may be estimated from climatological data; or it may be entered directly. See Section 6.4.3 for details related to estimation of mixing layer thickness.

#### 4.5 STACK PLUME RISE

RASCAL estimates final plume rise for stacks using Briggs' equations (1969, 1975, and 1984) as implemented by Petersen and Lavdas (1986) in the INPUFF 2.0 code and Ramsdell, Simonen, and Burk (1994) in the RATCHET code. In general, the numerical constants in the equations are dimensional, and the appropriate metric (SI) units should be assumed.

Plume rise is caused by vertical momentum of the exhaust gases in a stack and buoyancy due to difference in density between the exhaust gases and the atmosphere. Equations for both momentum- and buoyancy- dominated plume rise are included in TADPLUME and TADPUFF. In general, one factor or the other will dominate. For a given set of stack and atmospheric conditions, the temperature difference between the stack effluent and the atmosphere determines which factor is dominant. The initial step in the plume- rise calculation is to determine the critical temperature difference given the stack effluent and atmospheric conditions. If the difference in temperature is less than the critical temperature, plume rise is calculated using momentum-rise equations; otherwise, it is calculated using buoyancy-rise equations. Plume rise is corrected for stack downwash, when the stack exit velocity is less than five times the wind speed.

#### 4.5.1 Unstable and Neutral Atmospheric Conditions

In unstable and neutral atmospheric conditions, plume rise is dominated by momentum if the atmospheric temperature is greater than the effluent. When plume rise is dominated by momentum, the plume rise is estimated using Petersen and Lavdas' Eq. A-9 (1986).

$$\Delta h = 6 r_s w_p u(h_s)^{-1} , \quad (4.18)$$

where

$\Delta h$  = plume rise estimate (m),  
 $r_s$  = stack radius (m),  
 $w_p$  = effluent initial vertical velocity (m/s),  
 $u(h_s)$  = stack height wind speed (m/s).

If the ambient air temperature is less than the effluent temperature, a critical temperature is calculated from either Petersen and Lavdas' Eq. A-3

$$\Delta t_c = 0.0187 w_p^{1/3} T_p r_s^{-2/3} \quad (4.19)$$

or Petersen and Lavdas' Eq. A-4

$$\Delta t_c = 0.00456 \left( \frac{w_p^2}{r_s} \right)^{1/3} T_p , \quad (4.20)$$

where  $\Delta t_c$  is the critical temperature difference (K) and  $T_p$  is the effluent temperature (K). The choice between Eq. (4.19) and (4.20) is based on the value of a buoyancy-flux parameter,  $F_b$ . The buoyancy-flux parameter is defined by Petersen and Lavdas' Eq. A-2 as

$$F_b = g \left[ (T_p - T_a) / T_p \right] w_p r_s^2 , \quad (4.21)$$

where  $g$  is gravitational acceleration (9.8 m/s<sup>2</sup>), and  $T_a$  is the air temperature (°K). If  $F_b$  is less than 55, the critical temperature is given by Eq. (4.19), otherwise it is given by Eq. (4.20). Equation (4.18) is used as long as the temperature difference,  $T_p - T_a$ , is less than  $\Delta t_c$ .

When the temperature difference is greater than  $\Delta t_c$ , the plume rise is calculated using either Petersen and Lavdas' Eq. A-7

$$\Delta h = 21.42 F_b^{3/4} u(h_s)^{-1} \quad (4.22)$$

or Petersen and Lavdas' Eq. A-8

$$\Delta h = 38.71 F_b^{0.6} u(h_s)^{-1} , \quad (4.23)$$

again depending on the value  $F_b$ . Equation (4.22) is used when  $F_b$  is less than 55, otherwise Eq. (4.23) is used.

#### 4.5.2 Stable Atmospheric Conditions

As in unstable and neutral conditions, plume rise is dominated by momentum if the atmospheric temperature exceeds the effluent temperature. If the effluent temperature is greater than the ambient temperature, a  $\Delta t_c$  is calculated to differentiate between momentum- and buoyancy- dominated plumes. The  $\Delta t_c$  is given by Petersen and Lavdas' Eq. A-11

$$\Delta t_c = 0.0196 w_p T_a S^{1/2} , \quad (4.24)$$

where  $S$  is a stability parameter associated with the frequency of vertical oscillation of air parcels in a stable atmosphere. The square root of this parameter is known as the Brunt-Väisälä frequency discussed in texts on the atmospheric boundary layer, e.g., Panofsky and Dutton (1984) or Stull (1988). It is defined by

$$S = g T_a^{-1} \frac{\partial \theta}{\partial z} , \quad (4.25)$$

where  $\partial \theta / \partial z$  is the potential temperature lapse rate shown in Petersen and Lavdas' Eq. A-10. Following Petersen and Lavdas, potential temperature lapse rates of  $0.02^\circ\text{K/m}$  and  $0.035^\circ\text{K/m}$  are assumed in TADPLUME and TADPUFF for Pasquill-Gifford stability classes E and F, respectively. A lapse rate of  $0.05^\circ\text{K/m}$  is assumed for G stability class following Ramsdell, Simonen, and Burk (1994).

In stable conditions when the temperature difference is less than  $\Delta t_c$ , plume rise is momentum dominated and a plume rise estimate is made using Eq. (4.18). The plume rise is also estimated using Petersen and Lavdas' Eq. A-16

$$\Delta h = \frac{1.5}{S^{1/6}} \left( \frac{F_o w_p T_a}{\pi u(h_s) T_p} \right)^{1/3} , \quad (4.26)$$

where  $F_o$  is the stack flow ( $\text{m}^3/\text{s}$ ). The two plume rise estimates are compared, and the smaller value is selected.

When plume rise is determined to be buoyancy dominated in stable conditions, the stack-height wind speed is compared with a critical wind speed to determine whether conditions are calm or windy. The critical wind speed,  $u_c$ , is calculated using Petersen and Lavdas' Eq. A-15

$$u_c = 0.2746 F_b^{1/4} S^{1/8} . \quad (4.27)$$

If the wind speed is less than the critical speed, the plume rise is calculated using Petersen and Lavdas' Eq. A-14)

$$\Delta h = 4.0 F_b^{1/4} S^{-3/8} \quad (4.28)$$

Otherwise, the rise is calculated using Petersen and Lavdas' Eq. A-13

$$\Delta h = 2.6 \left( \frac{F_b}{u(h_s)S} \right)^{1/3} \quad (4.29)$$

### 4.5.3 Effective Release Height

If the isolated stack option is selected in STDose, the plume height is equal to an effective release height. The effective release height has three components: stack height, plume rise, and stack down wash. It is calculated as

$$h_e = h_s + \Delta h + \Delta h_d \quad (4.30)$$

where  $h_s$  is the stack height and  $\Delta h_d$  is the stack down wash. The stack height is entered by the user, and the calculation of plume rise is previously described. Stack down wash occurs when the stack exit velocity is less than or approximately the same magnitude as the stack-height wind speed. It is an aerodynamic effect that reduces the stack height by up to three stack diameters. Down wash is calculated in Petersen and Lavdas' Eq. A-1 as

$$\Delta h_d = 4 r_s \left[ \frac{w_p}{u(h_s)} - 1.5 \right] \quad (4.31)$$

when the ratio between the exit velocity and stack-height wind speed is less than 1.5. Otherwise, the down wash is set to 0.0.

If the isolated stack option is not selected, the release is treated as if it occurs from the surface of the building. A default release height of 10 m is assumed unless another, greater release height is entered.

## 4.6 DEPOSITION

RASCAL 3.0 calculates deposition for iodine and particles using the dry and wet deposition models used in MESORAD (Scherpelz, et al. 1986; Ramsdell, et al. 1988) and earlier versions of RASCAL. The activity deposited each time step is the product of the total deposition rate and the time-step duration. At any time, the surface contamination (activity/m<sup>2</sup>) is the sum of the activity deposited in the current time step plus previously deposited activity.

The dry deposition rate is calculated using a constant deposition velocity of 0.003 m/s (0.3 cm/s). This deposition velocity is used because data summarized by Sehmel (1984) indicate that it is a reasonable value for iodine assuming that about one-third of the iodine in the atmosphere is associated with particles, another one-third is in the form of reactive gases (e.g., I<sub>2</sub> or HI) and the remaining one-third is in the form of non reactive gases (e.g., CH<sub>3</sub>I). A deposition velocity of 0.003 m/s is slightly high for 1 μm particles of other materials. The dry deposition rate is given by

$$\omega'_d = -v_d \chi \quad , \quad (4.32)$$

where  $\omega'_d$  is the deposition rate in (activity/m<sup>2</sup>)/s and  $v_d$  is the dry deposition velocity.

The wet deposition rate is calculated using a washout model. In the washout model, the wet deposition rate is

$$\omega'_w = -\lambda_p \int_0^\infty \chi dz \quad , \quad (4.33)$$

where  $\lambda_p$  is a washout coefficient that is a function of the precipitation type. The washout coefficients used in RASCAL are listed in Table 4.2. These coefficients, which were used in previous versions of RASCAL, are based on analyses of experimental data by Engelmann (1968). TADPLUME and TADPUFF convert the washout coefficients to s<sup>-1</sup> for use in the models. Hanna, Briggs, and Hosker (1982) and Slinn (1984) point out that the washout model is appropriate only for monodisperse aerosols and highly reactive gases.

The total deposition rate at any point is the sum of the dry and wet deposition rates at that point. In TADPLUME, the total deposition rate is a function of position only because the concentration in the plume is a function of position. In TADPUFF, the total deposition rate is a function of position because the concentration varies in space, and meteorological conditions may vary in space. In both models, the total deposition rate is a function of time at a point because both the concentration and precipitation may change with time.

**Table 4.2 RASCAL Washout Coefficients<sup>a</sup>**

Precipitation Type	Washout Coefficient (h <sup>-1</sup> )
1 (light rain)	0.79
2 (moderate rain)	2.2
3 (heavy rain)	4.0
4 (light snow)	0.36
5 (moderate snow)	1.2
6 (heavy snow)	2.3

<sup>a</sup>Source: Engelmann 1968.



RASCAL calculates and stores deposition by radionuclide for all radionuclides except noble gases. Noble gases are assumed not to deposit. However, RASCAL 3.0 does calculate the surface contamination from Xe isotopes that result from decay of iodine, assuming that the Xe is trapped within the remaining iodine. The Xe isotopes are not included in ground-shine dose calculations, but the Cs daughters of Xe are included in the ground-shine dose calculations. In general, the contribution of these daughters to the total dose is small.

#### **4.7 DEPLETION**

Both atmospheric models in RASCAL 3.0 calculate depletion caused by wet deposition; only TADPUFF accounts for depletion from dry deposition. TADPLUME does not account for depletion from dry deposition because the calculation is relatively time consuming, and dry deposition generally does not result in significant depletion of the plume near the source.

In TADPUFF, the activity in the puffs ( $Q$ ) is updated every 5 min. The activity removed from each puff is determined by integrating the total deposition rate under the puff in space and time. In TADPLUME, the fraction of activity remaining in the plume at each distance during periods of precipitation is estimated assuming an exponential decrease in activity with travel time, i.e.,  $Q'(x) = Q_0 \exp(-\lambda_p x/u)$ .

#### **4.8 DECAY AND INGROWTH**

TADPLUME and TADPUFF calculate decay and ingrowth at 5-min intervals for both airborne and deposited radionuclides. The decay schemes used include as many as four progeny and account for branched decay chains. The 5-min decay and ingrowth calculations continue to the end of the calculation period specified by the user. If the duration of the calculation period specified by the user is less than 96 h (4 days), TADPLUME and TADPUFF will continue ground-shine dose calculations until 96 h have elapsed from the beginning of the model run specified by the user. Decay and ingrowth calculations during this extended period are made at 1-h intervals.

#### **4.9 DOSE CALCULATIONS**

One of the areas in which RASCAL 3.0 differs significantly from earlier RASCAL versions is dose calculations. The calculation of dose commitments from inhalation of activity (Section 4.9.1) and the calculation of ground-shine doses (Section 4.9.2) are generally unchanged, except that the dose calculations can now treat temporal variations in the activity release rate and radionuclide mix. The cloud-shine calculations have been revised to improve consistency between the TADPLUME and TADPUFF cloud-shine dose estimates and to decrease TADPUFF computational time. Calculation of open- and closed- window dose rates has been added to both TADPLUME and TADPUFF. The cloud-shine calculations are discussed in Section 4.9.3, and the calculations of open- and closed-window dose rates is discussed in Section 4.9.4.

#### 4.9.1 Organ Committed Dose Equivalents Due to Inhalation

Organ committed dose equivalents and committed effective dose equivalents are calculated for 15-min periods in both TADPLUME and TADPUFF. These dose equivalents are the sums over all radionuclides of products of the exposure to the radionuclide during the 15-min period times a radionuclide and organ specific dose factor and the breathing rate. The general expression for the organ-committed dose equivalents is

$$D_{15} = \sum_n \left[ v_b DF_n \int_0^{15} \chi_n(t) dt \right], \quad (4.34)$$

where

$D_{15}$  = organ-committed dose equivalent due to inhalation during a 15-min period,  
 $v_b$  = breathing rate,  
 $DF_n$  = radionuclide n and organ specific dose factor,  
 $\chi_n$  = radionuclide n concentration,  
 $t$  = time.

Dose factors used in RASCAL 3.0 are from *Federal Guidance Report No. 11* (Eckerman, Wolbarst, and Richardson 1988).

At the end of each 15-min period, the committed dose equivalents at each receptor node are written to TADPLUME and TADPUFF output files. They are then set to zero prior to beginning model calculations for the next 15-min period.

#### 4.9.2 Ground-Shine Doses

TADPLUME and TADPUFF calculate ground-shine dose equivalents as the sum over all radionuclides of product of the surface contamination by the radionuclide and a radionuclide-specific dose factor. The general expression for the ground-shine dose equivalent is

$$D_{gs} = \sum_n \left[ DF_n \int_t^{t+15} \omega_n(t) dt \right], \quad (4.35)$$

where

$D_{gs}$  = dose equivalent during the period,  
 $DF_n$  = radionuclide n specific ground-shine dose factor,  
 $\omega_n$  = radionuclide n surface concentration,  
 $t$  = time.

Note that the integration in Eq. (4.35) is from  $t$  to  $t+15$  min. These integration times are used because the surface concentration at any time is cumulative from the beginning of the event but the dose is set to

zero at the beginning of the period. After the surface is contaminated, ground-shine doses can be incurred, even if airborne material is not present.

### 4.9.3 Cloud-Shine Doses

Earlier versions of RASCAL calculated cloud-shine doses using either a semi-infinite cloud model or a finite-plume model based on the model developed for MESORAD (Scherpelz, et al. 1986). The first of these models assumes that activity is uniformly distributed through a large volume, and the second assumes that activity is concentrated in a finite number of points distributed through a volume to represent the actual activity distribution. The use of the semi-infinite cloud model is usually inappropriate in the immediate vicinity of the release point, and application of the MESORAD finite-plume model to cloud-shine dose estimates near the release point in TADPLUME did not prove satisfactory. Consequently, the cloud-shine dose models in RASCAL 3.0 have been significantly revised from those used in earlier RASCAL versions.

Cloud-shine models based on line sources and plane sources have been developed that are analogous to the point-source model used in MESORAD. These models are used, along with the point-source model, until plumes and puffs grow to sufficient size that the assumptions associated with the semi-infinite cloud model are met. In the MESORAD point-source model, point-source dose rates were calculated as a function of distance for each radionuclide from gamma energies. This calculation, which was repetitive and time consuming, has been deleted. The finite-plume, cloud-shine models in RASCAL 3.0 make use of precalculated dose rate vs distance curves. These curves are provided in the radionuclide database for each radionuclide for a 1 Ci (0.01 Sv) point source, and a 1 Ci/m (0.01 Sv/m) infinite-line source. The remainder of this section describes the RASCAL 3.0 cloud-shine models.

#### 4.9.3.1 TADPUFF Cloud-Shine Dose Calculations

There are three stages in TADPUFF cloud-shine dose calculations. Near the source where puff dimensions are small compared to the mean path length of photons, TADPUFF uses a revised version of the point-kernel dose model used in previous versions of RASCAL. When the puff radius becomes sufficient ( $\sigma_y = 400$  m), cloud-shine dose rates beneath the centerline of the plume are calculated using an infinite-slab model. The dose rate at ground level is calculated assuming that the activity in the plume is equally divided among ten horizontal slabs with slab heights determined by the release height and vertical dispersion coefficients. The change in dose rate with distance from slabs is due only to buildup and absorption of photons; the change in dose rate across the plume is proportional to the crosswind variation of activity concentration in the slab. This model will be discussed further. Finally, when the vertical dimensions of the plume become sufficient ( $\sigma_z = 400$  m), cloud-shine is calculated using a semi-infinite cloud model.

Previous versions of RASCAL used the MESORAD finite-puff, cloud-shine model (Scherpelz et al. 1986, Ramsdell et al. 1988). This model first calculates composite characteristics (photon energies, photons per disintegration, etc.) of the gamma radiation from the radionuclide mix in a puff. Next, the model calculates the dose rate vs distance from a point source having the composite characteristics using

$$D'_p(\rho) = \frac{2.13 \times 10^6}{4\pi\rho^2} \sum_{\gamma} \left[ f_{\gamma} B_{\gamma}(\mu_{\gamma}, \rho) e^{-\mu_{\gamma}\rho} E_{\gamma} T_{\gamma} W_{\gamma} \right], \quad (4.36)$$

where

$D'_p(\rho)$  = dose rate in (rem/h)/Ci,  
 $\rho$  = distance from point source,  
 $f_\gamma$  = fraction of disintegrations producing  $\gamma$ s of energy,  $E_\gamma$ ,  
 $B_\gamma(\mu_\gamma, \rho)$  = buildup factor for air,  
 $\mu_{a\gamma}$  = linear attenuation factor for air,  
 $E_\gamma$  = gamma energy,  
 $T_\gamma$  = mass energy absorption coefficient for tissue ( $\mu_{tr}/\rho$ ),  
 $W_\gamma$  = ratio of whole body dose to surface dose.

The constant  $2.13 \times 10^6$  is a collection of unit conversion constants to give dose rate in (rem/h)/Ci. The components of the constant are described following Eq. 19 in Scherpelz, et al. (1986). Previous versions of RASCAL used a constant value of 592, which gives dose rates in (rem/s)/Ci.

The model then calculates the dose rate at ground level as a function of horizontal distance from the ground-level position of center of the puff. This calculation involves summation over volume elements distributed throughout the puff.

$$D'(r) = \sum_i \sum_j \sum_k D'_p(\rho_{ijk}) M_{ijk} \quad , \quad (4.37)$$

where

$D'(r)$  = dose rate at  $r$ ,  
 $r$  = distance from the receptor to the projection of the puff center on the ground,  
 $i, j, k$  = indices associated with the volume elements,  
 $D'_p(\rho_{ijk})$  = dose rate at distance  $\rho$  from a point source in volume element  $ijk$ ,  
 $\rho_{ijk}$  = distance from the center of the volume element  $ijk$  to the receptor,  
 $M_{ijk}$  = fraction of the total puff activity in volume element  $ijk$ .

For purposes of cloud-shine calculation, puffs were assumed to be circular cylinders with three layers. The volume elements were defined in 3, 5, or 8 annular rings with either 6 or 16 sectors. The fraction of activity in volume elements varied by annulus and level. Finally, the dose at a receptor for a period is accumulated by summing the product of dose rates and the time step for all puffs for all time steps in the period.

In RASCAL 3.0, this process has been modified by eliminating the calculation of composite characteristics from the gamma energies. In its place, the TADPUFF calculates the dose rate vs distance from a point source that has all of the activity in the puff. Thus, Eq. (4.36) is replaced by

$$D'_p(\rho) = \sum_{n=1}^N Q_n D'_{pn}(\rho) \quad (4.38)$$

where

$N$  = number of radionuclides,

$Q_n$  = activity of radionuclide  $n$  in the puff,

$D'_{pn}(\rho)$  = dose rate at distance  $\rho$  from a 1-Ci point source of radionuclide  $n$ .

The overall puff geometry remains the same in TADPUFF as it was in earlier versions of RASCAL. However, the internal geometry has changed. In TADPUFF, the puff is divided into ten layers with each layer containing one-tenth of the activity. The number of annular rings has been fixed at six, with each ring containing one-sixth of the puff activity, and the number of sectors has been fixed at 12. With these changes, the number of volume elements has been increased, and the fraction of activity in each volume element becomes 1/720 of the total activity. In TADPUFF, Eq. (4.37) becomes

$$D'(r) = \frac{1}{720} \sum_i \sum_j \sum_k D'_p(\rho_{ijk}) \quad (4.39)$$

As before, symmetry is used to reduce the computational load.

When the horizontal dispersion parameter reaches 400 m, the puff radius is large enough that the horizontal variations in the cloud-shine dose rate are directly proportional to the horizontal variation in concentration in the puff. At this point, MESORAD changed to a semi-infinite cloud model, and previous versions of RASCAL changed to calculating dose rates beneath the center of the puff using the finite-puff model and dose rates elsewhere using the horizontal variation in concentration. TADPUFF changes from the point-source based cloud-shine model used in earlier versions of RASCAL to a new plane-source based model. The plane-source model assumes that the puff is a vertical cylinder as is assumed in the point-source model. However, rather than assuming that activity is distributed among volume elements, the activity is assumed to be concentrated on ten horizontal slabs (planes).

To calculate the activity in each slab, the concentration at the center of the puff ( $y=0$ ) is first integrated vertically from the bottom of the puff to the top. This is similar to the integration done in calculating the depletion from wet deposition

$$\langle \chi \rangle_n = \int_{-\infty}^{\infty} \frac{Q_n}{(2\pi)^{3/2} \sigma_y^2 \sigma_z} \exp \left[ -0.5 \left( \frac{r}{\sigma_y} \right)^2 \right] \exp \left[ -0.5 \left( \frac{h_e}{\sigma_z} \right)^2 \right] dz = \frac{Q_n}{2\pi\sigma_y^2} \exp \left[ -0.5 \left( \frac{r}{\sigma_y} \right)^2 \right], \quad (4.40)$$

where  $\langle \chi \rangle_n$  is the vertically integrated concentration of radionuclide  $n$  at the center of the puff. This concentration is then divided by the number of slabs (ten) to get the concentration in each slab.

Within the cylinder, the vertical position of the slabs is determined by the effective release height, the mixing-layer thickness, and the vertical-dispersion coefficient. When a Gaussian distribution is partitioned so the area under the curve is divided into ten equal parts and the center of mass of each part is determined, these centers of mass fall at  $\pm 0.127\sigma$ ,  $\pm 0.385\sigma$ ,  $\pm 0.674\sigma$ ,  $\pm 1.037\sigma$ , and  $\pm 1.645\sigma$ . Using this as a basis, the slab heights are initially estimated as  $h_e \pm 0.127\sigma_z$ ,  $h_e \pm 0.385\sigma_z$ ,  $h_e \pm 0.674\sigma_z$ ,  $h_e \pm 1.037\sigma_z$ , and  $h_e \pm 1.645\sigma_z$ . The initial heights may lie below ground level or above the top of the mixing layer. Any heights that fall outside these bounds are adjusted to account for reflection by the

boundaries. Signs of heights that are negative are changed to positive, and heights ( $h_p$ ) that are above the mixing layer are replaced by  $2H-h_p$ .

The dose rate at ground level from a slab is calculated as

$$D'_{sl}(r,z) = \frac{0.1 \sum_n Q_n DF_{pn}}{2\pi\sigma_y^2} \exp\left[-0.5\left(\frac{r}{\sigma_y}\right)^2\right] (1 + k\mu z) \exp(-\mu z) , \quad (4.41)$$

where

$z$  = height of the slab above the receptor, which is assumed to be at 1 m (m),  
 $DF_{pn}$  = dose factor radionuclide  $n$  for an infinite plane [(rem/s)/(Ci/m<sup>2</sup>)],  
 $\mu$  = total gamma ray absorption coefficient for air (m<sup>-1</sup>),  
 $k$  = ratio of energy in scattered photons to absorbed energy.

The infinite plane dose factor is approximated by

$$DF_{pn} = DF_{sien}/241.2 , \quad (4.42)$$

where  $DF_{sien}$  is the semi-infinite cloud dose factor [(rem/s)/(Ci/m<sup>3</sup>)] and 241.2 is a constant with units of meters evaluated by comparing dose rates calculated by Eq. (4.35) with semi-infinite cloud dose rates in plumes for which the semi-infinite cloud model is appropriate. Semi-infinite cloud dose factors contained in *Federal Guidance Report No. 12* (Eckerman and Ryman 1993) are used to estimate the infinite-plane dose factors. These calculations were carried out for 30 radionuclides that are typically released in reactor accidents involving fuel damage. The standard deviation of the estimates of the constant value was 0.04.

In Eq. (4.41), the term  $(1 + k\mu z)$  represents the buildup factor due to scattered photons, and  $\exp(-\mu z)$  represents the absorption of energy by the air. These terms are discussed by Healy and Baker (1968) and Healy (1984). In RASCAL 3.0,  $\mu$  and  $k$  are assumed to be constants with values appropriate for ~0.7 MeV photons ( $\mu=0.01$ ,  $k=1.4$ ) based on Figure 16.4 of Healy (1984).

Ultimately, the dose rate at a receptor is

$$D'_{sl}(r) = \frac{0.1 \sum_n Q_n DF_{pn}}{2\pi\sigma_y^2} \exp\left[-0.5\left(\frac{r}{\sigma_y}\right)^2\right] \sum_{i=1}^{10} (1 + k\mu z_i) \exp(-\mu z_i) , \quad (4.43)$$

where the summation is over all slabs.

When the vertical extent of the puff is sufficient for the semi-infinite cloud model to be appropriate ( $\sigma_z > 400$  m, or a uniformly-mixed plume with a vertical depth  $> 600$  m), the cloud-shine dose rate is calculated using the semi-infinite cloud model

$$D'(r) = [\chi(r)/Q] \sum_n Q_n D'_{\text{slab } n} \quad , \quad (4.44)$$

where  $[\chi(r)/Q]$  is calculated using Eq. (4.2) or a variation thereof, as appropriate. The semi-infinite dose factors from *Federal Guidance Report No. 12* (Eckerman and Ryman 1993) are used in this calculation.

#### 4.9.3.2 TADPLUME Cloud-Shine Dose Calculations

A new set of models has been developed for cloud-shine dose calculations in TADPLUME. These calculations proceed in a manner similar to the calculations in TADPUFF. Near the source, the plume is divided into a large number of equal-strength line sources spaced to properly represent the distribution of activity in the plume. The dose rates from these line sources are used to calculate the ground-level dose rate as a function of horizontal distance from the plume axis. This relationship is then used to calculate dose rates and 15-min doses at receptor locations. When the width of the plume is sufficient ( $\sigma_y = 400$  m), TADPLUME switches from the line-source model to an infinite-slab model. Finally, when the vertical dimensions of the plume are sufficient to make the semi-infinite cloud model appropriate ( $\sigma_z = 400$  m or a uniformly-mixed plume with a thickness of 600 m), TADPLUME switches to a semi-infinite cloud model.

Dose rates from line sources are calculated using

$$D'_i(\rho) = \sum_{n=1}^N Q'_{ln} D'_n(\rho) \quad , \quad (4.45)$$

where

$D'_i(\rho)$  = dose rate (rem/s) at a distance  $\rho$  from an infinite line source of  $Q'_{ln}$  (Ci/m),  
 $Q'_{ln}$  = line-source strength (Ci/m),  $Q'_{ln} = Q'_n / u$  where  $Q'_n$  is in Ci/s,  
 $D'_n(\rho)$  = line-source dose rate factor [(rem/s)/(Ci/m)] for radionuclide  $n$ .

Equation (4.45) is analogous to Eq. (4.38) with changes in the definitions of source term and dose factors.

The line-source dose rates are combined to get the plume dose rate by summing over all line sources, just as the point-source dose rates were combined to get a puff dose rate. The number of line sources used is determined by the horizontal dispersion parameter,  $\sigma_y$ . If  $\sigma_y > 200$  m, 100 lines ( $10 \times 10$ ) are used to describe the concentration distribution in the plume. Otherwise, the concentration distribution is described by 36 lines ( $6 \times 6$ ). In either case, the lines are spaced horizontally and vertically such that all lines represent the same fraction of the activity in the plume. The plume dose rate is given by

$$D'(y) = \frac{C_R}{N_l} \sum_i \sum_j D'_i(y_{ij}) \quad , \quad (4.46)$$

where

$D'(y)$  = plume dose rate ,  
 $y$  = distance from the ground-level projection of the center of the plume,  
 $C_R$  = finite line correction factor,  
 $N_l$  = number of line sources (36 or 100),  
 $i, j$  = line source indices,  
 $D'_l(y_{ij})$  = infinite line, line-source dose rate.

The finite-line source correction factor is included in Eq. (4.46) to account for the fact that the plume does not extend upwind of the release point. A correction factor could be calculated by numerical integration of a rather complex equation. However, an approximate correction factor of adequate accuracy for emergency response dose calculations can be calculated using

$$C_R = 0.5 \left[ 1 + \frac{x}{(R^2 + h_e^2)^{1/2}} \right], \quad (4.47)$$

where

$x$  = downwind distance (m) to a point beneath the plume centerline at the intersection of the plume centerline and a perpendicular line passing through the receptor,  
 $R$  = distance (m) from the release point to the receptor,  
 $h_e$  = effective release height.

In the case of a ground-level release and a receptor on the plume centerline, the correction factor will be one. However, generally the correction factor is less than one. For a 0.7 MeV photon, the correction factor given by Eq. (4.47) corresponds to a receptor at a position approximately 100 m off of the plume centerline. Doses will be slightly over estimated for receptors that are closer than 100 m and slightly under estimated for receptors that are farther than 100 m from the centerline.

When the horizontal dispersion parameter exceeds 400 m, TADPLUME shifts from a line-source based, finite-plume model to an infinite-plane model. The infinite-plane model used by TADPLUME is similar to the model used by TADPUFF. The differences between the two models are associated with the calculation of concentrations, not with the cloud-shine calculation. Thus, Eq. (4.43) for TADPUFF becomes

$$D'_{sl}(r) = \frac{0.1 \sum_n Q'_n D F_{pn}}{2 \pi \sigma_y u} \exp \left[ -0.5 \left( \frac{r}{\sigma_y} \right)^2 \right] \sum_{i=1}^{10} (1 + k \mu z_i) \exp(-\mu z_i) \quad (4.48)$$

for TADPLUME.

Finally, when the vertical extent of the plume is sufficient ( $\sigma_z = 400$  m, or a uniformly mixed plume with a 600 m vertical extent), TADPLUME shifts to a semi-infinite plume, cloud-shine model. Equation (4.44) for TADPUFF becomes



$$D'(r) = [\chi(r)/Q'] \sum_n Q'_n DF_{sien} , \quad (4.49)$$

where  $\chi(r)/Q'$  is calculated using Eq. (4.5) or a variation thereof, as appropriate.

#### 4.9.4 Open- and Closed-Window Dose Rates

Calculation of open- and closed-window dose rates is a new feature in RASCAL 3.0. These dose rates, which are reported in mrad/h, are intended for use in comparisons with field radiation measurements. The open-window dose rate has four components. These components are gamma and beta radiation from airborne activity and gamma and beta radiation from surface contamination. The closed-window dose rates have only the gamma radiation components.

The gamma dose rate from airborne activity is calculated using the same algorithms used in TADPUFF and TADPLUME for finite-plume, cloud-shine doses with adjustment for the difference in energy absorption coefficients of tissue and air. The gamma dose rate is calculated as

$$D'_{\text{gair}} = D' \frac{DF_{\text{sicair}}}{DF_{\text{sictissue}}} , \quad (4.50)$$

where  $D'$  is the cloud-shine dose rate calculated by TADPLUME or TADPUFF for tissue. Semi-infinite cloud-dose factors for tissue from *Federal Guidance Report No. 12* (Eckerman and Ryman 1993) are used in this calculation along with semi-infinite cloud-dose factors for air calculated by A. L. Sjoreen using the methods listed in (Scherpelz 1986). The semi-infinite dose factors for air are included in the RASCAL 3.0 radionuclide database. They are passed to TADPLUME and TADPUFF as needed.

The beta dose rates from airborne activity are calculated using the semi-infinite cloud model with appropriate dose factors. Beta semi-infinite cloud dose factors, which were extracted from the original data used in producing *Federal Guidance Report No. 12* by its authors, are included in the RASCAL 3.0 radionuclide database and passed to TADPLUME and TADPUFF as needed.

The gamma and beta ground-shine dose rates are calculated using the same models used to calculate external doses to the body, with dose factors for air in place of dose factors for tissue. These dose factors, which were extracted from the original data used in producing *Federal Guidance Report No. 12* by its authors, are included in the RASCAL 3.0 radionuclide database and passed to TADPLUME and TADPUFF as needed.

## 4.10 REFERENCES

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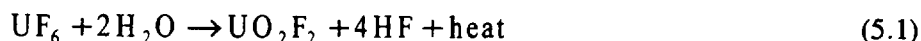
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## 5 UF<sub>6</sub> MODEL

UF6PLUME is a special version of TADPLUME developed to treat potential releases of UF<sub>6</sub>, HF, and UO<sub>2</sub>F<sub>2</sub>, or a combination of UF<sub>6</sub>, HF, and UO<sub>2</sub>F<sub>2</sub>. Modifications to TADPLUME include the introduction of a dense gas model to treat the gravitationally driven spread of UF<sub>6</sub> releases, a chemical/thermodynamic model to treat the reaction of UF<sub>6</sub> with water vapor in the atmosphere, and a plume rise model to treat the vertical displacement of HF/UO<sub>2</sub>F<sub>2</sub> plumes when their densities becomes less than the density of air. Minor modifications were also made to input and output routines to accommodate the additional information required by UF6PLUME.

The dense gas and chemical/thermodynamic models are implemented in control volumes that move downwind at the 10-m level wind speed. The control volumes are initially defined by the release rates of UF<sub>6</sub>, HF, and UO<sub>2</sub>F<sub>2</sub>. As the control volumes move downwind, the volume of UF<sub>6</sub> is deformed by gravitational settling, and air and water vapor are mixed into the UF<sub>6</sub> volume. The chemical reaction



is assumed to occur instantaneously as the mixing takes place. The result of the reaction is a decrease of mass and volume of the control volume containing UF<sub>6</sub> and increase in the mass and volume in the HF/UO<sub>2</sub>F<sub>2</sub> control volume. The temperatures of these two control volumes are assumed to be identical and are determined from the initial temperature of the released material, the air temperature, and the heat reaction of UF<sub>6</sub> and water vapor.

The output of the dense gas and chemical/thermodynamic model calculations is used as input to atmospheric dispersion and deposition calculations. This input is a function of distance from the release point to the point at which all UF<sub>6</sub> has been converted to HF and UO<sub>2</sub>F<sub>2</sub>. Beyond this point, the HF and UO<sub>2</sub>F<sub>2</sub> source terms remain constant with correction for deposition and decay as described in Section 4.

### 5.1 UF<sub>6</sub> MODEL ASSUMPTIONS AND EQUATIONS

The following assumptions were made in development of the UF<sub>6</sub> model.

1. The UF<sub>6</sub> plume is released at or near ground level.
2. An initial UF<sub>6</sub> control volume is defined by the UF<sub>6</sub> release rate and density.
3. The initial cross section of the UF<sub>6</sub> control volume is square with

$$A_{\text{uf6}} = \frac{Q'_{\text{uf6}}}{\rho_{\text{uf6}} u}, \quad (5.2)$$

where

$A_{uf6}$  = cross-sectional area ( $m^2$ ),  
 $Q'_{uf6}$  =  $UF_6$  release rate ( $g/s$ ),  
 $\rho_{uf6}$  =  $UF_6$  density ( $g/m^3$ ),  
 $u$  = wind speed at 10 m ( $m/s$ ).

4. There is no diffusion of the  $UF_6$  plume.
5. Deformation of the  $UF_6$  control volume is determined by gravitational slumping of the  $UF_6$ .
6. The rate of change of the  $UF_6$  control volume width is given by

$$\frac{dw_{uf6}}{dt} = k \left[ g \frac{(\rho_{uf6} - \rho_{air})}{\rho_{uf6}} H_{uf6} \right], \quad (5.3)$$

where

$w_{uf6}$  =  $UF_6$  control volume width (m),  
 $t$  = time (s),  
 $k$  = a slumping constant (dimensionless),  
 $g$  = gravitational constant ( $m/s^2$ ),  
 $\rho_{air}$  = density of air ( $g/m^3$ ),  
 $H_{uf6}$  = thickness of the control volume (m).

7. The slumping constant has a theoretical value of 1.4 but may be given a lower value to account for surface resistance or to tune the model. A value of 1.3 is used as default in the current version of the  $UF_6$  model in RASCAL.
8. Air is entrained into the  $UF_6$  control volume only through the top. Entrainment through the sides is negligible because after only a few seconds the area of the top of the volume is much larger than the area of the sides.
9. The rate of entrainment of air into the  $UF_6$  control volume is given by

$$\frac{dV_{air}}{dt} = w_e w_{uf6} u, \quad (5.4)$$

where

$V_{air}$  = air entrainment rate ( $m^3/s$ ),  
 $w_e$  = an entrainment velocity ( $m/s$ ).

10. The entrainment velocity is given by

$$w_e = \frac{\rho_{air} u_*^3}{(\rho_{UF_6} - \rho_{air}) g h_{UF_6}}, \quad (5.5)$$

where  $u_*$  is a scaling velocity (m/s) associated with atmospheric turbulence.

11. The water available for reaction with  $UF_6$  is determined by a combination of the water vapor in the entrained air and precipitation entering the  $UF_6$  control volume.
12. The water available for reaction is given by

$$m_{H_2O} = \rho_{H_2O} V_{air} + p_r w_{UF_6} \rho_{H_2O} l, \quad (5.6)$$

where

$m_{H_2O}$  = the rate at which water becomes available for reaction (g/s),

$\rho_{H_2Ov}$  = density of water vapor in the ambient air (g/m<sup>3</sup>),

$P_r$  = precipitation rate (m/s),

$\rho_{H_2Ol}$  = density of liquid water (g/m<sup>3</sup>).

13. The reaction between  $UF_6$  and water is assumed to occur at the top of the  $UF_6$  control volume. The volume of  $UF_6$  involved in the reaction is subtracted from the  $UF_6$  control volume, and the masses of air, HF, and  $UO_2F_2$  are added to the HF/ $UO_2F_2$  control volume. The volume of the HF/ $UO_2F_2$  control volume is increased by the volumes of the air and HF. The  $UO_2F_2$  formed in the  $UF_6/H_2O$  reaction is present as small particles that are assumed to have negligible volume. The temperature and volumes of the control volumes are adjusted to conserve enthalpy in constant pressure reaction.
14. Potential heat exchange with the ground and possible reaction of  $UF_6$  with water on the ground surface are assumed to be negligible. However, these phenomena could be added to the model at a later date.
15. The ground is assumed to be a sink for  $UF_6$  that may be deposited on the ground. Any  $UF_6$  condensing in the  $UF_6$  control volume is assumed to deposit on the ground. Wet deposition of  $UF_6$  is not modeled because all water entering the  $UF_6$  control volume is assumed to react with  $UF_6$  to produce HF and  $UO_2F_2$ .

## 5.2 CHEMICAL/THERMODYNAMIC MODEL

The chemical/thermodynamic model in UF6PLUME is based on the description contained in NUREG/CR-4360, *Calculational Methods for Analysis of Postulated  $UF_6$  Releases* (Williams 1985). The initial release for UF6PLUME may be  $UF_6$  or a mixture of  $UF_6$ , HF, and  $UO_2F_2$ . However, the chemical/thermodynamic model is only invoked when the release includes  $UF_6$ . A release of HF or  $UO_2F_2$ , or a combination of HF and  $UO_2F_2$  is treated as a release of passive contaminants.

Air, water vapor, and HF are assumed to be ideal gases; a compressibility factor is used to account for deviation of UF<sub>6</sub> behavior from that of an ideal gas. Although UF<sub>6</sub> cannot exist as a liquid at atmospheric pressures, equations for the density, vapor pressure, and enthalpy of liquid UF<sub>6</sub> are included in UF6PLUME because they were included in the computer code published by Williams (1985).

### 5.2.1 Compressibility Factor

Dewitt (1960) cites work by D. W. Magnuson in presenting the following relationship for UF<sub>6</sub> compressibility factor

$$Z = \frac{T_r^3}{(T_r^3 + 4.892 \times 10^5 P)} \quad (5.7)$$

where

Z = the compressibility factor,  
T<sub>r</sub> = the temperature (°R),  
P = the pressure (psia).

### 5.2.2 UF<sub>6</sub> Density

The density of UF<sub>6</sub> is given by the following relationships. The relationships for the UF<sub>6</sub> liquid and vapor are based on the work of Dewitt (1960), and the relationship for the density of UF<sub>6</sub> solid was derived by Williams (1985) based on data presented by Dewitt. The density of solid UF<sub>6</sub> is given by

$$\rho_{uf6s} = 330.0 - 0.180 t_f \left( \frac{MW}{352} \right) \quad (5.8)$$

where

ρ<sub>uf6s</sub> = the density of the solid (lb<sub>m</sub>/ft<sup>3</sup>),  
t<sub>f</sub> = the temperature (°F),  
MW = the molecular weight.

The density of liquid UF<sub>6</sub> is given by

$$\rho_{uf6l} = (250.6 - 0.1241 t_f + 2.620 \times 10^{-4} t_f^2) \left( \frac{MW}{352.0} \right) \quad (5.9)$$

and the density of UF<sub>6</sub> vapor is given by

$$\rho_{uf6v} = \frac{MW \cdot P \cdot Z}{R \cdot T_r} \quad (5.10)$$



where R is the universal gas constant, 10.73 (psia · ft<sup>3</sup>)/(lb-mol °R).

### 5.2.3 UF<sub>6</sub> Vapor Pressure

The following relationships, based on the work of Dewitt (1960), describe the vapor pressure of UF<sub>6</sub>. The constants in the relationships assume English units for pressure, temperature, and volume. From 32°F to the triple point of 147.3°F, the vapor pressure of UF<sub>6</sub> the solid phase is

$$P_{uf6s} = \exp \left[ 10.44 + 9.642 \times 10^{-3} t_f - \frac{3.90 \times 10^3}{(t_f + 298.1)} \right], \quad (5.11)$$

where  $P_{uf6s}$  is the vapor pressure (psia) and  $t_f$  is the temperature (°F). From the triple point (147.3°F) to 240°F, the vapor pressure is given by

$$P_{uf6vl} = \exp \left[ 12.16 - \frac{4.668 \times 10^3}{(t_f + 367.5)} \right] \quad (5.12)$$

and from 276°F to the critical temperature (446°F) the vapor pressure is given by

$$P_{uf6vh} = \exp \left[ 13.76 - \frac{6.976 \times 10^3}{(t_f + 511.9)} \right]. \quad (5.13)$$

Between 250°F and 276°F, the vapor pressure is estimated by a weighted average of  $P_{uf6vl}$  and  $P_{uf6vh}$

$$P_{uf6v} = P_{uf6vl} (276.0 - t_f) + P_{uf6vh} \left[ \frac{(t_f - 240.0)}{36.0} \right]. \quad (5.14)$$

### 5.2.4 UF<sub>6</sub> Enthalpy

Williams (1985) provides the following equations for the enthalpy of UF<sub>6</sub> using 25°C (77°F) as a base. The equations are to a large extent based on data of Dewitt (1960). For solid UF<sub>6</sub>, the enthalpy is given by

$$H_{uf6s} = 50.446 - 5.70531 \times 10^{-2} T_r + 1.27509 \times 10^{-4} T_r^2 - 9645.63 T_r^{-1}, \quad (5.15)$$

where  $H_{uf6s}$  is the enthalpy (Btu/lb<sub>m</sub>). For liquid UF<sub>6</sub>, the enthalpy is given by

$$H_{uf6l} = 30.6133 + 5.10057 \times 10^{-2} T_r + 5.13165 \times 10^{-5} T_r^2 - 6.139.34 T_r^{-1} + 0.18268 \left[ \frac{(P - P^\circ)}{r_l} \right], \quad (5.16)$$

where

$H_{\text{uf6l}}$  = the enthalpy,  
 $P$  = the atmospheric pressure (psia),  
 $P^\circ$  = the vapor pressure over liquid  $\text{UF}_6$  (psia),  
 $\rho_l$  = the density of the liquid ( $\text{lb}_m/\text{ft}^3$ ).

The last term in this relationship is a correction for supersaturated liquids, assuming an incompressible fluid. Finally, the enthalpy for  $\text{UF}_6$  vapor is given by

$$H_{\text{uf6v}} = 43.2614 + 9.21307 \times 10^{-2} T_r + 6.26265 \times 10^{-6} T_r^2 + 2951.71 T_r^{-1} + 3.0939 \times 10^{-3} T_r (Z|_{P,T} - Z|_{14.7,T}) \quad (5.17)$$

The last term in this relationship is a compressibility correction. This term is small in the atmosphere because atmospheric pressure is always near 14.7 psia.

### 5.2.5 Uranium Enrichment

William's (1985) model includes correction terms for the molecular weight to account for enrichment. The correction terms are retained in UF6PLUME. The molecular weight of enriched uranium is input to UF6PLUME along with the release rates. However, the corrections terms have only a small effect on the results of model computations.

### 5.2.6 HF-H<sub>2</sub>O System

William's (1985) model treats HF and H<sub>2</sub>O as a system for computation of vapor pressures and enthalpy assuming that the HF and H<sub>2</sub>O are vapors in equilibrium with a condensed phase. It is unlikely that a condensed phase will occur in the atmosphere because of the exothermic nature of the  $\text{UF}_6/\text{H}_2\text{O}$  reaction. However, the equations for the condensed phase are included in UF6PLUME for completeness. HF vapor in the atmosphere is assumed to exist as a set of polymers linked by hydrogen bonding. The effects of this self association are included in the HF vapor pressure and enthalpy calculations.

### 5.2.7 HF Self Association

According to Williams (1985), Beckerdrite, Powell, and Adams (1983) report that the self association of HF is reasonably modeled by assuming equilibrium among an HF monomer  $(\text{HF})_1$ , an HF trimer  $(\text{HF})_3$ , and an HF hexamer  $(\text{HF})_6$ . The partial pressure of HF is given by

$$P_{\text{HF}} = P_{(\text{HF})_1} + K_3 P_{(\text{HF})_1}^3 + K_6 P_{(\text{HF})_1}^6, \quad (5.18)$$

where the second and third terms on the right are the partial pressures of the polymers and  $K_3$  and  $K_6$  are equilibrium coefficients. The equilibrium coefficients have been determined experimentally by Strohmeier and Briegleb (Beckerdrite, Powell, and Adams 1983). Using these data, Williams (1985) derived the following relationships to estimate the coefficients

$$K_3 = \exp(2.3884 \cdot 0T_r^{-1} - 51.2393) \quad (5.19)$$

and

$$K_6 = \exp(40319.6T_r^{-1} - 87.7927) \quad (5.20)$$

With self association, the effective molecular weight for HF for vapor-phase densities and mole fractions is greater than the molecular weight of the HF monomer. It is

$$M W_{HF} = \frac{[P_{(HF)_1} M W_{(HF)_1} + K_3 P_{(HF)_1}^3 M W_{(HF)_3} + K_6 P_{(HF)_1}^6 M W_{(HF)_6}]}{P_{HF}} \quad (5.21)$$

### 5.2.8 Partial Vapor Pressures of HF

If a condensed phase exists in the HF-H<sub>2</sub>O system, the vapor pressure of HF is calculated using relationships of the form

$$P_{HF} = \exp(A T_r^{-1} + B) \quad (5.22)$$

where the model parameters are a function of the weight fraction of HF in the condensed phase. Williams (1985) gives estimates of the coefficient values based on a figure supplied by Allied Chemical (Brian C. Rogers). The differences between partial vapor pressures estimated using the model and the figure, range from about 1% for weight fractions near 1.0 to a maximum of 5% at weight fractions below 0.5. If a condensed phase does not exist, the partial vapor pressure of HF is calculated using an iterative procedure along with estimation of the effective molecular weight.

### 5.2.9 Partial Vapor Pressure of H<sub>2</sub>O

As long as UF<sub>6</sub> continues to exist in the vapor phase, all water entering the plume will be used by the UF<sub>6</sub>/H<sub>2</sub>O reaction to form HF and UO<sub>2</sub>F<sub>2</sub>. Under these conditions, the partial vapor pressure in the HF-H<sub>2</sub>O system will be zero. Following conversion of all of the UF<sub>6</sub>, an initial estimate is made of the H<sub>2</sub>O partial vapor pressure from the mass of water in the plume using the ideal gas law. The phase composition of the HF-H<sub>2</sub>O system is determined by comparing the sum of the HF partial pressure and the initial estimate of the H<sub>2</sub>O partial pressure with the total pressure of HF and H<sub>2</sub>O for an azeotropic mixture. If the sum is less than the total pressure for the azeotropic mixture, there is no condensation phase and the initial H<sub>2</sub>O partial pressure estimate is used. If condensation occurs, an iterative procedure is used to determine the partial pressure of H<sub>2</sub>O. The procedure is described in detail by Williams (1985).

### 5.2.10 Enthalpy of HF-H<sub>2</sub>O Vapor Mixtures

The enthalpy of HF-H<sub>2</sub>O vapor mixtures is given by

$$H_{\text{hfh2ov}} = 1051.0 + 0.472T_f - \left[ 376.0 + 0.136T_f + 790.642W_{(\text{HF})_3} + 667.358W_{(\text{HF})_6} \right] W_{\text{hfv}} \quad (5.23)$$

where

$W_{(\text{HF})_3}$  and  $W_{(\text{HF})_6}$  = the weight fractions of the HF polymers with respect to total HF,  
 $W_{\text{Hfv}}$  = the weight fraction of HF in the HF-H<sub>2</sub>O vapor.

The heat of association for (HF)<sub>3</sub> is -790.642 Btu/lb<sub>m</sub> (HF)<sub>3</sub> formed, and the heat of association of (HF)<sub>6</sub> is -667.358 Btu/lb<sub>m</sub> formed.

### 5.2.11 Enthalpy of HF-H<sub>2</sub>O Liquid Mixtures

The enthalpy of liquid HF-H<sub>2</sub>O mixture is given by a relationship of the form

$$H_{\text{hfh2ol}} = A_i + B_i W_{\text{HfL}} + C_i W_{\text{HfL}}^2 \quad (5.24)$$

where the coefficients  $A_i$ ,  $B_i$ , and  $C_i$  are functions of the weight fraction  $W_{\text{HfL}}$  of HF in the HF-H<sub>2</sub>O liquid mixture. Williams (1985) provides correlations for estimating the coefficients that are based on an enthalpy-concentration diagram provided by Brian C. Rogers at Allied Chemical.

### 5.2.12 UO<sub>2</sub>F<sub>2</sub> Enthalpy

UO<sub>2</sub>F<sub>2</sub> is formed as a product of the UF<sub>6</sub>-H<sub>2</sub>O reaction. It is a solid with a heat capacity of 0.0821 Btu/(lb<sub>m</sub> °F). The enthalpy at any temperature, relative to a reference temperature is

$$H_{\text{uo2f2}} = 0.0821(t_f - t_{\text{ref}}) \quad (5.25)$$

where  $t_f$ , the UO<sub>2</sub>F<sub>2</sub> temperature, and  $t_{\text{ref}}$ , the reference temperature, are in °F or Rankine. The reference temperature is 77°F in UF6PLUME.

### 5.2.13. Mixture Enthalpies and Plume Temperature

Mixing and reactions in UF6PLUME are assumed to take place under constant pressure. The following reference conditions are assumed for enthalpy calculations: a pressure of 1013.25 mb (1 atmosphere, 760 mm Hg, or 14.696 psia), a temperature of 25°C (77°F); a vapor state for UF<sub>6</sub>, H<sub>2</sub>O, and air; monomeric vapor for HF; and solid for UO<sub>2</sub>F<sub>2</sub>.

In UF6PLUME, the enthalpy of the plume is calculated for the control volume as the control volume moves downwind. The control volume initially consists of the volume of the UF<sub>6</sub> plus the volume of the entrained air and water vapor and has an enthalpy equal to the sum of enthalpies of the UF<sub>6</sub>, air, and H<sub>2</sub>O. With the UF<sub>6</sub>-H<sub>2</sub>O reaction, the enthalpy of the control volume increases because of the heat release and the changes in the masses of the plume constituents.

The  $\text{UF}_6\text{-H}_2\text{O}$  reaction is limited by one constituent or the other. If the available water is the limiting factor, the heat of reaction is calculated as

$$H_{\text{rxn}} = 25.199 \times 10^3 \frac{m_{\text{h}_2\text{o}}}{\text{MW}_{\text{h}_2\text{o}}} , \quad (5.26)$$

where

$H_{\text{rxn}}$  = heat of reaction,  
 $m_{\text{h}_2\text{o}}$  = mass of water available for the reaction,  
 $\text{MW}_{\text{h}_2\text{o}}$  = molecular weight of water.

Otherwise, the heat of reaction is calculated as

$$H_{\text{rxn}} = 50.398 \times 10^3 \frac{m_{\text{u}}}{\text{MW}_{\text{u}}} . \quad (5.27)$$

With completion of the  $\text{UF}_6\text{-H}_2\text{O}$  reaction, the enthalpy of the plume in the control volume is

$$H_{\text{plume}} = \Delta H_{\text{air}} + \Delta H_{\text{h}_2\text{o v}} + \Delta H_{\text{uf}_6} + \Delta H_{\text{hfh}_2\text{o}} + \Delta H_{\text{uo}_2\text{f}_2} + H_{\text{rxn}} . \quad (5.28)$$

The change in enthalpy of air is

$$\Delta H_{\text{air}} = 0.24037 m_{\text{air}} (t_{\text{air}} - 77.0) \quad (5.29)$$

and, the change in enthalpy associated with entrained water is

$$\Delta H_{\text{h}_2\text{o}} = (0.99783 m_{\text{h}_2\text{o le}} + 0.472 m_{\text{h}_2\text{o vc}}) (t_{\text{air}} - 77.0) . \quad (5.30)$$

Finally, an iterative procedure is used to arrive at a plume temperature that gives the same mixture enthalpy. During this procedure, the phase composition of the  $\text{HF-H}_2\text{O}$  mixture and  $\text{UF}_6$  are adjusted as the temperature changes. The plume temperature is used in plume-rise calculations.

### 5.3 DISPERSION AND DEPOSITION OF HF AND $\text{UO}_2\text{F}_2$

The  $\text{UF}_6$  model works in two stages. In the first stage, the model calculates the spread of  $\text{UF}_6$ , the conversion of  $\text{UF}_6$  to HF, and  $\text{UO}_2\text{F}_2$ , and the plume rise of the HF and  $\text{UO}_2\text{F}_2$ . The products of this stage are  $\text{UF}_6$ , HF, and  $\text{UO}_2\text{F}_2$  source terms and the plume rise of HF and  $\text{UO}_2\text{F}_2$ , all as a function of distance from the release point. In the second stage, a straight-line Gaussian model based on TADPLUME is used to calculate airborne concentrations and deposition of HF and  $\text{UO}_2\text{F}_2$  at receptors on a polar grid. The distance-dependent source terms calculated in the first stage are used as long as  $\text{UF}_6$  is present. After the  $\text{UF}_6$  is gone, the HF and  $\text{UO}_2\text{F}_2$  source terms are depleted to account for deposition.

The  $\text{UF}_6$  chemical and thermodynamics models are run in the first stage while the control volume moves downwind in small time steps. The maximum time step is 2 s. Time steps decrease to 1 s when the

wind speed increases to 4 m/s, and to 0.5 s when the speed exceeds 8 m/s. As the control volume moves downwind, plume rise is calculated using the stable plume equations discussed in Section 4.5.2. In addition, transition plume rise is calculated using

$$\Delta h_t = 1.6 F_b^{1/3} x^{2/3} u^{-1} \quad (5.31)$$

where  $\Delta h_t$  is the transition rise (Briggs 1984). The smaller of the transition and final rise is selected as the plume rise.

Dispersion of the HF and  $\text{UO}_2\text{F}_2$  plumes is calculated using the dispersion parameters that are used in TADPLUME. As long as there is  $\text{UF}_6$  present, the HF and  $\text{UO}_2\text{F}_2$  plumes are assumed to be uniformly mixed in the vertical because the plumes are being fed by the  $\text{UF}_6\text{--H}_2\text{O}$  reaction. Normalized HF and  $\text{UO}_2\text{F}_2$  concentrations in this range are given by

$$\chi / Q' = \frac{1}{(2\pi)^{1/2} u \sigma_y H} \exp \left[ -\frac{1}{2} \left( \frac{y}{\sigma_y} \right)^2 \right], \quad (5.32)$$

where  $H$  is the thickness of the plume. The thickness of the plume is equal to the plume rise plus the vertical dispersion ( $3\sigma_z$ ).

At the point that the last  $\text{UF}_6$  is converted to HF and  $\text{UO}_2\text{F}_2$ , the plume is assumed to become elevated. The effective release height at this point is calculated assuming that the ground-level concentrations of the uniformly-mixed and elevated plumes are equal. The effective release height,  $\Delta h_f$ , is

$$\Delta h_f = -2.0 \sigma_z^2 \log \left[ \frac{(\pi/2)^{1/2} \sigma_z}{H} \right]. \quad (5.33)$$

This effective release height is assumed for the remainder of the dispersion calculations.

Assuming the mixing-layer thickness is significantly greater than the vertical dimension of the plume, the normalized concentrations of HF and  $\text{UO}_2\text{F}_2$  are calculated as

$$\chi / Q' = \frac{1}{\pi u \sigma_y \sigma_z} \exp \left[ -\frac{1}{2} \left( \frac{y}{\sigma_y} \right)^2 \right] \exp \left[ -\frac{1}{2} \left( \frac{\Delta h_f - z}{\sigma_z} \right)^2 \right] \quad (5.34)$$

after all  $\text{UF}_6$  has been converted to HF and  $\text{UO}_2\text{F}_2$ . The receptor height,  $z$ , is assumed to be 1 m.

UF6PLUME generates the following products:

- airborne uranium exposure (g-s)/m<sup>3</sup>,
- inhaled uranium (mg),
- dose commitment from inhaled uranium (rem),

- deposited uranium ( $\text{g}/\text{m}^2$ ),
  - average HF concentration (ppm by volume),
  - 1-h equivalent HF concentration (ppm by volume), and
  - HF deposition ( $\text{g}/\text{m}^2$ ).

The airborne uranium exposure and uranium deposition are calculated, accounting for deposition and depletion. The inhaled uranium and the dose commitment are calculated from the airborne uranium exposure. Similarly, an HF exposure and HF deposition are calculated, accounting for deposition and depletion. The average HF concentration is calculated from HF exposure. The 1-h equivalent HF concentration is an effective concentration calculated for short-duration releases for comparison with toxicity limits. It is calculated as

$$C_{1\text{he}} = C(t) \left( \frac{t}{3600} \right)^{1/2}, \quad (5.35)$$

where

$C_{1\text{he}}$  = 1-h equivalent concentration (ppm),  
 $C(t)$  = average concentration for duration  $t$  (ppm),  
 $t$  = duration of the exposure to concentration  $C(t)$  (s).

UF6PLUME does not calculate cloud-shine or ground-shine doses.

## 5.4 REFERENCES

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## **6 METEOROLOGICAL DATA PROCESSOR**

The meteorological data processor, **METPROC**, is the **STDose** module used for entering meteorological data and preparing the data for use by the atmospheric transport and diffusion models in **RASCAL 3.0**. In earlier **RASCAL** versions, this function was handled directly by the user interface. It was necessary to separate the function from the interface to expand capabilities of **TADPLUME** and **TADPUFF**.

Meteorological data for the site (event location) and as many as 35 additional meteorological stations may be entered and processed for use by the **RASCAL 3.0** atmospheric models using **METPROC**. All data must be entered manually at the present time. Future version of the meteorological data processor may include options for importing meteorological data files.

The following sections describe the technical aspects of the meteorological data requirements and the meteorological data processing.

### **6.1 MODEL DOMAIN**

Model domain refers to the area covered by the dose calculations in **STDose**. The model domain for **TADPUFF** is square. In **RASCAL 3.0**, **STDose** has three options for the **TADPUFF** model domain. They are squares that are 20, 50, and 100 miles (32, 80, and 160 km) on a side. The model domain is selected when dose calculations are started. **METPROC** creates a meteorological file for each domain for use by **TADPUFF**. These files describe the spatial and temporal variation of meteorological conditions at nodes on a Cartesian grid. **METPROC** also creates a smaller file of meteorological data for the release point for use by **TADPLUME** and **UF6PLUME**. This file describes the temporal variation of meteorological conditions at the center of the polar grid used by these straight-line models.

Meteorological data must be entered for at least one location, generally the release site. If data are entered for only one location, the data will be assumed to be representative for the center of the domain.

### **6.2 METEOROLOGICAL STATIONS**

Locations for which meteorological data are entered are called meteorological stations. Meteorological stations may be within or near the model domain. Spatial fields of winds, stability, etc., are produced from the station meteorological data. Section 6.3 discusses the meteorological data input.

Information on each station must be available to **METPROC** before **METPROC** can use station meteorological data in generating the meteorological fields needed by **TADPUFF**. Files containing the required information for potential release sites are included with **RASCAL 3.0**. Each file contains the information for the location of the site and for other meteorological stations near the site. However, the file for a specific site may not include information for all meteorological stations near the site, or the



information for a meteorological station may become outdated. Therefore, METPROC provides the means to add meteorological stations to the file or update information in the file.

The following information is needed for each meteorological station

- A station identification. The station identification can be any 10 letter character; the release site ID is appropriate for the first station in the station list; FAA or ICAO location indicators are appropriate for national weather service or other stations that have them.
- The latitude (positive north of the equator and negative south of the equator) and longitude (positive east of the prime meridian and negative west of the prime meridian) of the station in decimal degrees.
- The elevation of the station (m). The elevation should be the height of the station above mean sea level.
- The surface roughness for the station (m). Meteorological texts such as Panofsky and Dutton (1984) and Stull (1988) provide guidance on estimating surface roughness. If no other information is available, a surface roughness of 0.2 m may be used.
- The height at which the wind measurements are made (m). The instrument height should be height above ground level.

METPROC uses station positions to place station data in the proper locations in the modeling domain; station elevations are used in the potential flow model that adjusts wind fields for topographic effects (Section 6.5.1), and the surface roughness and height of wind measurement are used in calculating wind speed variation with height (Section 6.4.2). The following information is used to identify the engineering units associated with the meteorological data for the station and permit METPROC to convert data value to units used in model calculations

- stability data type (Pasquill-Gifford stability class,  $dT/dz$  in  $^{\circ}\text{C}/100\text{ m}$ , or  $dT/dz$  in  $^{\circ}\text{F}/100\text{ ft}$ ,
- height interval for  $dT/dz$ ,
- units of height interval for  $dT/dz$  (1=m, 2= ft, 9=undefined),
- units for wind speed (1=m/s, 2=mph, 3=knots),
- units for temperature (1= $^{\circ}\text{C}$ , 2= $^{\circ}\text{F}$ ) for the first station, not used for other stations.

A longer station name may be included for each station for better identification.

The first station in the station file is the station at the source of the release (the site). The latitude and longitude of the first station will define the coordinates of the center of the model domain grid. Distances from the center of the grid to the other stations are calculated using

$$x_{rs} = r_e \Delta\lambda_{rs} \cos \phi_s \quad (6.1)$$

and

$$y_{rs} = r_e \Delta\phi_{rs} , \quad (6.2)$$

where

$x_{rs}$  = distance of the station east (+) or west (-) of the source (center of the grid) (km),  
 $y_{rs}$  = distance of the station north (+) or south (-) of the source (center of the grid) (km),  
 $r_e$  = radius of the earth (= 6370 km),  
 $\phi_s$  = latitude of the center of the grid (first station),  
 $\Delta\lambda_{rs}$  = longitude difference between the station and the source (center of the grid) (radians),  
 $\Delta\phi_{rs}$  = latitude difference between the station and the source (center of the grid) (radians).

### 6.3 METEOROLOGICAL DATA INPUT

Station meteorological data are entered for specific dates and times. The data may be actual observations (measurements) or they may be taken from meteorological forecasts. If available, the following data should be entered for each station:

- surface-level wind direction and speed,
- estimated atmospheric stability,
- precipitation class, and
- estimated mixing height.

All of these data are used in the transport, diffusion, and deposition calculations. In addition, the following data should be entered for the first station (center of the grid):

- ambient air temperature,
- pressure (station), and
- humidity measurement (dew point temperature, relative humidity, or wet bulb temperature).

The air temperature is used in plume rise calculations in TADPLUME, TADPUFF, and UF6PLUME. The air temperature, station pressure, and humidity are used in the thermodynamic calculations in UF6PLUME. Station pressure and humidity are used only by UF6PLUME.

The following subsections describe the meteorological variables in more detail.

### 6.3.1 Surface Winds

The surface winds are made up of the wind direction (the direction from which the wind is blowing) and the wind speed. Wind directions must be entered in degrees. Wind speed can be entered as m/s, mph, or knots. The wind-speed and wind speed unit are passed to the meteorological data processing program in the observation file. METPROC converts all wind speeds to m/s. Both a wind direction and wind speed are required. The acceptable range for wind directions is 0 through 360°. The acceptable range for wind speeds is 0 through 30 m/s. A wind speed of 0.4 m/s will be answered in UF6PLUME if the wind speed is less than 0.4 m/s.

### 6.3.2 Atmospheric Stability Class

Atmospheric stability may be entered either as a stability class (A—extremely unstable through G—extremely stable) based on the general classification scheme discussed by Pasquill (1961), Gifford (1961), and Turner(1964) or as temperature variation with height ( $dT/dz$ ). If  $dT/dz$  is entered, it will be converted to a stability class by METPROC using the conversion table shown in Table 6.1 (NRC, 1972). If the temperature difference measurement is over a height interval different from those shown in Table 6.1, the measurement is adjusted to the appropriate interval.

**Table 6.1 Estimated Pasquill-Gifford Stability Class Based on NRC Delta TM Method**

Stability Class	$dT/dz$ ( $^{\circ}\text{C}/100\text{ m}$ )	$dT/dz$ ( $^{\circ}\text{F}/100\text{ ft}$ )
A	$< -1.9$	$< -1$
B	$< -1.7$	$< -0.9$
C	$< -1.5$	$< -0.8$
D	$< -0.5$	$< -0.3$
E	$< 1.5$	$< 0.8$
F	$< 4$	$< 2.2$
G	$\geq 4$	$\geq 2.2$

METPROC has two options related to modification of station stability classes. The first option allows METPROC to replace a missing stability class with an estimate based on the time of day, the wind speed at the station, and whether there is precipitation or not. The second option allows METPROC to compare the entered stability class with ranges of stability classes that would be expected given the time

of day and meteorological conditions and replace values that are out of the expected range with more likely values.

When the first option is selected, Table 6.2 is used to estimate the stability class from wind speed, precipitation type, and the time of day. Factors discussed by Turner (1964) were used in selecting the stability classes for the table. Daytime is defined as one hour after sunrise to one hour before sunset. Nighttime is defined as one hour before sunset to one hour after sunrise.

**Table 6.2 Estimated Atmospheric Stability Class for Missing Stability Classes**

Wind Speed (m/s)	No or Light Precipitation	Moderate or Heavy Precipitation
Daytime		
≤ 6.0	3	3
> 6.0	4	4
Nighttime		
≤ 3.0	6	5
3.1 - 5.0	5	5
> 5.0	4	4

When the second option is selected, Table 6.3 is used to determine the reasonable range of stability classes given the time of day, wind speed, and precipitation type. These ranges are based on factors discussed by Turner (1964). If a meteorological station stability class falls within the reasonable range, the stability class is not modified. But if the stability class falls outside the range, the stability class is changed to the closest stability class within the range.

### 6.3.3 Precipitation Class

Wet deposition in TADPLUME, TADPUFF, and UF6PLUME and the reaction between UF<sub>6</sub> and water in UF6PLUME are affected by precipitation. Information on precipitation may be entered for each station during meteorological data entry by selecting one of seven precipitation classes, or unknown, if appropriate. In addition to none, the precipitation classes are light, moderate, and heavy rain; and light, moderate and heavy snow. In the context of RASCAL 3.0, rain includes drizzle, freezing rain, and freezing drizzle; and snow includes snow grains, snow pellets, ice pellets, ice crystals, and hail. METPROC estimates precipitation rates from precipitation classes. Estimation of precipitation rates is covered in Section 6.4.6.

**Table 6.3 Limits of Atmospheric Stability Classes Based on  
Time of Day, Wind Speed, and Precipitation**

<b>Wind Speed (m/s)</b>	<b>No or Light Precipitation</b>	<b>Moderate or Heavy Precipitation</b>
<b>Daytime</b>		
≤ 3.0	1-5	3-5
3.1 - 5.0	2-4	3-4
> 5.0	3-4	3-4
<b>Nighttime</b>		
≤ 3.0	3-7	3-5
3.1 - 5.0	4-6	4-5
5.1 - 6.0	4-5	4-5
> 6.0	4	4

#### **6.3.4 Mixing Height**

TADPLUME and TADPUFF use the mixing height to limit vertical dispersion. Mixing heights may be entered with the other meteorological data for a station. However, this information is generally not available. Consequently, unless the option of entering mixing-height data is specifically selected, METPROC will estimate mixing heights from wind speed and stability. There is also an option of using climatological mixing-height estimates in place of measured or calculated values.

#### **6.3.5 Temperature**

The ambient air temperature should be entered for the first meteorological station. If the meteorological data are to be used for consequence analysis for a ground-level release not involving UF<sub>6</sub>, and it is not snowing, the temperature may be omitted without affecting doses.

#### **6.3.6 Pressure**

The station atmospheric pressure (not sea-level pressure at the station) is needed for thermodynamic calculations in UF6PLUME. However, the calculations are not particularly sensitive to the pressure as long as the pressure is within a few percent of the actual value. METPROC includes default pressures for fuel-cycle facilities that should be adequate for most purposes because atmospheric pressures rarely vary by more than ±5%. METPROC will convert pressures entered in other units to millibars.

### 6.3.7 Humidity

Information on humidity is needed for chemical reaction and thermodynamic calculations in UF6PLUME. Humidity information may be entered for the first station as dew point temperature, relative humidity, or wet bulb temperature. METPROC includes default humidity information based on climatological data for fuel-cycle facilities. However, actual data should be entered whenever possible because the calculations are very sensitive to humidity, and humidities have a wide range of variation in the atmosphere.

### 6.3.8 Temporal Interpolation of Input Values

The atmospheric models in RASCAL 3.0 expect meteorological data on the 15-min time interval typically used to record meteorological data at U.S. nuclear facilities. Data from other meteorological stations are not likely to be available on that interval. Consequently, METPROC will estimate missing 15-min data for each station by linear interpolation between observed values. For example, if 10:00 and 11:00 observations are entered for a station, METPROC will estimate values for 10:15, 10:30, and 10:45. METPROC will not interpolate between observed and forecast values, or between two forecast values.

The interpolation procedures are as follows:

#### Winds

- If the wind (either speed or direction) is missing for the earlier observation, the winds at all times between the two observations are also assumed to be missing.
- If the wind is missing for the later observation but not for the earlier observation, the winds are set to the wind of the earlier for times within 12 h of the earlier observation, otherwise they are assumed to be missing.
- If the winds for both the earlier and later observation are valid, the winds are interpolated as follows:
  1. The wind speed and direction are converted to U (east-west) and V (north-south) components.
  2. The U and V component are linearly interpolated (i.e.,  $U(t) = (U_1 - U_e)\{(t-t_e)/(t_1-t_e)\} + U_e$  where  $U_1$ ,  $U_e$ ,  $t_1$ ,  $t_e$  are the U component and time of the later and earlier observations, respectively).
  3. The U and V components are converted back to speed and direction.

### **Atmospheric Stability**

- If the atmospheric stability for the earlier observation is missing, the atmospheric stabilities at all times between the two observations are assumed to be missing.
- If the atmospheric stability for the later observation is missing but not for the earlier observation, then the atmospheric stabilities are set to the value of the earlier observation as long as the elapsed time from the earlier observation is less than 12 h. After 12 h, the stabilities are set to missing.
- If both observations have valid atmospheric stabilities, the atmospheric stability is estimated using linear interpolation between the two observations. If the atmospheric stability is given by a Pasquill-Gifford stability class (1-7), then the interpolation is rounded to the nearest integer.

### **Precipitation Class**

- If the precipitation class for the earlier observation is missing, the precipitation class for all times between the two observations will be set to missing.
- If the precipitation class for the later observation is missing but not for the earlier observation, then precipitation classes are set to the precipitation class of the earlier observation as long as the elapsed time from the earlier observation is less than 12 h. After 12 h, the precipitation classes are set to missing.
- If both observations have valid precipitation classes, then the precipitation class for the earlier observation is used when the time is less than or equal to half way between the two observations. If the time is greater than half way between the two observations, the precipitation class of the later observation is used.

### **Mixing Height**

- Unless the mixing height is being entered directly (not calculated from the meteorological data or from climatology), the method of estimating mixing heights being used for the earlier observation will continue to be used.
- If the mixing heights are being entered directly, the technique used to interpolate stability is used to estimate the missing mixing heights (see previous statement).

### **Temperature, Pressure, and Moisture**

- The same technique previously explained used to estimate missing stabilities is used for temperature, pressure, and humidity.

If data are missing between observed and forecast values, persistence will be used to estimate missing

values for all times up to the time of the forecast.

For each station, data for all times before the first date and time with an entered value are assumed to be missing. Likewise, data for all dates and times past the entered value are assumed to be missing.

## 6.4 OTHER METEOROLOGICAL PARAMETERS

Meteorological data entered for a station are used to evaluate additional parameters. The following subsections describe these additional parameters.

### 6.4.1 Monin-Obukhov Length

The Monin-Obukhov length ( $L$ ) is a scaling length for vertical motions in atmospheric boundary layer studies that is used as a measure of atmospheric stability. It is used in wind profile, turbulence, and mixing-layer depth calculations. Golder (1972) provides a graphical means for converting from Pasquill-Gifford stability classes to Monin-Obukhov lengths using the surface roughness length (Section 6.4.2). METPROC uses a procedure to convert stability classes to Monin-Obukhov lengths that was developed by Ramsdell, Simonen, and Burk (1994) based on Golder's work.

### 6.4.2 Winds

The RASCAL 3.0 atmospheric dispersion models are measured at 10 m above ground level for ground-level release calculations and release height winds for elevated release calculations. Wind measurements are not always made at these heights. Therefore, METPROC adjusts wind speeds for the difference between the measurement height and the height required for model calculations. A diabatic wind-profile model, which accounts for the effects of surface roughness and atmospheric stability on variation of wind speed with height, is used for this adjustment. No attempt is made to model the variation of wind direction with height.

The diabatic profile model is derived from atmospheric boundary layer similarity theory proposed by Monin and Obukhov (1954). The basic hypothesis of similarity theory is that a number of parameters in the atmospheric layer near the ground, including wind profiles, should be universal functions of the friction velocity, a length scale, and the height above the ground. The length scale is referred to as the Monin-Obukhov length and the ratio  $z/L$  is related to atmospheric stability.

The diabatic wind profile is

$$u(z) = \frac{u_*}{k} \left[ \ln \left( \frac{z}{z_0} \right) - \psi \left( \frac{z}{L} \right) \right], \quad (6.3)$$



where

$u(z)$  = wind speed at height  $z$  (m/s),  
 $u_*$  = friction velocity (boundary-layer scaling velocity) (m/s),  
 $k$  = von Karman constant ( $\approx 0.4$ ),  
 $z_0$  = surface roughness length (m),  
 $\psi(z/L)$  = stability correction factor,  
 $L$  = Monin-Obukhov length (m).

The surface roughness length is associated with small-scale topographic features. It arises as a constant of integration in the derivation of the wind profile equations and is used in several boundary-layer relationships. Texts on atmospheric diffusion, air pollution and boundary-layer meteorology (Panofsky and Dutton 1984, Stull 1988) contain tables that give approximate relationships between surface roughness and land use, vegetation type, and topographic roughness.

The term  $\Psi(z/L)$  accounts for the effects of stability on the wind profile. In stable atmospheric conditions,  $\Psi(z/L)$  has the form  $-\alpha z/L$  where  $\alpha$  has a value of 5. In neutral conditions  $\Psi(z/L)$  is equal to zero, and the diabatic profile simplifies to a logarithmic profile.

In unstable air,  $\Psi(z/L)$  is more complicated. According to Panofsky and Dutton (1984), the most common form of  $\Psi(z/L)$  for unstable conditions, based on the work of Businger et al. (Paulson 1970) is

$$\Psi\left(\frac{z}{L}\right) = \ln \left( \left[ \frac{(1+x^2)}{2} \right] \left[ \frac{(1+x)}{2} \right]^2 \right) - 2 \tan^{-1}(x) + \frac{\pi}{2} \quad (6.4)$$

where  $x = (1-16z/L)^{1/4}$ . Equation (6.4) is used to estimate the friction velocity ( $u_*$ ) from the wind speed, surface roughness, and Monin-Obukhov length. In unstable and neutral conditions, the use of Eq. (6.4) is limited to the lowest 100 m of the atmosphere. In stable conditions, the upper limit for application of Eq. (6.4) is the smaller of 100 m or three times the Monin-Obukhov length.

### 6.4.3 Mixing Height

Heating of the surface and surface friction combine to generate turbulence that mixes material released at or near ground level through a layer that varies in thickness from a few meters to a few kilometers in thickness. This layer is referred to as the mixing layer. The atmospheric models in RASCAL 3.0 use the mixing height (also referred to as the mixing-layer depth and mixing-layer thickness) to limit vertical diffusion.

METPROC has three methods for obtaining estimates of the mixing height at meteorological stations. The mixing height may be entered directly, or it may be estimated by the program from either current meteorological data or climatological information. Of the later two options, estimation of mixing height

from current meteorological data is preferable to estimating the mixing height from climatological data, if sufficient data are available.

METPROC uses algorithms developed by Ramsdell, Simonen, and Burk (1994 ) for estimating mixing height from current meteorological data. The algorithms are based relationships derived by Zilitinkevich (1972) for stable and neutral conditions. For stable atmospheric conditions, the relationship is

$$H = k \left( \frac{u_* L}{f} \right)^{1/2}, \quad (6.5)$$

where

$H$  = mixing height (m),  
 $k$  = von Karman constant (0.4),  
 $u_*$  = friction velocity (m/s),  
 $L$  = Monin-Obukhov length (m),  
 $f$  = Coriolis parameter (1/s).

A 50-m mixing height is used if the mixing height calculated by Equation 6.5 is less than 50 m. Similarly, if the calculated mixing height is greater than 2000 m, the mixing height is set to 2000 m.

For neutral and unstable conditions, the mixing height is calculated by

$$H = \frac{\beta u_*}{f}, \quad (6.6)$$

where  $\beta$  is a constant set to 0.2. If the mixing height calculated by Equation 6.6 is less than 250 m, the mixing height is set to 250 m, and if the calculated mixing height is greater than 2000 m, the mixing height is set to 2000 m.

The mixing-layer thickness may also be estimated from climatological data. When this option is selected, the mixing-layer thickness is estimated from typical morning and afternoon thicknesses for each month using the method used in the Environmental Protection Agency's meteorological preprocessor code, PCRAMMET (EPA 1999). The monthly morning and afternoon mixing-layer thicknesses were calculated from daily data obtained from the Environmental Protection Agency's Support Center for Regulatory Air Models (<http://www.epa.gov/scram001/>). The following rules are used in estimating mixing-layer thicknesses from the monthly values.

- From midnight to sunrise—use the morning mixing height.
- From sunrise to 1400—linearly interpolate between morning and afternoon mixing heights.
- From 1400 to sunset—use the afternoon mixing height.

- From sunset to midnight—use exponential interpolation between the afternoon and morning mixing heights. For the last day of the month, use the morning of the next month.

The exponential interpolation of the mixing height is given by

$$H(t) = a \cdot \exp\left(-\frac{bt}{24}\right), \quad (6.7)$$

where

$H(t)$  = mixing height at time  $t$  (m),  
 $a = H_{\text{morn}}/\exp(-b)$ ,  
 $b = 24 \ln(H_{\text{aft}}/H_{\text{morn}})/(24 - t_{\text{sunset}})$ ,  
 $H_{\text{morn}}$  = morning mixing height (m),  
 $H_{\text{aft}}$  = afternoon mixing height (m),  
 $t_{\text{sunset}}$  = time of sunset (h).

The following equations (Stull 1988) are used in calculating sunset and sunrise times

$$\sin \nu = \sin \phi \sin \delta_s - \cos \phi \cos \delta_s \cos(T_0), \quad (6.8)$$

where

$\nu$  = local elevation of the sun,  
 $\phi$  = latitude of the station,  
 $\delta_s$  = solar declination angle (angle of the sun above the equator),  
 $T_0$  = local time.

The solar declination angle is calculated using

$$\delta_s = \phi_r \cos\left(\frac{2\pi(d - d_r)}{d_y}\right), \quad (6.9)$$

where

$\phi_r$  = latitude of the tropic of Cancer ( $23.45^\circ$ ),  
 $d$  = Julian calendar day of the year,  
 $d_r$  = Julian calendar day of the summer solstice (173),  
 $d_y$  = average number of days per year (365.25).

The local time is defined as

$$T_0 = \left( \frac{\pi_{utc}}{12} - \lambda_e \right), \quad (6.10)$$

where

$\pi_{utc}$  = time at the prime meridian,  
 $\lambda_e$  = longitude (in radians) of the station.

Sunrise and sunset are calculated by setting the solar elevation angle to  $-0.833^\circ$  (the sun appears to rise and set when it is  $0.833^\circ$  below the horizon) and solving for  $T_0$  using Eq. (6.10). Sunset is  $24 \text{ h} - T_0$ . The equations for sunrise and sunset do not take into account the ellipticity of the earth's orbit, but it is accurate to about  $\pm 16 \text{ min}$ .

#### 6.4.4 Dry Air and Water Vapor Density

UF6PLUME requires estimates of the air density and water content of the atmosphere. These two variables are estimated from the air temperature, station pressure, and humidity for the event site. (The event site is assumed to be at the location of the first meteorological station. The method used to calculate the dry air density and water-vapor density depends upon the variables used for humidity and whether the temperature, pressure, and moisture variables exist.

The water vapor density is given by

$$\rho_v = \frac{e}{R_v T}, \quad (6.11)$$

where

$\rho_v$  = water vapor density ( $\text{kg/m}^3$ ),  
 $e$  = vapor pressure (Pa),  
 $R_v$  = gas constant =  $461.5 \text{ J/kg K}$ ,  
 $T$  = temperature (K),

and the dry air density can be estimated by

$$\rho_d = \frac{(p - e)}{RT}, \quad (6.12)$$

where

$\rho_d$  = dry air density ( $\text{kg/m}^3$ ),

$p$  = total station pressure (Pa),  
 $R$  = gas constant for dry air = 287.0 J/kg K.

The method used to calculate the vapor pressure ( $e$ ) depends upon the moisture variable. If the moisture variable is the dew point and precipitation is not occurring, then the vapor pressure is given by

$$e = e_s(t_d) , \quad (6.13)$$

where  $e_s(t)$  [mb] is the saturation vapor pressure at temperature  $t$  ( $^{\circ}\text{C}$ ). According to Rogers and Yau (1989), the saturation vapor pressure is given by

$$e_s(t) = 6.112 \exp\left(17.67 \frac{t}{t + 243.5}\right) . \quad (6.14)$$

If the moisture is defined by the relative humidity and precipitation is not occurring, then the vapor pressure is given by

$$e = \frac{RH \cdot e_s(t)}{100} , \quad (6.15)$$

where  $RH$  is the relative humidity (percent) and  $e_s(t)$  is given by Eq. (6.14).

If the moisture is given by the wet bulb temperature and precipitation is not occurring, then the vapor pressure is given by

$$e = e_s(t) - \left(\frac{p}{0.622}\right) \cdot \left[\frac{1004(t - t_w)}{2.5 \times 10^6}\right] , \quad (6.16)$$

where  $t_w$  is the wet bulb temperature [ $^{\circ}\text{C}$ ].

If precipitation is occurring, the air is assumed to be 95% saturated, so the vapor pressure is given by

$$e = 0.95 e_s(t) , \quad (6.17)$$

where  $e_s(t)$  is given by Eq. (6.14). During precipitation, Eq. (6.17) is used regardless of the moisture variable.

If the temperature is missing, a climatological temperature estimate will be taken from the site climatology file, if available. A temperature of  $15^{\circ}\text{C}$  will be assumed if a climatology file is not available. If the pressure is missing, a pressure of 1000 mb is assumed. Finally, if the moisture variable is missing, a relative humidity of 60% is assumed unless there is precipitation. During periods of precipitation, the relative humidity is assumed to be 95%.

### 6.4.5 Precipitation Rate

The RASCAL 3.0 atmospheric codes use precipitation rate to calculate wet deposition rate. When the precipitation class for a station is other than none or unknown, METPROC estimates a precipitation rate (mm/h) for the station using the precipitation class and a precipitation rate zone. Each site in the RASCAL 3.0 database is assigned to one of three precipitation rate zones. The precipitation zones, originally defined in Ramsdell, Simonen, and Burk (1994) are based on annual precipitation. Zone 1 is for areas where the annual precipitation is less than 10 in., zone 2 is for areas where the annual precipitation is between 10 and 20 in., and zone 3 is for areas where the annual precipitation exceeds 20 in. Generic sites and sites not known to RASCAL 3.0 are assigned to precipitation rate zone 3. The precipitation rates assigned by METPROC are listed in Table 6.4. These rates, based on data collected in the Pacific northwest, should be conservative for most nuclear facilities in the United States.

**Table 6.4 Precipitation Rates as a Function of Precipitation Climate Zone**

Precipitation Class	Precipitation Rate (mm/h)		
	Zone 1	Zone 2	Zone 3
1	0.4	0.6	0.7
2	3.8	3.8	3.8
3	3.8	3.8	8.5
4	0.3	0.3	0.7
5	1.7	1.7	3.8
6	1.7	1.7	3.8

## 6.5 CALCULATING SPATIALLY VARYING METEOROLOGICAL CONDITIONS

TADPUFF takes into account both spatial and temporal variations in the atmospheric conditions. METPROC provides gridded fields of the atmospheric stability class, the inverse Monin-Obukhov length, the east-west (u) and north-south (v) components of the wind, the mixing height, and the precipitation class and precipitation rate for each of the three TADPUFF model domains. The following subsections describe the preparation of the fields from the station data.

### 6.5.1 Winds

TADPUFF uses wind fields to calculate movement of puffs. These are fields of u (east-west) and v (north-south) components of the wind vector. The wind fields are created from station wind data using a  $1/r^2$  interpolation scheme, where r is the distance from the grid point to the station. This interpolation

scheme, which was used in earlier NRC codes such as MESOI (Ramsdell, Athey, and Glantz 1983) and MESORAD (Scherpelz, et al. 1986; Ramsdell et al. 1988), is common in spatial interpolation of the wind fields (Hanna, Briggs, and Hosker 1982).

If the meteorological stations reporting data are well placed with respect to major topographic features, the wind fields developed by interpolation will give reasonable puff trajectories. However, with one meteorological station or a small number of stations, the wind fields may not properly reflect the effects of topography. METPROC includes an option to use a simple one-layer model to adjust wind fields for topography based on site topographic data. Topographic data are included in RASCAL 3.0 for all sites in the database. The wind-field model is a two-dimensional adaption of the wind fitting program described by Ross et al. (1988) that is used in the NUATMOS and MATTHEW codes.

The wind-field model uses the wind fields created by interpolation as a starting point. The thickness of the mixing layer is calculated for each node in the model domain by computing the difference between the top of the boundary layer and the terrain elevation. For those nodes where the terrain rises above the top of the boundary layer, the program assumes that the boundary-layer thickness is 0.01 m and sets the wind to zero. This technique is simple to implement and has proven effective at generating flows that avoid obstacles such as mountain ridges.

The initial wind field is adjusted using methods of variational calculus to produce a non-divergent wind field in the boundary layer, subject to the constraint of minimum difference between the initial wind field and the adjusted wind field. The equation for adjusting the wind field involves solving Poisson's equation. The code uses a nine-point Laplacian operator and a simultaneous relaxation technique to obtain the solution.

The model has been tested and shows that the winds produced by the model flow around obstacles that are well resolved by the grid. Obstacles having width of three grid points or greater are considered well resolved. Smaller obstacles may or may not be resolved, depending on their shape and orientation relative to the grid. For example, a ridge one grid point wide is well resolved if it runs in the x or y direction, but if that same ridge is at 45° to the grid, it is not resolved.

The adjusted wind field is most accurate near stations and along trajectories that pass near stations. Wind fields are less accurate elsewhere. Thus, it is desirable to have wind data near the release point and, if possible, at downwind locations.

Sites not included in the RASCAL 3.0 database and the generic site do not have topographic data files. Therefore, the option of modifying wind fields for topographic effects is not available for these sites.

### **6.5.2 Stability and Precipitation**

The stability class and precipitation fields (precipitation class and precipitation rate) are based on data for the closest meteorological station. Fields created in this manner include stability class, inverse Monin-Obukhov length, precipitation class, and precipitation rate. This procedure avoids averaging that would

minimize the effects of extreme stability or instability. It also provides maximum detail in treating isolated precipitation events.

### **6.5.3 Mixing Height**

Estimates of station mixing height are not considered particularly reliable. Therefore, the spatial variation of the mixing height is modeled using two steps. The initial step is create a mixing height field using the mixing height for the closest station for each point in the field. If there is only one station the process is terminated after this step. The second step is taken when there are two or more stations. In this step, the mixing height at each point in the field is replaced by an average of the initial mixing height and the mixing heights at 24 surrounding points. This second step smooths the mixing height field.

## **6.6 CALCULATING METEOROLOGICAL CONDITIONS AT THE SOURCE**

All of the RASCAL 3.0 atmospheric dispersion models require information about the wind speed, wind direction, atmospheric stability, precipitation class, precipitation rate, mixing-layer depth, and temperature at the source. If these meteorological data are available for the first station, which is considered to be at the source, then those data are used. If no data are available for the first station, the wind speed, wind direction, atmospheric stability, current weather, precipitation rate, and mixing-layer depth will be estimated from the spatial meteorological data field. For the temperature, a default climatological value will be used if it exists. The default climatological temperature varies by month and is obtained from the climate file. If the climate file does not exist for the site, the temperature will be set to 15°C.

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## 7 DOSE CALCULATIONS IN FMDOSE

FMDose is designed to compute doses after a radiological emergency has begun. It allows field measurement data to be used in decision making regarding measures taken to protect the health of the public and emergency workers. FMDose computes doses, derived intervention levels (DILs), and emergency-worker turn-back guidance at a single field measurement location. Doses are to people standing outdoors. Computational methods are based on the FRMAC Assessment Manual (DOE 1995). All calculations require the user to enter at least one air or ground concentration and a meter reading.

The dose factors used are not listed in this document. They are available within the RASCAL 3.0 radionuclide help files. The air-submersion and ground-shine dose factors are for effective dose from *Federal Guidance Report No. 12* (EPA 1993). The 50-year committed-effective-dose equivalent and thyroid inhalation dose factors are from *Federal Guidance Report No. 11* (EPA 1991). Four-day bone marrow, lung, and small-intestine wall inhalation dose factors are for an adult and were computed using the methods described in the previous reference. The committed effective dose equivalent is a weighted sum of selected organ doses and is defined in *ICRP Publication 26* (ICRP 1977).

For emergency worker guidance and early-phase doses based on air concentrations, all radionuclide concentrations are assumed to be constant over the exposure period. All other dose and DIL calculations include decay and decay-product ingrowth. Weathering is included in decay of ground concentrations. FMDose uses different weathering functions in computing the amount of material resuspended from the ground and the amount of material remaining on the ground. For clarity, the equations for doses and DILs presented here do not explicitly include the decay integral or daughter ingrowth.

If data are entered in mass units, their specific activity is used to compute the activity present. If enriched uranium is included in the measurements, its specific activity is computed based on its enrichment as described in Section 3.1.1.

Because the user chooses the input and output units used, the calculations all include factors to convert the units of the data to match the output units. This factor is not explicitly included in the following discussion.

### 7.1 EARLY-PHASE DOSES

The early phase dose extends from before a major release until the risk of a major release has ended and the areas with major contamination have been identified. Early-phase doses include up to 4 days of exposure to ground shine and the actual time of exposure to contaminated air as the plume passes. Early-phase doses are used to project where early-phase protective action guides (PAGs) may be exceeded and where early health effects are possible.

The early-phase doses that FMDose computes are total effective dose equivalent (TEDE), total acute

dose, and several organ-specific inhalation doses. TEDE is the sum of 4-day ground shine, air submersion, and 50-year committed effective dose equivalent (CEDE) from inhalation. Total acute bone dose is the sum of ground shine over the selected exposure period, air submersion, and 4-day red bone marrow inhalation doses over the exposure period selected by the user.

### 7.1.1 Inhalation Doses

Inhalation dose results from inhaling contaminated air. The inhalation doses that FMDose calculates are for 50-year CEDE and thyroid and 4-day bone, lung, and small-intestine wall. In addition a 50-year thyroid dose is calculated using only the air concentrations of isotopes of iodine. This dose is used in the decision to administer KI. The inhalation dose,  $D_{Io}$ , is computed as

$$D_{Io} = BR \times T_A \times \sum_{i=1}^N C_{Ai} \times DCF_{Ioi} \quad (7.1)$$

where

- BR = breathing rate (1.2 m<sup>3</sup>/h),
- $T_A$  = selected exposure time for air,
- N = number of radionuclides,
- $C_{Ai}$  = entered air concentration of radionuclide i,
- $DCF_{Ioi}$  = inhalation dose factor for radionuclide i and organ o.

If the user does not enter air concentration measurements, FMDose uses the activity resuspended from the ground instead. This calculation is described in Section 7.7.

### 7.1.2 Cloud-Submersion Dose

The cloud-submersion dose results from standing in contaminated air. The cloud-submersion dose,  $D_S$ , is

$$D_S = T_A \times \sum_{i=1}^N C_{Ai} \times DCF_{Si} \quad (7.2)$$

where  $DCF_{Si}$  is the effective submersion dose factor for radionuclide i.

If the user does not enter air concentration measurements, the activity resuspended from the ground is used in their place. This calculation is described in Section 7.7.

### 7.1.3 Ground-Shine Dose

The ground-shine dose is the gamma dose from standing on contaminated ground. FMDose computes ground shine at 1 m above the ground surface. The dose is reduced by a correction factor to account for ground surface roughness. The early-phase, ground-shine dose for all radionuclides,  $D_G$ , is

$$D_G = G_{\text{CORR}} \times \sum_{i=1}^N (DCF_{Gi} \times E_{Gi}) , \quad (7.3)$$

where

$G_{\text{CORR}}$  = selected ground surface correction factor (default: 0.7),

$DCF_i$  = effective dose factor from exposure to contaminated ground for radionuclide  $i$ ,

$E_{Gi}$  = exposure to the ground over the selected exposure period.

#### 7.1.4 TEDE Dose

TEDE is an estimate of the total dose from all pathways. The TEDE is used to compare to early-phase PAGs. TEDE, is

$$TEDE = D_{IE} + D_S + D_G , \quad (7.4)$$

where

$D_{IE}$  = 50-year committed effective dose equivalent from inhalation [Eq. (7.1)],

$D_S$  = effective dose equivalent from air submersion [Eq. (7.2)],

$D_G$  = effective dose equivalent from ground shine over 4 days [Eq. (7.3)].

## 7.2 EMERGENCY WORKER TURN-BACK GUIDANCE

Emergency worker turn-back guidance defines the self-reading dosimeter reading that should result in acceptable doses to workers who perform various kinds of emergency services. This calculation is from Method M.2.2 of the FRMAC assessment manual (DOE 1995). Emergency worker guidance values,  $EW_{TB}$ , are computed as

$$EW_{TB} = \frac{L_{EW}}{1 + \left( \frac{1.0 - ER}{MR} \times D_{IE} \right)} , \quad (7.5)$$

where

$L_{EW}$  = specific turn-back limit,

$ER$  = respiratory protection efficiency entered by the user,

$D_{IE}$  = 50-year committed effective dose equivalent rate (rem/h) computed as the dose from 1 h of exposure [Eq. (7.3)],

$MR$  = meter reading.

When KI is taken, FMDose reduces the inhalation dose by 95% of the contribution of the thyroid dose to effective dose (0.03) for all the isotopes of iodine. FMDose writes a table that includes the results of the calculations both with and without KI taken and with and without respiratory protection.

The turn-back limits used in the calculations are shown in Table 7.1

**Table 7.1 Emergency Worker Turn-Back Limits<sup>a</sup>**

<b>Emergency Worker Activity</b>	<b>Limit (rem)</b>
All	5
Protecting valuable property	10
Life saving	250
Life saving: to exceed this limit the worker should be a volunteer and be trained on the impact of radiation exposure	> 250

<sup>a</sup> Source: EPA 1992.

### 7.3 EARLY-PHASE EXPOSURE-RATE DILs

Early-phase DILs are used to promptly assess deposition to identify locations where the early-phase TEDE PAG may be exceeded after the plume passes. DILs are calculated from both air and ground concentrations, if the user has entered both. FMDose also computes a ground-only DIL that includes an estimate of the air concentrations that resulted from resuspension of activity on the ground. Both total DIL and radionuclide-specific DILs are calculated. This calculation is from Method M.3.2 of the FRMAC assessment manual (DOE 1995).

The total DIL is computed as

$$DIL_{EG} = P_E \times \frac{MR}{D_{TEDE}} \quad , \quad (7.7)$$

where  $P_E$  is the early-phase PAG for this DIL.

The  $D_{TEDE}$  includes 4 days of ground shine and 1 h of air submersion and inhalation. Doses used in the early-phase DIL calculations are computed as described in Section 7.1.4.

The radionuclide specific DILs are computed as

$$DIL_{EG} = P_{EG} \times \frac{C_{Gi}}{D_{TEDE}} \quad . \quad (7.8)$$

## 7.4 INTERMEDIATE-PHASE DOSES

The intermediate phase begins after the source of a major release is under control. FMDose computes ground-shine dose and inhalation dose from resuspension. The intermediate-phase doses that FMDose computes are for the first year, the second year, and fifty years. Note that the second year intermediate-phase dose is the dose from the first 2 years minus the dose from the first year. The intermediate-phase TEDE does not include an air submersion dose because it is assumed that the plume has passed before the intermediate phase begins.

FMDose computes the intermediate-phase ground-shine dose as shown in Eq. (7.3), using the appropriate exposure periods. The inhalation dose is computed as shown in Eq. (7.1), with the air concentration being estimated from resuspension using the appropriate exposure period as described in Section 7.7.

If the user enters a re-entry delay time, FMDose computes first- and second-year doses with delay. Dose with re-entry delay,  $D_{WD}$ , is computed as

$$D_{WD} = D_{(T+D)} - D_D \quad (7.9)$$

where

$D_{(T+D)}$  = dose for the selected period plus the re-entry delay,  
 $D_D$  = dose for the re-entry delay period.

In addition, the first-year dose from a meter reading is computed. This value is used to estimate the first-year dose from a meter reading taken 1 m above the ground. It is valid for only the mix entered. It is computed as

$$D_{First} = \frac{D_{G1st} + D_{IE1st}}{1.4 \times D_{G1st}} \quad (7.10)$$

## 7.5 INTERMEDIATE-PHASE DEPOSITION DILs

Intermediate-phase DILs are used to assess deposition to identify locations where the relocation PAG and long-term objectives may be exceeded after the plume passes. FMDose computes the intermediate-phase deposition exposure-rate total DIL the same way as the early-phase total DILs [Eq. (7.6)] using the intermediate-phase exposure periods, except that the external dose is always used to estimate the meter reading. FMDose assumes that there is no air submersion dose in the intermediate phase. The intermediate-phase deposition marker radionuclide DILs are computed the same way as the early-phase, radionuclide-specific DILs [Eq. (7.7)]. The DILs for first year, second year, and 50 years are computed for a range of times from 0 to 100 days since the release or contamination event. FMDose presents the results both graphically and as a table.

## 7.6 GROUND EXPOSURE AND WEATHERING

Ground-shine doses and DILs are dependent on ground contamination. They include the explicit calculation of radiological decay and daughter ingrowth and weathering of the material on the ground. The exposure to radionuclide  $i$  on the ground,  $E_{Gi}$ , is computed as (EPA 1992)

$$E_{Gi} = 0.37 \times \left( \int_{j=0}^{T_g} C_{Gi} \times e^{-2.05E-5} \right) + 0.63 \times \left( \int_{j=0}^{T_g} C_{Gi} \times e^{-3.10E-3} \right), \quad (7.11)$$

where

$L$  = number of daughters in radionuclide chain  $i$ ,  
 $C_{gi}$  = concentration of radionuclide  $i$  on the ground.

## 7.7 AIR CONCENTRATION DUE TO RESUSPENSION

Intermediate-phase doses from inhalation and air immersion are always computed from the activity assumed to be resuspended from the ground. FMDose computes early-phase doses from resuspended activity when the user has not entered any air concentration measurements. The concentration of activity in the air that results from material resuspended from the ground is computed as (NCRP 1999)

$$C_{Ai} = C_{Gi} \times (R \times e^{-0.01T_g} + 10^{-9}), \quad (7.12)$$

where  $R$  is the resuspension rate entered by the user.

Note that because the computed resuspension factor is a function of time, the resuspension calculation is included in the decay calculation.

## 7.8 REFERENCES

International Commission on Radiological Protection (ICRP). 1977. "Recommendations of the International Commission of Radiological Protection." ICRP Publication 26, Pergamon Press, Oxford.

National Council on Radiation Protection and Measurements (NCRP). 1999. *Recommended Screening Limits for Contaminated Surface Soil and Review of Factors Relevant to Site-Specific Studies*. NCRP Report 129, NCRP, Bethesda, Md.

U.S. Department of Energy (DOE). 1995. *FRMAC Assessment Manual for Interim Use and Comment*. U.S. Department of Energy.



U.S. Environmental Protection Agency (EPA). 1988. "Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion." *Federal Guidance Report No. 11*. EPA-520/11-88-020, U.S. Environmental Protection Agency.

U.S. Environmental Protection Agency (EPA). 1992. "Manual of Protective Action Guides and Protective Actions for Nuclear Incidents." EPA-520/1-75-001A, U.S. Environmental Protection Agency.

U.S. Environmental Protection Agency (EPA). 1993. "External Exposure to Radionuclides in Air, Water, and Soil." *Federal Guidance Report No. 12*. EPA-402-R-93-081, U.S. Environmental Protection Agency.

## 8 DECAY CALCULATIONS

Almost all modules in RASCAL 3.0 require some kind of decay calculation. All use the same data and basic method of calculation. Because STDose requires that decay calculations be performed at least every 15 min, it was determined that a significant amount of calculation time could be saved by precalculating decay over that period for all of the radionuclides in RASCAL. Since the STDose calculations may also require decay over longer or shorter periods, decay was also precomputed for 1 and 5 min, 1 h, and 1, 14, and 182 days. One implication of this is that in RASCAL 3.0, decay cannot be calculated for less than 1 min. Only FMDose calculates decay directly. In FMDose, the decay equations had to be modified to include the weathering of material on the ground. For this reason the precalculated decay file could not be used.

### 8.1 DECAY DATA FILES

The decay data used in RASCAL 3.0 is the decay data used in creating the dose factors in *Federal Guidance Report No. 12* (USEPA 1993). FMDose reads this file directly. The decay data file used by STDose and decay was created by running a program called Chain, that was originally written by K. F. Eckerman to read the decay data used in creating the dose factors in *Federal Guidance Report No. 12* and to solve the Bateman equations.

The precalculated decay data is stored in two binary, direct-access files called DECAY.DAT and INTDECAY.DAT. These files contain data for all 825 radionuclides in *Federal Guidance Report No. 12*, sorted in alphabetical order. Decay has been precomputed for 1, 5, and 15 min, 1 h, and 1, 14, and 182 days. Each line in the file contains the names and resulting activities of the parent nuclide and its daughters. DECAY.DAT contains the activity (Ci) of each radionuclide remaining after the decay period. INTDECAY.DAT contains the integrated activity (Ci sec) of each radionuclide calculated over the decay period.

### 8.2 IMPLEMENTATION

This section discusses the implementation of the decay calculations in STDose, FMDose, and DecayCalc. The calculation of decay in TADPUFF and TADPLUME are discussed in Section 4.8.

#### 8.2.1 STDose and DecayCalc

The decay calculations for the source term calculation of STDose and DecayCalc are performed by the same subroutines. These subroutines compute decay incrementally, starting with the longest time period for which decay data have been precalculated and stored. For each time period, the activity of the parent and its daughter products are summed. The process is repeated until the correct decay time is reached. For example, assuming that 72 min of decay are required, the subroutines find the required nuclide

decay data using a binary search and then sum it for 1 h, then for 5 min twice, then for 1 min twice.

STDose extracts the required 5-min and 15-min decay data for the radionuclides in the source term and passes them in a file to TADPUFF or TADPLUME for the calculation of decay during atmospheric transport.

In STDose only, the activities of the short-lived daughters are initially set equal to their parents. These are listed in Table 8.1. (Note that only 0.16 of the  $^{135}\text{I}$  is set to  $^{135\text{m}}\text{Xe}$ .) The activities of the parents and daughters may not remain equal throughout the accident because reduction mechanisms may affect them differently.

**Table 8.1 Short-lived Daughters Whose Activities are Set Equal to Their Parents' Activities**

Parent	Daughter
$^{44}\text{Ti}$	$^{44}\text{Sc}$
$^{68}\text{Ge}$	$^{68}\text{Ga}$
$^{88}\text{Kr}$	$^{88}\text{Rb}$
$^{99}\text{Mo}$	$^{99\text{m}}\text{Tc}$
$^{106}\text{Ru}$	$^{106}\text{Rh}$
$^{109}\text{Cd}$	$^{109\text{m}}\text{Ag}$
$^{113}\text{Sn}$	$^{113\text{m}}\text{In}$
$^{126}\text{Sn}$	$^{126\text{m}}\text{Sb}$ $^{126}\text{Sb}$
$^{129\text{m}}\text{Te}$	$^{129}\text{Te}$
$^{135}\text{I} (\times 0.16)$	$^{135\text{m}}\text{Xe}$
$^{137}\text{Cs}$	$^{137\text{m}}\text{Ba}$
$^{144}\text{Ce}$	$^{144}\text{Pr}$

### 8.2.2 FMDose

FMDose calculates decay directly. The Chain program has been modified to be called as a subroutine. FMDose calls Chain for each parent radionuclide. Depending on the calculation being performed, it returns either the activity remaining after the decay period or the amount of integrated activity for each parent and its daughters integrated over the decay period and assuming an initial activity of one. These

results are multiplied by the actual activity of the parent. The activities of short-lived daughters are not automatically set equal to their parents, as is done in STDose and DecayCalc.

### **8.3 REFERENCES**

U. S. Environmental Protection Agency (EPA). 1993. "External Exposure to Radionuclide in Air, Water, and Soil." *Federal Guidance Report No. 12*, EPA-402-R-93-081, U.S. Environmental Protection Agency.

APPENDIX. NUCLEAR REACTOR FACILITY DATA USED IN STD05E

Name	Facility Type	Containment Type	Number Fuel Assemblies	Steam Generator Type	Amount of Coolant (gal)	Containment Volume ft <sup>3</sup>	Design Leak Rate %/d	Design Pressure psi	Rated Power MW(t)	Avg Fuel Burnup - Reactor	Avg Fuel Burnup - Spent Fuel Storage	Status
Arkansas - Unit 1	PWR	Dry Ambient	177	Once-Through	188824	2100000	0.2	59	2568	22000	15000	Operational
Arkansas - Unit 2	PWR	Dry Ambient	177	U-Tube	206985	1800000	0.1	54	2815	22000	15000	Operational
Beaver Valley - Unit 1	PWR	Sub-atmospheric	157	U-Tube	195000	1800000	0.1	54	2652	22000	15000	Operational
Beaver Valley - Unit 2	PWR	Sub-atmospheric	157	U-Tube	195000	1800000	0.1	54	2652	22000	15000	Operational
Big Rock Point	BWR	Dry Ambient	84	N/A	0	1200000	0.5	27	240	22000	15000	Decommissioned
Braidwood - Unit 1	PWR	Dry Ambient	193	U-Tube	250808	2900000	0.1	61	3411	22000	15000	Operational
Braidwood - Unit 2	PWR	Dry Ambient	193	U-Tube	250808	2900000	0.1	61	3411	22000	15000	Operational
Browns Ferry - Unit 1	BWR	Mark I	764	N/A	164650	160000	0.5	56	3293	22000	15000	Operational
Browns Ferry - Unit 2	BWR	Mark I	764	N/A	164650	160000	0.5	56	3293	22000	15000	Operational
Browns Ferry - Unit 3	BWR	Mark I	764	N/A	164650	160000	0.5	56	3293	22000	15000	Operational
Brunswick - Unit 1	BWR	Mark I	560	N/A	127900	160000	0.5	62	2436	22000	15000	Operational
Brunswick - Unit 2	BWR	Mark I	560	N/A	121800	160000	0.5	62	2436	22000	15000	Operational
Byron - Unit 1	PWR	Dry Ambient	193	U-Tube	250808	2900000	0.1	61	3411	22000	15000	Operational
Byron - Unit 2	PWR	Dry Ambient	193	U-Tube	250808	2900000	0.1	61	3411	22000	15000	Operational

APPENDIX. NUCLEAR REACTOR FACILITY DATA USED IN STD0SE (cont.)

Name	Facility Type	Containment Type	Number Fuel Assemblies	Steam Generator Type	Amount of Coolant (gal)	Containment Volume ft <sup>3</sup>	Design Leak Rate %/d	Design Pressure psi	Rated Power MW(t)	Avg Fuel Burnup - Reactor	Avg Fuel Burnup - Spent Fuel Storage	Status
Callaway	PWR	Dry Ambient	193	U-Tube	262132	2500000	0.1	60	3565	22000	15000	Operational
Calvert Cliffs - Unit 1	PWR	Dry Ambient	217	U-Tube	198529	2000000	0.33	50	2700	22000	15000	Operational
Calvert Cliffs - Unit 2	PWR	Dry Ambient	217	U-Tube	198529	2000000	0.33	50	2700	22000	15000	Operational
Catawba - Unit 1	PWR	Ice Condenser	193	U-Tube	250808	1200000	0.2	30	3411	22000	15000	Operational
Catawba - Unit 2	PWR	Ice Condenser	193	U-Tube	250808	1200000	0.2	30	3411	22000	15000	Operational
Clinton	BWR	Mark III	624	N/A	144700	250000	0.65	15	2894	22000	15000	Operational
Comanche Peak - Unit 1	PWR	Dry Ambient	193	U-Tube	250808	3000000	0.1	50	3411	22000	15000	Operational
Comanche Peak - Unit 2	PWR	Dry Ambient	193	U-Tube	250808	3000000	0.1	50	3411	22000	15000	Operational
Cooper	BWR	Mark I	548	N/A	119050	150000	0.5	56	2381	22000	15000	Operational
Crystal River - Unit 3	PWR	Dry Ambient	177	Once-Through	187059	2000000	0.25	55	2544	22000	15000	Operational
D. C. Cook - Unit 1	PWR	Ice Condenser	193	U-Tube	238971	1200000	0.25	12	3250	22000	15000	Operational
D. C. Cook - Unit 2	PWR	Ice Condenser	193	U-Tube	250808	1200000	0.25	12	3411	22000	15000	Operational
Davis-Besse	PWR	Dry Ambient	177	Once-Through	203823	2900000	0.5	40	2772	22000	15000	Operational
Diablo Canyon - Unit 1	PWR	Dry Ambient	193	U-Tube	245441	2600000	0.1	47	3338	22000	15000	Operational
Diablo Canyon - Unit 2	PWR	Dry Ambient	193	U-Tube	250808	2600000	0.1	47	3411	22000	15000	Operational

APPENDIX. NUCLEAR REACTOR FACILITY DATA USED IN STD05E (cont.)

Name	Facility Type	Containment Type	Number Fuel Assemblies	Steam Generator Type	Amount of Coolant	Containment Volume	Design Leak Rate	Design Pressure	Rated Power	Avg Fuel Burnup - Reactor	Avg Fuel Burnup - Spent Fuel Storage	Status
					(gal)	ft <sup>3</sup>	%/d	psi	MW(t)			
Dresden - Unit 2	BWR	Mark I	724	N/A	126350	160000	0.5	62	2527	22000	15000	Operational
Dresden - Unit 3	BWR	Mark I	724	N/A	126350	160000	0.5	62	2527	22000	15000	Operational
Duane Arnold	BWR	Mark I	368	N/A	82900	130000	0.5	56	3430	22000	15000	Operational
Edwin I. Hatch - Unit 1	BWR	Mark I	560	N/A	127900	150000	1.2	56	2436	22000	15000	Operational
Edwin I. Hatch - Unit 2	BWR	Mark I	560	N/A	127900	150000	1.2	56	2436	22000	15000	Operational
Fermi - Unit 2	BWR	Mark I	764	N/A	171500	160000	0.5	56	3430	22000	15000	Operational
Fort Calhoun	PWR	Dry Ambient	133	U-Tube	110294	1100000	0.2	56	1500	22000	15000	Operational
Generic BWR Mark I	BWR	Mark I	550	N/A	170000	250000	0.54	60	2500	22000	15000	Generic
Generic BWR Mark II	BWR	Mark II	550	N/A	170000	350000	0.58	50	3000	22000	15000	Generic
Generic BWR Mark III	BWR	Mark III	700	N/A	170000	1250000	0.36	15	3400	22000	15000	Generic
Generic PWR with Ice Condenser Containment	PWR	Ice Condenser	200	U-Tube	250000	1200000	0.25	15	3500	22000	15000	Generic
Generic PWR with Large, Dry Containment	PWR	Dry Ambient	200	U-Tube	250000	2500000	0.1	50	3800	22000	15000	Generic

APPENDIX. NUCLEAR REACTOR FACILITY DATA USED IN STDOSE (cont.)

Name	Facility Type	Containment Type	Number Fuel Assemblies	Steam Generator Type	Amount of Coolant (gal)	Containment Volume ft <sup>3</sup>	Design Leak Rate %/d	Design Pressure psi	Rated Power MW(t)	Avg Fuel Burnup - Reactor	Avg Fuel Burnup - Spent Fuel Storage	Status
Ginna	PWR	Dry Ambient	121	U-Tube	111765	1000000	0.1	60	1520	22000	15000	Operational
Grand Gulf - Unit 1	BWR	Mark III	800	N/A	191650	270000	0.35	15	3833	22000	15000	Operational
H. B. Robinson - Unit 2	PWR	Dry Ambient	157	U-Tube	169118	2100000	0.1	42	2300	22000	15000	Operational
Haddam Neck	PWR	Dry Ambient	157	U-Tube	0	1700000	0.1	40	1825	22000	15000	Decommissioned
Hope Creek - Unit 1	BWR	Mark I	764	N/A	164650	170000	0.5	62	3293	22000	15000	Operational
Indian Point - Unit 2	PWR	Dry Ambient	193	U-Tube	225809	2600000	0.1	47	3071	22000	15000	Operational
Indian Point - Unit 3	PWR	Dry Ambient	193	U-Tube	222426	2600000	0.1	47	3025	22000	15000	Operational
James A. Fitzpatrick	BWR	Mark I	560	N/A	126800	110000	0.5	56	2436	22000	15000	Operational
Joseph M. Farley - Unit 1	PWR	Dry Ambient	157	U-Tube	195000	2000000	0.3	54	2652	22000	15000	Operational
Joseph M. Farley - Unit 2	PWR	Dry Ambient	157	U-Tube	70000	2000000	0.3	54	2652	22000	15000	Operational
Kewaunee	PWR	Dry Ambient	121	U-Tube	121324	1300000	0.5	46	1650	22000	15000	Operational
LaCrosse	BWR	Mark I	0	N/A	70000	0	0	0	165	22000	15000	Decommissioned
LaSalle - Unit 1	BWR	Mark II	764	N/A	166150	200000	0.5	45	3323	22000	15000	Operational
LaSalle - Unit 2	BWR	Mark II	764	N/A	166150	200000	0.5	45	3323	22000	15000	Operational
Limerick - Unit 1	BWR	Mark II	764	N/A	172900	240000	0.5	56	3293	22000	15000	Operational



APPENDIX. NUCLEAR REACTOR FACILITY DATA USED IN STD0SE (cont.)

Name	Facility Type	Containment Type	Number Fuel Assemblies	Steam Generator Type	Amount of Coolant (gal)	Containment Volume ft <sup>3</sup>	Design Leak Rate %/d	Design Pressure psi	Rated Power MW(t)	Avg Fuel Burnup - Reactor	Avg Fuel Burnup - Spent Fuel Storage	Status
Limerick - Unit 2	BWR	Mark II	764	N/A	172900	240000	0.5	56	3293	22000	15000	Operational
Maine Yankee	PWR	Dry Ambient	217	U-Tube	0	1900000	0.1	55	2700	22000	15000	Decommissioned
McGuire - Unit 1	PWR	Ice Condenser	193	U-Tube	250808	1200000	0.2	28	3411	22000	15000	Operational
McGuire - Unit 2	PWR	Ice Condenser	193	U-Tube	250808	1200000	0.2	28	3411	22000	15000	Operational
Millstone - Unit 1	BWR	Mark I	580	N/A	0	150000	0.5	62	2011	22000	15000	Decommissioned
Millstone - Unit 2	PWR	Dry Ambient	217	U-Tube	198529	1900000	3	54	2700	22000	15000	Operational
Millstone - Unit 3	PWR	Sub-atmospheric	193	U-Tube	250808	10000000	0.9	45	3411	22000	15000	Operational
Monticello	BWR	Mark I	484	N/A	83500	130000	0.5	56	1670	22000	15000	Operational
Nine Mile Point - Unit 1	BWR	Mark I	532	N/A	92500	180000	0.5	62	1850	22000	15000	Operational
Nine Mile Point - Unit 2	BWR	Mark II	764	N/A	173350	300000	1.1	45	3323	22000	15000	Operational
North Anna - Unit 1	PWR	Sub-atmospheric	157	U-Tube	212721	1800000	0.1	45	2893	22000	15000	Operational
North Anna - Unit 2	PWR	Sub-atmospheric	157	U-Tube	212721	1800000	0.1	45	2893	22000	15000	Operational
Oconee - Unit 1	PWR	Dry Ambient	177	Once-Through	188824	1900000	0.5	59	2568	22000	15000	Operational

APPENDIX. NUCLEAR REACTOR FACILITY DATA USED IN STD05E (cont.)

Name	Facility Type	Containment Type	Number Fuel Assemblies	Steam Generator Type	Amount of Coolant (gal)	Containment Volume ft <sup>3</sup>	Design Leak Rate %/d	Design Pressure psi	Rated Power MW(t)	Avg Fuel Burnup - Reactor	Avg Fuel Burnup - Spent Fuel Storage	Status
Oconee - Unit 2	PWR	Large, Dry	177	Once-Through	188824	1900000	0.5	59	2568	22000	15000	Operational
Oconee - Unit 3	PWR	Large, Dry	177	Once-Through	188824	1900000	0.5	59	2568	22000	15000	Operational
Oyster Creek	BWR	Mark I	560	N/A	96500	180000	0.5	62	1930	22000	15000	Operational
Palisades	PWR	Dry Ambient	204	U-Tube	186029	1600000	0.2	55	2530	22000	15000	Operational
Palo Verde - Unit 1	PWR	Dry Ambient	241	U-Tube	279412	2600000	0	60	3800	22000	15000	Operational
Palo Verde - Unit 2	PWR	Large, Dry	241	U-Tube	285000	2600000	0	60	3800	22000	15000	Operational
Palo Verde - Unit 3	PWR	Large, Dry	241	U-Tube	285000	2600000	0.1	60	3800	22000	15000	Operational
Peach Bottom - Unit 2	BWR	Mark I	764	N/A	172900	180000	0.5	58	3293	22000	15000	Operational
Peach Bottom - Unit 3	BWR	Mark I	764	N/A	172900	180000	0.5	58	3293	22000	15000	Operational
Perry - Unit 1	BWR	Mark III	748	N/A	178950	280000	0.2	15	3579	22000	15000	Operational
Pilgrim - Unit 1	BWR	Mark I	580	N/A	99900	150000	0.5	56	1998	22000	15000	Operational
Point Beach - Unit 1	PWR	Dry Ambient	121	U-Tube	111691	1000000	0.4	60	1518	22000	15000	Operational
Point Beach - Unit 2	PWR	Dry Ambient	121	U-Tube	111691	1000000	0.4	60	1518	22000	15000	Operational
Prairie Island - Unit 1	PWR	Dry Ambient	121	U-Tube	121322	1300000	0.5	41	1650	22000	15000	Operational
Prairie Island - Unit 2	PWR	Dry Ambient	121	U-Tube	121322	1300000	0.5	41	1650	22000	15000	Operational

APPENDIX. NUCLEAR REACTOR FACILITY DATA USED IN STD050 (cont.)

Name	Facility Type	Containment Type	Number Fuel Assemblies	Steam Generator Type	Amount of Coolant (gal)	Containment Volume ft <sup>3</sup>	Design Leak Rate %/d	Design Pressure psi	Rated Power MW(t)	Avg Fuel Burnup - Reactor	Avg Fuel Burnup - Spent Fuel Storage	Status
Quad-Cities - Unit 1	BWR	Mark I	724	N/A	125550	160000	0.5	56	2511	22000	15000	Operational
Quad-Cities - Unit 2	BWR	Mark I	724	N/A	125550	160000	0.5	56	2511	22000	15000	Operational
Rancho Seco	PWR	Large, Dry	177	N/A	0	2000000	0.1	59	2772	22000	15000	Decommissioned
River Bend - Unit 1	BWR	Mark III	624	N/A	144700	260000	0.26	15	2894	22000	15000	Operational
Salem - Unit 1	PWR	Dry Ambient	193	U-Tube	250808	2600000	0.1	47	3411	22000	15000	Operational
Salem - Unit 2	PWR	Dry Ambient	193	U-Tube	250808	2600000	0.1	47	3411	22000	15000	Operational
San Onofre - Unit 1	PWR	N/A	0	N/A	0	1400000	0.5	47	1347	22000	15000	Decommissioned
San Onofre - Unit 2	PWR	Dry Ambient	217	U-Tube	249265	2300000	0.3	60	3390	22000	15000	Operational
San Onofre - Unit 3	PWR	Dry Ambient	217	U-Tube	249265	2300000	0.3	60	3390	22000	15000	Operational
Seabrook - Unit 1	PWR	Dry Ambient	193	U-Tube	250808	2700000	0.5	65	3411	22000	15000	Operational
Sequoyah - Unit 1	PWR	Ice Condenser	193	U-Tube	250808	1200000	0.5	11	3411	22000	15000	Operational
Sequoyah - Unit 2	PWR	Ice Condenser	193	U-Tube	250808	1200000	0.5	11	3411	22000	15000	Operational
Shearon Harris - Unit 1	PWR	Dry Ambient	157	U-Tube	204044	2500000	0.3	45	2775	22000	15000	Operational
South Texas Project - Unit 1	PWR	Dry Ambient	193	U-Tube	279412	3300000	0.3	56	3800	22000	15000	Operational

APPENDIX. NUCLEAR REACTOR FACILITY DATA USED IN STD05E (cont.)

Name	Facility Type	Containment Type	Number Fuel Assemblies	Steam Generator Type	Amount of Coolant (gal)	Containment Volume ft <sup>3</sup>	Design Leak Rate %/d	Design Pressure psi	Rated Power MW(t)	Avg Fuel Burnup - Reactor	Avg Fuel Burnup - Spent Fuel Storage	Status
South Texas Project - Unit 2	PWR	Dry Ambient	193	U-Tube	279412	3300000	0.3	56	3800	22000	15000	Operational
St. Lucie - Unit 1	PWR	Dry Ambient	217	U-Tube	198529	2500000	0.5	44	2700	22000	15000	Operational
St. Lucie - Unit 2	PWR	Dry Ambient	217	U-Tube	198529	2500000	0.5	44	2700	22000	15000	Operational
Summer	PWR	Dry Ambient	157	U-Tube	213235	1800000	0.2	55	2775	22000	15000	Operational
Surry - Unit 1	PWR	Sub-atmospheric	157	U-Tube	187206	1800000	0.1	60	2441	22000	15000	Operational
Surry - Unit 2	PWR	Sub-atmospheric	157	U-Tube	187206	1800000	0.1	60	2441	22000	15000	Operational
Susquehanna - Unit 1	BWR	Mark II	764	N/A	172050	240000	0.5	53	3293	22000	15000	Operational
Susquehanna - Unit 2	BWR	Mark II	764	U-Tube	172050	240000	0.5	53	3293	22000	15000	Operational
Three Mile Island - Unit 1	PWR	Dry Ambient	177	Once-Through	188824	2000000	0.1	55	2568	22000	15000	Operational
Trojan	PWR	N/A	193	N/A	0	2000000	0.2	60	3411	22000	15000	Decommissioned
Turkey Point - Unit 3	PWR	Dry Ambient	157	U-Tube	169118	1600000	0.25	59	2200	22000	15000	Operational
Turkey Point - Unit 4	PWR	Dry Ambient	157	U-Tube	169118	1600000	0.25	59	2200	22000	15000	Operational
Vermont Yankee	BWR	Mark I	368	N/A	79650	130000	0.5	56	1593	22000	15000	Operational

APPENDIX. NUCLEAR REACTOR FACILITY DATA USED IN STD05E (cont.)

Name	Facility Type	Containment Type	Number Fuel Assemblies	Steam Generator Type	Amount of Coolant (gal)	Containment Volume ft <sup>3</sup>	Design Leak Rate %/d	Design Pressure psi	Rated Power MW(t)	Avg Fuel Burnup - Reactor	Avg Fuel Burnup - Spent Fuel Storage	Status
Vogtle - Unit 1	PWR	Dry Ambient	193	U-Tube	262132	2700000	0.1	52	3565	22000	15000	Operational
Vogtle - Unit 2	PWR	Dry Ambient	193	U-Tube	262132	2700000	0.1	52	3565	22000	15000	Operational
Washington Nuclear Power - Unit 2	BWR	Mark II	764	N/A	174300	200000	0.5	45	3323	22000	15000	Operational
Waterford - Unit 3	PWR	Dry Ambient	217	U-Tube	249268	2700000	0.5	44	3390	22000	15000	Operational
Watts Bar - Unit 1	PWR	Ice Condenser	193	U-Tube	250808	920000	0.5	15	3411	22000	15000	Operational
Wolf Creek - Unit 1	PWR	Dry Ambient	193	U-Tube	262132	2500000	0.1	60	3565	22000	15000	Operational
Yankee- Rowe	PWR	Large, Dry	76	U-Tube	0	1000000	3	34	600	22000	15000	Decommissioned
Zion - Unit 1	PWR	Dry Ambient	193	U-Tube	0	2900000	0.1	47	3250	22000	15000	Decommissioned
Zion - Unit 2	PWR	Dry Ambient	193	U-Tube	0	2900000	0.1	47	3250	22000	15000	Decommissioned

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(See instructions on the reverse)

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A. L. Sjoreen, ORNL (a), J. V. Ramsdell, Jr., PNNL (b), T. J. McKenna, IAEA (c), S. A. McGuire, NRC (d), C. Fosmire, Innovative Emergency Management (e), and G. F. Athey, Athey Consulting (f)

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10. SUPPLEMENTARY NOTES

Stephen. A. McGuire, NRC Project Manager

11. ABSTRACT (200 words or less)

The Radiological Assessment System for Consequence Analysis (RASCAL) 3.0 is the latest version of the RASCAL series of codes. RASCAL was developed for use by U. S. Nuclear Regulatory Commission personnel who conduct independent assessment of radiological accidents to prepare dose projections. It includes three sets of tools for use in consequence analysis: STDose, FMDose, and DecayCalc. STDose estimates: (1) source terms for radiological accidents, (2) atmospheric transport, diffusion, and deposition of effluents from the accidents, and (3) doses from exposures to the effluents. FMDose calculates doses from environmental measurements of activity in the air and on the ground. DecayCalc calculates activity of radionuclides present at a future time following decay and ingrowth. The current version of RASCAL includes computational techniques that are substantially modified from those used in the prior version of RASCAL and significantly expands the capabilities of STDose. The major changes to STDose are: (1) the inclusion of time-dependent source terms and source terms for fuel cycle and materials accidents, (2) the inclusion of radiological decay during atmospheric transport, (3) the addition of a UF6 atmospheric transport model, and (4) the ability to include meteorological data from multiple stations and the effects of terrain.

12. KEY WORDS/DESCRIPTORS (List words or phrases that will assist researchers in locating the report.)

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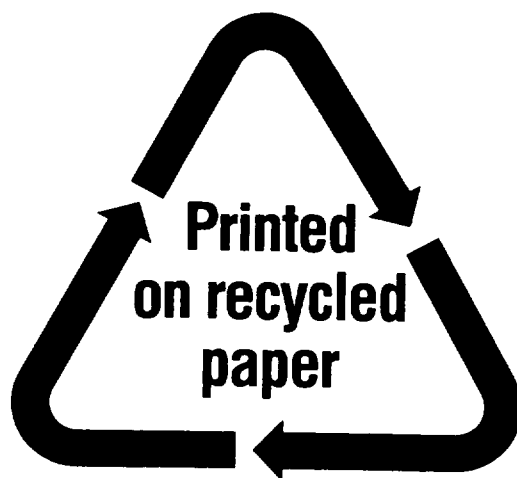
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