

HIGH LEVEL HAZARD SAFETY ANALYSIS VOL 3 OF 3

Main Category:	Safety & Failures
Sub Category:	-
Course #:	SAF-143
Course Content:	143 pgs
PDH/CE Hours:	8

OFFICIAL COURSE/EXAM (SEE INSTRUCTIONS ON NEXT PAGE)

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SAF-143 EXAM PREVIEW

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Exam Preview:

- 1. Liquid effluent releases to surface bodies generally require relatively long periods of time (e.g., hours to days) before the general public could be impacted.
 - a. True
 - b. False
- 2. Each principal water body has its own unique transport characteristics due to different boundary conditions and flow rates. Which water body matches the following description: Advective and turbulent flows throughout with variable boundaries?
 - a. Rivers
 - b. Estuaries
 - c. Small lakes and reservoirs
 - d. Oceans and large lakes
- 3. According to the reference material, two behaviors need to be captured to model contaminant transport in groundwater media. The first is movement of the carrier fluid and the second is the rate of absorption of the dissolved contaminants.
 - a. True
 - b. False
- 4. Four types of radiation are important to consider in DSAs: alpha (α), beta (β), gamma (γ), and neutron. Which types of radiation matches the description: consists of electromagnetic waves or photons, and have energy similar to that of x-rays?
 - a. Alpha
 - b. Beta
 - c. Gamma
 - d. Neutron

- 5. Acute health effects from short-term exposures to toxic chemicals differ with respect to mode of exposure or route of entry into the human body. Since the inhalation pathway is also considered the most impactful for toxic chemical exposures, most toxic chemical consequence assessments focus on inhalation exposures.
 - a. True
 - b. False
- 6. There are 14 classes of aquatic dispersion models that have been developed for application to surface water bodies. Using Table 7-1. Aquatic Dispersion Model Classes, which of the following class of aquatic dispersion model matches the characteristics: Transient, homogeneous, analytical solution?
 - a. Partially-mixed model
 - b. Numerical model
 - c. Completely-mixed model
 - d. Transient source model
- 7. According to the reference material, the principal advantage of AEGLs is that they have been established for eight exposure times ranging from 10 minutes to _ hours.
 - a. 2
 - b. 4
 - **c**. 6
 - d. 8
- 8. According to the reference material, the atmospheric variables of temperature and moisture (e.g., relative humidity, wet-bulb temperature) do directly affect the magnitudes of the atmospheric dilution and diffusion for radionuclide release evaluations.
 - a. True
 - b. False
- 9. Using Table 9-3. Uranium Compound PAC/TEELs, which of the concentrations below corresponds to PAC/TEEL-3 of Uranium Telluride?
 - a. 26
 - b. 50
 - c. 51
 - d. 62
- 10. The organ weighting factors represent the fraction of the total health risk resulting from uniform whole-body irradiation that could be attributed to that particular tissue or organ. Using Table 8-2. Organ Weighting Factors, what is the ICRP-60 weighting factor for the liver?
 - a. 0.01
 - b. 0.05
 - c. 0.12
 - d. 0.20

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ACRONYMS

AC	Administrative Control or Alternating Current
ACGIH	American Conference of Government Industrial Hygienists
AED	Aerodynamic Equivalent Diameter
AEGL	Acute Exposure Guideline Level
AICC	Adiabatic, Constant-Volume Combustion
AIHA	American Industrial Hygienist Association
AMAD	Activity Median Aerodynamic Diameter
ANS	American Nuclear Society
ANSI	American National Standards Institute
APAC	Accident Phenomenology and Consequence
ARF	Airborne Release Fraction
ASCE	American Society of Civil Engineers
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
BC	Building Construction
BDBA	Beyond Design Basis Accident
BEBA	Beyond Evaluation Basis Accident
BEU	Beyond Extremely Unlikely
BLEVE	Boiling Liquid Expanding Vapor Explosion
BNL	Brookhaven National Laboratory
BR	Breathing Rate
BST	Building Source Term
CCPS	Center for Chemical Process Safety
CDC	Centers for Disease Control
CFAST	Consolidated Model of Fire and Smoke Transport
CFD	Computational Fluid Dynamics
CFR	Code of Federal Regulations
CMM	Chemical Mixture Methodology
CR	Central Registry
CSE	Criticality Safety Evaluation
CTH	Cloud Top Height
CW	Co-located Worker
DBA	Design Basis Accident
DCF	Dose Conversion Factor
DDT	Deflagration to Detonation Transition
DF	Decontamination Factor
DG	Dense Gas
DNFSB	Defense Nuclear Facilities Safety Board
DOE	Department of Energy
DOS	Disk Operating System
DOT	Department of Transportation
DR	Damage Ratio
DSA	Documented Safety Analysis
DTA	Differential Thermal Analysis

EBA EDE	Evaluation Basis Accident Effective Dose Equivalent		
EEGL	Emergency Exposure Guidance Level		
EFCOG	Energy Facility Contractor Group		
EG	Evaluation Guideline		
EPA	Environmental Protection Agency		
ERPG	Emergency Response Planning Guideline		
EU	Extremely Unlikely		
FDC	Flood Design Category		
FDT	Fire Dynamics Tool		
FGR	Federal Guidance Report		
FHA	Fire Hazards Analysis		
FMEA	Failure Modes and Effects Analysis		
FTF	Filter Test Facility		
FW	Facility Worker		
GEP	Good Engineering Practice		
GNB	Gaussian Neutrally Buoyant		
GRF	German Research Foundation		
HA	Hazard Analysis		
HAZOP	Hazard and Operational Analysis		
HC	Hazard Category		
HCN	Health Code Number		
HDBK	Handbook		
HE	High Explosive		
HEPA	High Efficiency Particulate Air		
HPR	Highly Protected Risk		
HRR	Heat Release Rate		
HSDB	Hazardous Substances Data Bank		
IACR	International Association of Cancer Registries		
ICRP	International Council on Radiation Protection		
IDLH	Immediately Dangerous to Life and Health		
IEEE	Institute of Electrical and Electronics Engineers		
ILA	Immediate Landscaped Area		
INL	Idaho National Laboratory		
IST	Initial Source Term		
JFD	Joint Frequency Distribution		
LANL	Los Alamos National Laboratory		
LCF	Latent Cancer Fatality		
LEL	Lower Explosive Limit		
LET	Linear Energy Transfer		
LFL	Lower Flammability Limit		
LOC	Level of Concern		
LPF	Leak Path Factor		
LPG	Liquified Petroleum Gas		

MAR	Material at Risk		
MAK-Wert	Maximale Arbeitsplatz-Konzentration		
MOI	Maximally Exposed Offsite Individual		
MW	Molecular Weight		
NAC/AEGL	National Advisory Committee for Acute Exposure Guideline Levels		
NARAC	National Atmospheric Release Advisory Center		
NASA	National Aeronautics and Space Administration		
NCRP	National Council on Radiation Protection		
NDC	Natural Phenomena Hazard Design Category		
NEPA	National Environmental Policy Act		
NFDRS	National Fire Rating Danger System		
NIOSH	National Institute for Occupational Safety and Health		
NIST	National Institute of Standards and Technology		
NNSA	National Nuclear Security Administration		
NNSS	Nevada Nuclear Security Site		
NOAA	National Oceanic and Atmospheric Administration		
NPH	Natural Phenomena Hazard		
NQA	Nuclear Quality Assurance		
NRC	Nuclear Regulatory Commission		
NTSB	National Transportation Safety Board		
OSHA	Occupational Safety and Health Administration		
PAC	Protective Action Criteria		
PBL	Planetary Boundary Layer		
PC	Performance Category		
PDC	Precipitation Design Category		
PEL	Permissible Exposure Level		
PHA	Preliminary Hazard Assessment		
PISA	Potential Inadequacy of the Safety Analysis		
PNNL	Pacific Northwest National Laboratory		
PRA	Probabilistic Risk Assessment		
PrHA	Process Hazard Analysis		
PSO	Program Secretarial Office		
PUREX	Plutonium Uranium Redox Extraction		
PWHA	Probabilistic Wind Hazard Assessment		
ΡΟΡΛ	Persource Conservation and Persovery Act		
RCKA	Resource Conservation and Recovery Act Recommended Exposure Level		
REL	Recommended Exposure Level		
RG	Regulatory Guide		
RTECS	Regulatory Guide Registry of Toxic Effects of Chemical Substances		
KILCS	Registry of Toxic Effects of Chemical Substances		
SAC	Specific Administrative Control		
SAWG	Safety Analysis Working Group		
SBAA	Safety Basis Approval Authority		
SC	Safety Class		
SCAPA	Subcommittee for Consequence Assessment and Protective Actions		
SDC	Seismic Design Category		

SDS	Safety Data Sheet		
SFPE	Society of Fire Protection Engineers		
SIH	Standard Industrial Hazard		
SIZ	Structure Ignition Zone		
SME	Subject Matter Expert		
SMP	Safety Management Program		
SNL	Sandia National Laboratories		
SNM	Special Nuclear Material		
SQA	Software Quality Assurance		
SRDT	Solar Radiation Delta Temperature		
SRNL	Savannah River National Laboratory		
SRS	Savannah River Site		
SS	Safety Significant		
SSC	Structures, Systems, and Components		
ST	Source Term		
STD	Standard		
STEL	Short-Term Exposure Level		
STP	Standard Temperature and Pressure		
TBP	Tri-Butyl Phosphate		
TED	Total Effective Dose		
TEDE	Total Effective Dose Equivalent		
TEEL	Temporary Emergency Exposure Limit		
TF	Topographical Feature		
TLV	Threshold Limit Value		
TNO	The Netherlands Organization		
TNT	Trinitrotoluene		
TRU	Transuranic		
TSL	Technical Support Level		
TSR	Technical Safety Requirement		
TWA	Time-Weighted Average		
UFI	Upper Explosive Limit		
UFL	Upper Flammability Limit		
	Underwriters Laboratories		
USO	Unreviewed Safety Question		
002	Sineviewed Surery Question		
V & V	Verification & Validation		
VDC	Volcanic Design Category		
VP	Vapor Pressure		
WDC	Wind Design Category		
WEEL	Workplace Environmental Exposure Limit		
WIPP	Waste Isolation Pilot Plant		

Note: Definitions related to the DOE hazard and accident analysis process can be found in 10 CFR §830.3, DOE-STD-3009-2014 (or other Part 830 safe harbor), or DOE-HDBK-3010-94, *Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities*. Other definitions related to accident phenomenology for evaluation of potential consequences, such as physical and chemical effects, are provided in references cited in the text.

7 AQUATIC DISPERSION AND GROUNDWATER TRANSPORT

7.1 OVERVIEW

Although a less frequent consequence of a radiological accident, a discharge of a liquid radionuclide effluent is considered in hazard evaluation or accident analysis for DOE facilities for unique situations. Slowly developing dose pathways from accidental releases are generally not analyzed in DSAs due to the relatively long time for potential liquid releases from facilities to reach dose receptors, and the ability of programmatic controls to mitigate any release or ingestion prior to a prolonged exposure period needed to significantly contribute to the overall DBA consequence. At least one DOE site historically evaluated water pathway release events, but only in the context of BDBAs. DOE-STD-3009-2014, Section 3.2.4.2 provides the following discussions regarding liquid releases to water pathways:

For some types of facilities such as liquid processing with the potential for significant spills to the environment outside the facility, the surface and groundwater pathways may be more important, and accident releases usually would be expected to develop more slowly than airborne releases. More time would also be available for implementing preventive and mitigative measures.

However, quick-release accidents involving other pathways, such as a major tank rupture that could release large amounts of radioactive liquid effluents to water pathways, should be considered.⁸⁶

This chapter addresses potential dose consequences via surface water pathways at significant uptake locations, that is, maximum exposure locations that could affect the unmitigated dose estimates to the CW and the MOI. Moreover, the dose contribution from water pathways may be important to the overall 50-yr Total Effective Dose (TED), including the airborne pathway, for the selection of SS or SC controls and derivation of TSRs. The event may also warrant discussion in DSA Section 3.3.2.6, Environmental Protection, as described in DOE-STD-3009-2014, Section 4, to ensure that the facility design and operational features are available to reduce the potential for large liquid effluent releases to the environment.

Liquid effluent releases to surface water bodies can occur from accidents involving liquid process lines, waste tanks, cooling or evaporation systems, and primary-to-secondary leakage paths, as well as from other off-normal conditions. Such releases to surface bodies generally require relatively long periods of time (e.g., hours to days) before the general public could be impacted. However, the availability of longer response times enables the execution of various administrative controls, such as protective actions (i.e., evacuation and sheltering) and food and water interdiction countermeasures.

Dose consequences from liquid effluent releases are dependent on the volume of release, the duration of the release, the soil characteristics in the area around the point of discharge and the configuration of drainage and containment networks that redirect effluents away from the release location. Examples of natural and anthropogenic drainage networks include discharge canals, sewers, viaducts, creeks, rivers, and lakes.

For the purposes of DSA preparation, industry- accepted models, summarized in two NRC guidance documents, should be consulted when relevant accident scenarios result in discharges to streams, rivers, lakes, or oceans that require subsequent analysis.

⁸⁶ See also Appendix A.3 of DOE-STD-3009-94 CN3)

7.2 NRC REGULATORY GUIDANCE ON AQUATIC DISPERSION AND DOSE CALCULATION

The following applicable NRC regulatory guides, both issued in 1977, should be consulted:

- Regulatory Guide 1.109, Calculation of Annual Doses to Man from Routine Releases of Reactor Effluents for the Purpose of Evaluating Compliance with 10 CFR Part 50 Appendix I; and
- Regulatory Guide 1.113, Estimating Aquatic Dispersion of Effluents from Accidental and Routine Reactor Releases for the Purpose of Implementing Appendix I.

Regulatory Guide 1.109 describes basic features of the dosimetric calculation models and suggests parameters for the estimation of radiation doses to man from effluent releases.

With respect to Regulatory Guide 1.113, this guidance:

- Describes the basic features of aquatic dispersion models and suggests methods of determining values of model parameters for the estimation of aquatic dispersion of both routine and accidental releases of liquid effluents;
- Describes general approaches for analysis of normal and accident releases into various types of surface water bodies;
- Provides guidance on the use of calculation models and specification of accompanying parametric values to perform aquatic dispersion of routine or accidental releases of radioactive material to a surface body of water. Groundwater pathway models are not addressed;
- Provides additional guidance on selection of model types rather than to specify models; Accordingly, the use of models other than those described Regulatory Guide 1.113 is acceptable; and
- Indicates that in situ tracer studies can provide accurate site-specific predictions as an alternative to modeling.⁸⁷

7.3 DOCUMENTED SAFETY ANALYSIS APPROACH

Each liquid effluent release assessment should be evaluated applying a graded approach as described in DOE-STD-3009, such as being commensurate to the hazard category of the facility, remaining operational time of the facility, magnitude of potential consequences, and the complexity of the aqueous pathways for exposure and environmental contamination. Methods for this evaluation are addressed in the remainder of this chapter.

In addition, regarding evaluation of environmental protection in the DSA, the primary focus of the DSA hazard evaluation or accident analysis should be on process design, SSCs, and engineered operational controls which would preclude any potential for a large liquid effluent release to the environment. If precluding large liquid effluent releases is not feasible, a secondary approach would be to impose engineering controls to limit the magnitude of the loss of process liquids. These controls include sewer networks to conduct liquids to a collection system (e.g., settlement basin and weir), or a berm or containment basin (e.g., dike) to limit the extent of the release within the facility or site control. Should additional preventive or mitigative controls be required, the results of the dose contribution from the

⁸⁷ Although specific surface-water models are considered in Regulatory Guide 1.113, representative of models found in the published literature at the time, the stated purpose is to use them as a framework for discussing the specific classes of models that they exemplify.

water pathway may provide insights on the effectiveness of these controls.

7.4 LIQUID EFFLUENT RELEASE KEY RECEPTORS

The dose contribution from the water pathway may or may not be significant compared to the airborne pathway dose contribution. Normally, the CW is evaluated at 100 m from the release, and the MOI is evaluated at the site boundary. However, the aqueous release pathway may result in a higher dose at locations beyond these distances. Therefore, the analysis should consider these farther onsite and offsite locations if it could affect the overall unmitigated maximum dose estimates for the CW and MOI. The CW and MOI are assumed to be located at the point of maximum concentration of the dispersed effluent stream at an uncontrolled onsite or offsite location, respectively.

Regulatory Guide 1.113 specifies that the location of surface water users and the types of water uses, out to a distance of 50 miles from the site, should be established to identify other important receptors for dose pathway analyses.

7.5 LIQUID EFFLUENT RELEASE REDISTRIBUTION MECHANISMS AND UPTAKE

Regulatory Guide 1.113 provides guidance on initial mixing, far-field mixing, deposition, and resuspension in sediments, as well as uptake mechanisms with respect to aquatic dispersion models. The following provides a brief summary of each physical mechanism.

7.5.1 INITIAL MIXING

The major factors in the initial mixing phase are momentum and buoyancy of the liquid effluent, the outfall location and configuration, and receiving water characteristics; principally the current and depth.

7.5.2 FAR-FIELD MIXING

The initial mixing will result in a homogeneous plume of radionuclides which ultimately yield to generally slower far-field aquatic transport and diffusion processes. In the far-field mixing region, much longer distances and time frames result in an appreciable reduction of the concentration of the radionuclide plume, as clean water further dilutes it.

The longer time frames associated with the aquatic dispersion process indicates that radiochemical physical transformations and radioactive decay and daughter ingrowth could be important factors in the dose calculation. Moreover, the size of the receiving water body and its overall transport behavior (e.g., current velocity) needs to also be considered.

Each principal water body has its own unique transport characteristics due to different boundary conditions and flow rates. The following describe such differences on the aquatic dispersion process:

- Rivers: Advective and turbulent flows throughout with variable boundaries.
- Estuaries: Established transitional zone between distinctly different water bodies, marked by oscillating tidal flow and weak net transport.
- Small lakes and reservoirs: Strong boundary limitations and weak transport.
- Oceans and large lakes: Large overall extent and appreciable advection of pollutants.

Depending on the analysis, the complexity of models for estimating the radionuclide concentration at some point in the far-field may range from simple dilution factor considerations, to solving the advection and dispersion equations in one-, two-, or three-dimensional spaces. The latter case is particularly true for river system discharges. The selection of the aquatic dispersion model should be based on the complexity of the system and the requirements of the analysis.

During surface water release events, some constituents may be present as volatilizing liquids or in a dissolved gas form. These contaminants can be released from the liquid-air interface as pressure changes are encountered. Equation 7-1 provides a simple approach to calculate the time-varying release rate, assuming that the radionuclide is uniformly mixed over the vertical water column.

$$[dC/dt]_e = K(C - C_s)$$
 Equation 7-1

Where,

 $[dC/dt]_e$ = Time-varying release rate (Ci/s)

K = Depth average loss coefficient (s⁻¹)

C = Vertically uniform gas concentration of the contaminant, with typical units for a radionuclide gas contaminant of activity per unit volume (Ci/m³)

 $C_s = Saturation value (Ci/m³)$

Note that the saturation value is usually set equal to zero.

As noted in Section 3.3.6 of NUREG/CR-3332, *Radiological Assessment: A Textbook on Environmental Dose Analysis*, K is related to the actual surface transfer coefficient, K_L by

$$K = K_i/H$$
 Equation 7-2

where,

 K_{L} = Surface transfer coefficient (m/s)

H = Water column height (m)

The water column height is the height of a conceptual "stack" of the water body layers receiving the radionuclide or chemical pollutant. The water column extends from the surface to the bottom of the water body of interest and includes all layers. Values of K_L are usually determined from experimentation or from the literature.

7.5.3 DEPOSITION AND RESUSPENSION IN SEDIMENTS

As contaminants are transported in the surface water body, adsorption processes may remove material from the aqueous phase and incorporate material onto sediments. This is similar to the atmospheric process of deposition. Both suspended and bed sediments may adsorb contaminants, although suspended sediments are usually more effective on a per unit weight basis. The process is reversible and while the initial reduction of contaminants from a water body can be pronounced, over longer periods of time these contaminants can be resuspended.

Examples of long-lived radionuclides that have been retained in sediments after chronic or acute release near DOE nuclear facilities have been Cs-137 and various Pu species. A counterexample is tritium, which due to the ubiquity of water and hydrogen in the environment, shows little to no evidence of preferential localization in sediments.

The extent to which a radiological species can be adsorbed is referred to as the equilibrium distribution coefficient, or K_d . The equilibrium distribution coefficient is a function of the state of the radionuclide and its concentration, the sediment characteristics, and the nature of the water body. K_d values are derived from field data and experimentation, and are defined as the amount of contaminant sorbed on sediment/amount of radionuclide left in solution.

7.5.4 UPTAKE MECHANISMS

The aquatic dispersion model can also be linked to dose through human uptake mechanisms, where the most important pathway is water ingestion. Moreover, additional uptake mechanisms may be of importance. This includes direct food ingestion from marine foodstuffs, or indirect food ingestion through use of contaminated irrigation water sources. External exposure is also of importance in some situations, including aquatic recreation or shoreline exposure. The need to evaluate these other pathways should be discussed with the DOE Safety Basis Approval Authority.

7.6 AQUATIC DISPERSION MODELS AND COMPARISONS

7.6.1 CLASSES OF AQUATIC DISPERSION MODELS

There are 14 classes of aquatic dispersion models that have been developed for application to surface water bodies. These are addressed in Regulatory Guide 1.113 and the model characteristics and surface water body applications are listed in Table 7-1.

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Class of Aquatic		Surface Water
Dispersion Model	Aquatic Dispersion Model Characteristics	Body Applications
Stream tube model	Steady-state, two-dimensional, analytical solution	Non-tidal rivers
Transient release model	Transient, two-dimensional, numerical quadrature solution	Non-tidal rivers
Gaussian diffusion model	Steady-state, three-dimensional, analytical solution	Open coastal waters
Transient source model	Transient, two-dimensional, numerical quadrature solution	Open coastal waters
Numerical model	Transient, two-dimensional, numerical solution of conservation equations of mass and momentum	Open coastal waters
Tidally-averaged analytical model	Steady-state, one-dimensional, analytical solution	Estuaries
Tidally-averaged, short- duration analytical model	Transient, one-dimensional, analytical or numerical quadrature solution	Estuaries
Tidally-averaged numerical model	Transient, one-dimensional, numerical solution of constituent transport equation	Estuaries
Intra-tidal numerical model	Transient, one-dimensional, numerical solution of conservation equations of mass, momentum, and constituent concentration	Estuaries
Completely-mixed model	Transient, homogeneous, analytical solution	Lakes, reservoirs, and cooling ponds
Plug-flow model	Steady-state, homogeneous, analytical solution	Lakes, reservoirs, and cooling ponds
Partially-mixed model	Steady-state, homogeneous, analytical solution	Lakes, reservoirs, and cooling ponds
Stratified reservoir lumped parameter model	Steady-state, homogeneous (within stratified layer), analytical solution	Lakes, reservoirs, and cooling ponds
Numerical stratified reservoir models	Transient, one- or two- dimensional, numerical solution of conservation equations of mass, momentum, and constituent concentration	Lakes, reservoirs, and cooling ponds

Table 7-1. Aquatic Dispersion Model Classes.

7.6.2 AQUATIC DISPERSION MODEL ATTRIBUTES AND CHARACTERISTICS

For a release from a large body of water such as a river, aquatic dispersion models have been developed that account for advection and dispersion effects. These models should take into account the required complexity necessary to account for change in concentrations. In many situations, a two-dimensional

model is sufficient.

Table 7-2 provides the analyst with the major attributes and characteristics to consider in the selection of an aquatic dispersion model for DSA preparation with respect to release type, dimensional dependence, contaminant transport, time dependence, solution technique and dose pathways. Overkill occurs when the analyst uses a more sophisticated model than is warranted and NCRP Report No. 76, *Radiological Assessment: Predicting the Transport, Bioaccumulation, and Uptake by Man of Radionuclides Released to the Environment*, warns against common misuses of aquatic dispersion models.

Attribute	Characteristics		
Release Type	Acute; Chronic		
Dimensional Dependence	One-dimensional; Two-dimensional; Three-dimensional		
Contaminant Transport	Solute; Particulate		
Time Dependence	Steady-state; Dynamic		
Solution Technique	Finite Element; Finite Difference		
Dose Pathways	Water Ingestion; Food Ingestion and Longer-Term Food Chain; Submersion; External Shine, Shoreline Exposure		

Table 7-2. Attributes and Characteristics of Aquatic Dispersion Models.

7.6.3 COMPARISON OF AQUATIC DISPERSION MODELS

Several aquatic dispersion models are available and five (5) of these codes are briefly summarized. More in-depth information may be located in the referenced model descriptions. A brief comparison of the release types, regulatory use, model types, and output of these 5 aquatic dispersion models is presented in Table 7-3.

7.6.3.1 LADTAP2

NUREG/CR-4013, *LADTAP II: Technical Reference and User Guide*, (LADTAP2) analyzes environmental doses following routine surface water releases of radiological liquid effluents from nuclear facilities. LADTAP2 provides a hydrological and exposure pathway and examines doses to individuals, population groups, and biota via ingestion and external exposures. Calculated population doses provide information for National Environmental Policy Act (NEPA) evaluations and for determining compliance with Appendix I of 10 CFR 50, *Domestic Licensing of Production and Utilization Facilities*.

LADTAP2 selects one of four hydrological models to represent mixing in the effluent impoundment system and receiving surface waters. The four model types are: (1) direct release to the receiving water; (2) plug-flow; (3) partially-mixed; and (4) completely-mixed. All but the direct release model account for radiological decay and daughter ingrowth during transit through the impoundment system. Optional models are available to estimate aquatic dispersion in non-tidal rivers and near shore lake environments.

The exposure pathway model estimates exposure of selected groups at various water usage locations in the environment. Water concentrations at usage locations are related to impoundment system effluent

concentrations by a dilution factor and the transit time that allows for radioactive decay during transport. Consequence calculations examine all potential pathways: ingestion of aquatic foodstuffs, irrigated terrestrial food crops, drinking water (freshwater sites only), boating and swimming.

7.6.3.2 STREAM2

STREAM2 (Chen, 1998) is an aqueous release emergency response code which analyzes the transport of pollutants from a release point to various points downstream on the Savannah River. This model is conservative and assumes a constant river flow, no transport losses, and uniform mixing in stream cross-sectional areas.

User input includes the time, date, type, location, calculation units, amount, and duration of the release. Input data are used to calculate the pollutant concentrations and transport time at downstream locations, which may be displayed in graphical and tabular form.

7.6.3.3 GENII 2.10.1

GENII Version 2.10.1 analyzes environmental contamination resulting from both far- and near-field scenarios. Annual, committed, and accumulated doses following acute and chronic releases can be calculated. Surface water transport is modeled using the same LADTAP2 mathematical models.

7.6.3.4 RIVER-RAD

RIVER-RAD uses a compartmental linear transfer technique to model radionuclide transport as a series of transfers between compartments, including the water and sediment sub-compartments. Radionuclide transfer pathways include upward volatilization from the water compartment, movement of radionuclides with the river flow rate, deposition (settling) and resuspension.

7.6.3.5 DISPERS

DISPERS (NUREG-0868) is a collection of mathematical models used for computing the dispersion and fate of routinely or accidentally released radionuclides in surface water and groundwater. Five programs, all of which are straightforward dispersion simulations, are included. These are SSTUBE, TUBE, RIVLAK, GROUND, and GRDFLX (see NUREG-0868).

	Aquatic Dispersion Model				
Parameter	LADTAP2	STREAM2	GENII 2.10.1	RIVER-RAD	DISPERS
Release types	Routine	Acute	Routine and acute	Routine and acute	Routine and acute
Regulatory use	NEPA and 10 CFR 50 Appendix I	Emergency response	Consequence assessment	Dispersion calculations	Dispersion calculations
Model and/or calculation types	Direct release; Plug-flow; Partially and Completely mixed	One- dimensional; WASP5 calculations	LADTAP2 models	Compartmental linear transfer model	Two- and three- dimensional models
Output	Dose and Concentration	Concentration	Dose and Concentration	Concentration	Concentration

Table 7-3. Comparison of Aquatic Dispersion Models.

7.7 GROUNDWATER TRANSPORT

7.7.1 OVERVIEW

Although radiological and chemical species release to the groundwater can be a concern for operating nuclear facilities, the principal facilities for which groundwater release is a likely pathway are mining and milling operations, and long-term waste disposal areas. Estimates of flow and transport in groundwater are important in assessing the performance of a disposal system because they are probable pathways between hazardous waste and the environment.

The concepts, models, and data development methods used in these models are outside the scope of the guidance given here, and can be found elsewhere.⁸⁸ The relative unimportance is due to the relatively small likelihood of acute release conditions needing to be addressed in the groundwater for most DOE facilities. Additionally, airborne and surface water pathways will tend to dominate the acute phase of accident consideration. However, the ultimate fate of the released contaminants for EIS and other types of safety analysis may need to address the groundwater pathway. The analyst seeking to apply a groundwater model as a tool to assist facility safety analysis should consult other compendia listing more detailed subject information.

7.7.2 GROUNDWATER FLOW AND CONTAMINANT TRANSPORT

Two behaviors need to be captured to model contaminant transport in groundwater media. The first is movement of the carrier fluid and the second is the mass transport of the dissolved contaminants.

In modeling contaminant releases to the groundwater, radionuclide travel may be in the unsaturated zone above the water table or in the zone of saturation. While flow is for the most part downward in the

⁸⁸ This material is excerpted from NUREG/CR-3332.

unsaturated region, flow is predominantly lateral in the saturated zone.

Flow can be governed by many anisotropies in the saturated region depending on the media and layers of sedimentation. From Chapter 4 of NUREG/CR-3332, and under the assumption of a homogeneous isotropic medium, the major flow direction can be assumed to follow Darcy's law where the flow volume per unit area (V_x) is shown in Equation 7-3:

$$V_x = -K dH/dx$$
 Equation 7-3

Where,

- K = Hydraulic conductivity, dependent on fluid and medium properties, which for an isotropic homogeneous saturated medium, determines rate at which water moves through a porous medium for a given hydraulic gradient (cm/s)
- H = Total head, which is pressure head + elevation head (cm)
- dH/dx = Hydraulic gradient in the direction of flow (cm)

This relationship assumes the gradient is constant over the increment. The actual velocity of a contaminant would be larger than the flow volume per unit area since water is moving through pore spaces.

It should be noted that the actual velocity of a contaminant would be larger than the flow volume per unit area since water is moving through pore spaces. The pore or seepage velocity U may be approximated by the effective porosity, as shown in Equation 7-4:

$$U = V_x / n_e$$
 Equation 7-4

Where,

 V_x = Volumetric flow rate per unit area in direction x (cm/s)

 $n_e = Effective porosity, open volume for flow per unit total volume of the medium of interest (dimensionless)$

Chapter 4 of NUREG/CR-3332 provides additional information.

7.7.3 TRITIUM IN SEDIMENTS

Examples of radionuclides that have been retained in sediments after chronic or acute release near nuclear facilities have been cesium and plutonium species. Recent work has shown that even tritium, in the form of organically bound tritium (OBT), can be retained in sediments near sources of OBT discharge (Morris, 2006).

7.7.4 GROUNDWATER TRANSPORT MODEL CONSIDERATIONS

Recommendations for the use of groundwater models is given by the National Council on Radiation Protection and Measurements (NCRP), which is an advisory body whose recommendations on radiation protection matters provide the scientific basis for U.S. standards (NCRP Report No. 76). The report summarizes both surface water and groundwater transport and dispersion models and provides general guidance on their use.

As the simplest and most conservative approach, the safety analyst can assume that no dispersion occurs as the contaminants are transported in the medium of interest, and that the transport velocity is constant.

More complex treatments consider that net convection in one dimension and dispersion in all three dimensions. Furthermore, the dispersion or velocity of transport can vary both spatially and temporally. As the modeling complexity grows, there is a commensurate difficulty in preparing input data and identifying the appropriate sources of information.

The transport of contaminants through the ground can be estimated using tracers, groundwater dating, or mathematical modeling. Mathematical modeling involves solving equations of mass transport for the water and for dissolved constituents such as radionuclides.

In applications involving high-level waste repositories, an additional equation for heat transport is required, but models for applications of this type are outside the scope of the Handbook. Results are obtained from the transport equations through simplifying approximations that allow analytical closed-form solutions or through numerical methods.

Numerical solutions generally employ one of following three solution techniques: finite differences, finite elements, or network analysis. Numerical methods generally require an extensive input data set. The availability of this data needs to be considered by the analyst as the lack of required data may make sophisticated numerical modeling impractical.

8 RADIOLOGICAL CONSEQUENCE ASSESSMENT

This chapter provides guidance to the safety analyst regarding evaluation of radiological doses and health risks. It discusses the different types of radiation and the effects these radiation types can have on the human body, its organs, and its tissues. The factors that are considered in estimating the dose a receptor may receive following the atmospheric release of radioactive material are covered in detail. Finally, the health risks associated with radiological doses and the standards for radiation protection, in terms of dose or air concentration, are discussed.

8.1 FUNDAMENTALS

Radiological doses arise from exposure to plumes of radioactive material, including deposition from plumes, and from exposure to prompt (direct) radiation from a criticality accident. The general modes of exposure include:

- Inhalation of radioactive material (particulates and gases) while immersed in a plume;
- Inhalation of particulates from deposited material that have been resuspended by traffic and/or by wind;
- Ingestion of food products through meat, vegetable and fish pathways and ingestion of water contaminated by deposition from the plume;
- Gamma radiation from the plume (cloudshine);
- Gamma radiation from particulates deposited on the ground from deposition (groundshine);
- Skin contamination from deposition;
- Prompt (direct) radiation from a criticality accident; and
- Direct radiation from a loss-of-shielding accident.

As described in Section 3.2.4.2 of DOE-STD-3009-2014, radiological consequences for the DSA accident analysis are presented as a TED based on integrated committed dose to all target organs, accounting for direct exposures, as well as a 50-yr dose commitment. The dose pathways to be considered are inhalation, direct shine, and ground shine. DOE-STD-3009-2014 also states that direct shine and ground shine from gamma emitters only need to be evaluated if they cause an upward change in the qualitative consequence level (see Table 2-8, Consequence Thresholds). DOE-STD-3009-2014 specifies that ingestion (except when the water pathway could significantly contribute to the overall radiological consequences), resuspension, and skin contamination need not be included in a DSA. Accordingly, slowly-developing dose pathways, such as ingestion of contaminated food, water supply contamination, or particle resuspension, are not included. However, quick-release accidents involving other pathways, such as a major tank rupture that could release large amounts of radioactive liquids to water pathways, should be considered (See Chapter 7). In this case, potential uptake locations should be the evaluation points for radiological dose consequences.

In the case of a criticality accident, doses arise from both the plume of fission products that may be released and from the prompt radiation. Prompt radiation from a criticality accident is of concern primarily for facility workers located near the accident site since effects from criticality accidents are generally confined to the near-field. Depending on the size and duration of the criticality accident, and evaluation of shielding provided by the structure, the prompt radiation dose contribution may also be important for the evaluation of consequences to 100 m co-located worker. The distance of concern for prompt radiation depends primarily upon the number of fissions in the first spike and the amount and type

of shielding (such as concrete walls) between the worker and the site of the criticality accident. (See Appendix B of this Handbook for additional information on criticality.)

On the other hand, for actinide exposure, inhalation of Pu-238, Pu-239, and Pu-240 particulates is the primary radiological concern as the body does not have effective excretory mechanisms to remove it. According to NUREG-1140, for actinide releases, cloudshine, groundshine, skin contamination, and ingestion doses are insignificant in comparison, with the exception of the release of significant gamma emitters where cloudshine doses would become meaningful. Radiological dose from inhalation of enriched uranium particulates is of lesser concern, although may still have significant consequences warranting the need to consider SS controls. Inhalation of depleted uranium particulates is trivial by comparison, and for depleted and natural uranium, chemical toxicity is normally of greater concern than its radioactivity. See Section 9.4.4 for the toxicity associated with uranium compounds. Skin absorption of tritium is a special case and should not be ignored.

8.1.1 TYPES OF RADIATION

Four types of radiation are important to consider in DSAs: alpha (α), beta (β), gamma (γ), and neutron. α , β , and γ radiations are emitted from atomic nuclei during radioactive disintegration, or decay, of the nucleus. Alpha particles are energetic helium nuclei, consisting of two protons and two neutrons, with a charge of +2⁸⁹. Beta particles are energetic electrons, with a charge of -1e, or positrons, with a charge of +1e; they have a mass about 0.01 percent that of the alpha particle. Gamma radiation consists of electromagnetic waves or photons, and have energy similar to that of x-rays. Being photons, gamma rays have neither charge nor mass. Gamma radiation accompanies alpha and beta radiation when an atomic nucleus disintegrates. Neutron radiation is emitted when a nucleus fissions, or breaks into fragments, such as during a criticality event.⁹⁰ Neutron radiation consists of energetic neutrons, particles with zero charge and mass similar to that of protons, that is, about 25 percent of the mass of alpha particles.

When any or all of these radiations strike an organ or tissue of the body, they can deposit some or all of their energy, causing cell damage. The manner of energy deposition varies with the type of radiation. Some types of radiation, principally alpha and beta, deposit their energy primarily through the production of ionization. When they strike an atom, they strip off an electron, thus ionizing the atom. The two charged particles formed, the electron and the ion, are referred to as an ion-pair. The electron that is stripped off the atom may be sufficiently energetic that it can cause further ionization. The amount of ionization created depends upon the mass, charge, and energy of the particle. Particulate radiation (α , β , neutron) can also deposit its energy through the dissociation of molecules and through elastic scattering, which causes heating.

Alpha-decay energy is on the order of several million electron volts $(MeV)^{91}$. For example, plutonium, uranium, and americium isotopes all emit alpha particles with energies on the order of 5 MeV. Because an alpha particle is doubly charged and massive, it can ionize many atoms before exhaustion. For example, an alpha particle traveling through air will create on the order of 50,000 ion pairs for each

⁸⁹ The basic unit of charge is that of the electron, but with a reversal of sign. The charge of an electron is -1.60E-19 coulomb.

⁹⁰ Neutrons can also be produced through (α , n) reactions, in which an alpha particle strikes the nucleus of an atom, causing the emission of a neutron. This is generally not important for dose calculations as the additional dose from the neutron radiation is balanced by the decreased dose from the lost alpha particle.

⁹¹ An electron volt (eV) is the kinetic energy of an electron after being accelerated through an electric potential difference of 1 V. It is equal to 1.60E-19 Joules.

centimeter it travels. Because it creates so much ionization, it deposits its energy quickly, and penetrates only a short distance into a tissue.

Beta-decay energy is on the order of tens of keV to a few MeV. For example, the beta-decay energy of Pu-241 is 21 keV. During beta decay, the emitted electron, or positron, is accompanied by an antineutrino or neutrino, with which it shares the energy. The beta-decay energy is the sum of the energies of the electron and neutrino. Thus, for Pu-241, the maximum energy the electron can have is 21 keV; normally, it will have only a fraction of this. Because the beta particle is singly charged and not very massive, it cannot create nearly as much ionization as an alpha particle. A beta particle traveling through air will create on the order of 100 ion pairs for each centimeter it travels. In addition to causing ionization, beta particles also can be scattered elastically by atomic electrons. Because a beta particle does not lose its energy as rapidly as does an alpha particle, and because of elastic scattering, it can penetrate more deeply into tissue. However, it travels an irregular path in tissue because of elastic scattering. This gives rise to the emission of electromagnetic radiation called *bremsstrahlung* (German for "braking radiation"), which in turn can deposit its energy in the surrounding tissue.

The energy of a gamma ray is on the order of tens of keV to a few MeV. For example, the energy of one of the several possible gamma rays that accompanies the alpha decay of Pu-239 is 52 keV. A gamma photon will create only about one ion-pair per centimeter in air. A gamma photon can also lose its energy through Compton scattering from electrons and even from interactions with the nucleus of an atom; although the latter are minor in comparison with photoionization and Compton scattering. Gamma radiation is capable of penetrating deeply into a person's body.

8.1.2 NUCLEAR FISSION

Nuclear fission yields two large fission fragments (nuclei of other isotopes), multiple neutrons, and other radiation (alpha particles, beta particles, or gamma rays). Fission fragments are highly radioactive. To reach a stable configuration, these fission products may continue emitting radiation for wide-ranging time periods; from milliseconds to many years.

The energy of a fission neutron is on the order of a few keV to about 10 MeV. Because the neutron has no charge, it will not create many ion-pairs. It loses it energy primarily through elastic scattering. However, it can also cause nuclear transformations, especially when it has slowed, through elastic scattering, and become a "thermal" neutron. These nuclear transformations can lead to the emission of other radiations, such as α and γ . Neutron absorption through nuclear transformation is primarily by hydrogen and nitrogen in the human body. Elastic scattering of neutrons is primarily by the hydrogen in the body. Like gamma radiation, neutron radiation is very penetrating.

Neutrons resulting from fission are categorized as either prompt or delayed. Prompt neutrons are emitted virtually simultaneously with fission (< 1E-14 second); whereas delayed neutrons may not be emitted for many seconds after fission. Prompt neutrons are "born" fast and are of high energy in the 1-20 MeV range, while delayed neutrons are born with an average energy of less than 0.5 MeV.





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8.1.3 RADIOACTIVITY

Radioactive decay is the spontaneous disintegration of a radioisotope accompanied by emission of ionizing radiation (α , β , and/or γ). It is the process by which a nucleus of an unstable atom reaches a more stable configuration by the release of energy or mass. The activity of a radioisotope is measured in units of rate of decay, commonly called disintegrations per second (dps). The SI unit is the Becquerel (Bq), defined as one dps. The historical, and still commonly used, unit of activity is the curie (Ci), which is equal to 3.7E+10 dps. Thus, 1 Ci = 3.7E+10 Bq. Lower radioisotope activities are measured in disintegrations per minute (dpm).

Specific activity is the activity per unit mass, and is measured in units such as Bq/kg or Ci/g. The specific activity of Ra-226 was originally defined as 1 Ci/g. The specific activity of a mixture of radionuclides is the sum, over all the radionuclides in the mixture, of the products of specific activities and mass fractions.

The activity of a sample of any given radionuclide decreases exponentially with time, providing it is not being created by the decay of another radionuclide. If N is the number of atoms of a specific type of radionuclide in a sample of material, the change in this number, dN, in a small interval of time, dt, is proportional to N and to dt. This is written

$$dN = -\lambda N dt$$
 Equation 8-1

where the negative sign is needed to show that *N* decreases with increasing time. The constant of proportionality, λ , is called the decay (or transformation) constant and is measured in inverse time units, such as s⁻¹. The disintegration rate, or activity (*A*), is given by

$$A = -dN/dt = \lambda N$$
 Equation 8-2

The solution to equation (8-1) is

$$N = N_0 e^{-\lambda t}$$
 Equation 8-3

where N_0 is the number of atoms at time t = 0. Thus, equation (8-2) can be written

$$A = A_0 e^{-\lambda t}$$
 Equation 8-4

where $A_0 = \lambda N_0$ is the activity at time t = 0.

Because the decay is exponential, the time interval to decrease the number of atoms in a sample by a given factor is a constant. For example, the time to decrease by a factor of two, called the half-life ($t_{\frac{1}{2}}$), is obtained by inverting equation (8-3):

$$t_{1/2} = -(1/\lambda) \ln(1/2 N_0/N_0) = (1/\lambda) \ln(2) = 0.693/\lambda.$$
 Equation 8-5

The half-life of Pu-239, for example, is 2.44E+04 yr, while that of U-235 is 7.1E+08 yr. The specific activity of U-235 is therefore about 30,000 times smaller than that of Pu-239, which is the main reason it does not present as great a radiological hazard as Pu-239 for a given amount of material as it is producing fewer decays, and therefore less energy, per unit time.

Instruments that measure the amount of radioactivity in a material usually present their results in terms of counts per minute (cpm). These are then converted to disintegrations per minutes (dpm) by knowing the efficiency of the counter and geometry of the measurement. In the case of surface contamination, the measurements are expressed in terms of activity per unit of area, such as cpm/100 cm², which are then converted to dpm/100 cm². To derive the amount of material involved, the dpm is divided by 60 to get dps, or Bq. This activity can then be converted to the number of atoms of the radionuclide present by dividing by the decay constant, or the number of grams present by dividing by the specific activity.

8.2 EFFECTS OF RADIATION ON THE BODY

Radiation damages the body as it deposits its energy, primarily through ionization, in organs and tissues. Because alpha radiation can be stopped by the body's outermost layer of dead skin cells, it poses no external hazard to the body; rather, its primary hazard is through inhalation and ingestion. Beta radiation can barely penetrate the skin to cause some damage; and it can also damage the eye. Like alpha radiation, its damage comes principally from inhalation and it also comes from ingestion. Gamma radiation and neutrons, on the other hand, can penetrate the body directly from external sources; material that emits gamma radiation and neutrons can, of course, be inhaled or ingested, but this is not the normal mode of exposure. Skin contamination from fallout from the plume causes tissue damage principally from β radiation.

Both short-term (acute) and long-term (chronic) exposures are important. External radiation from cloudshine, groundshine, skin contamination, or prompt radiation gives a short-term or even instantaneous dose, whereas internal radiation from inhalation and ingestion gives a long-term committed dose. A long-term dose can also arise from continual exposure to external radiation, as in a work place. If a radioactive particle is inhaled or ingested, it will cause damage as long as it remains in the body, because it contains many radioactive atoms that continue to disintegrate. An organ or tissue irradiated for an extended time (chronic exposure) may develop cancer or suffer other deleterious effects.

8.2.1 DOSE EVALUATIONS

The effects of exposure to ionizing radiation were originally defined in terms of the amount of ionization in air produced by gamma radiation and x-rays. The unit used was the Roentgen (R), now defined as the ratio $\Delta Q/\Delta m$, where ΔQ is the sum of all charges of one sign produced in air when all the electrons liberated by photons in a mass Δm of air are completely stopped in air. It is equal to 2.58×10^{-4} coulombs produced in 1 kg of air. This is equivalent to 1.61×10^{15} ion-pairs produced per kilogram of air, or an energy deposition of 87.3 ergs/g of air (Turner 1986). Absorption of 1 R of radiation in tissue corresponds to about 95 ergs/g of tissue; this unit is called the rep (roentgen-equivalent, physical). The rep is no longer used.

Today, dose is expressed as an absorbed dose, that is, the amount of energy deposited in matter, or as an equivalent dose, a measure of damage done in tissue. The traditional unit of absorbed dose is the rad (radiation absorbed dose) and is defined as 100 ergs absorbed in 1 g of material. The newer standard international unit is the gray (Gy), which is defined as 1 J absorbed in 1 kg of material. Thus, 1 Gy = 100 rad. This equality applies to any type of radiation absorbed in any type of material.

The dose of most interest in accident analysis is the equivalent dose, as this is a measure of the biological damage. The amount of damage depends upon the type of radiation, as well as the amount of energy absorbed. The equivalent dose H_T to a particular tissue *T* is equal to the absorbed dose D_T in that tissue times a radiation-weighting factor w_{R} .

$$H_T = w_R D_T$$
 Equation 8-6

where w_R is a measure of the amount of damage done by the radiation. If more than one type of radiation impacts the tissue, H_T is calculated by summing over all radiation types. Table 8-1 gives the radiation weighting factors from 10 CFR Part 20, *Standards for Protection Against Radiation*, for the four radiation types considered here. This table can also be located in ICRP-60.

Туре,	Energy Range	Radiation Weighting Factor, w _R
Alpha	any energy	20
Beta	any energy	1
Gamma	any energy	1
Neutrons	< 10 keV	5
	10 keV to 100 keV	10
>100 keV to 2 MeV		20
>2 MeV to 20 MeV		10
	> 20 MeV	5

 Table 8-1. Radiation Weighting Factors.

The traditional unit for equivalent dose is the rem (roentgen-equivalent man). The newer international unit is the sievert (Sv). The relation between them is the same as between gray and rad (1 Sv = 100 rem). Sometimes the unit centisieverts (cSv) is used in place of rem.

Example: Assume a medical x ray gives the lungs an absorbed dose of 1 rad (0.01 Gy). The equivalent dose would be 1 rem (0.01 Sv), as x-rays are similar to gamma rays and have a radiation weighting factor of one. On the other hand, if the absorbed dose of 1 rad to the lungs were from inhalation of plutonium, an alpha emitter, the equivalent dose would be 20 rem (0.2 Sv), as the radiation weighting factor for alpha radiation is 20.

The radiation-weighting factor is related to the stopping power of the material, expressed as Linear Energy Transfer (LET):

$$LET = dE/dx$$
 Equation 8-7

where dE is the average energy locally imparted to the medium by a charged particle traversing the distance dx. Alpha and beta particles have high and low LET, respectively. Gamma radiation, although not a charged particle, is considered equivalent to low LET radiation. Neutrons have a moderate to high LET, depending upon their kinetic energy.

The definition of equivalent dose does not differentiate between short-term and long-term dose, or between external and internal exposure. A related term is committed equivalent dose, which is the predicted dose from internal exposures over the remaining life of the individual, normally taken to be 50 years for adults (such as workers) or 70 years for children (as in the general population); it does not include external exposures. The committed equivalent dose is thus a subset of the equivalent dose. This

has led to some confusion as some have incorrectly used equivalent dose exclusively for external radiation, apparently as a counterpoint to committed equivalent dose, which is used exclusively for internal radiation.

Doses are also calculated for the body as a whole. This is done by summing over all organs the product of an organ weighting factor and the equivalent dose for that organ. This sum is called the effective dose, formerly called the effective dose equivalent (EDE), a term still used. The organ weighting factors represent the fraction of the total health risk resulting from uniform whole body irradiation that could be attributed to that particular tissue or organ; these factors are between zero and one; their sum over all organs and tissues is one. The weighting factors (also called tissue weighting factor) for the various organs are shown in Table 8-2, as taken from ICRP-60, *Recommendations of the International Commission of Radiological Protection*; for comparison, ICRP-26, *Recommendations of the ICRP*, values are also shown, as they may still be used for existing safety analyses in nonreactor nuclear facility DSAs.

0	Organ Weig	Organ Weighting Factor			
Organ	ICRP-26	ICRP-60			
Bladder	-	0.05			
Bone Marrow (red)	0.12	0.12			
Bone Surface (skeleton)	0.03	0.01			
Breast	0.15	0.05			
Colon	_	0.12			
Esophagus	_	0.05			
Gonads	0.25	0.20			
Liver	_	0.05			
Lung	0.12	0.12			
Skin	_	0.01			
Stomach	_	0.12			
Thyroid	0.03	0.05			
Remainder	0.30	0.05			

 Table 8-2. Organ Weighting Factors.

Example: Assume every organ listed in Table 8-2 (considering "remainder" as a single organ), receives a dose of 1 rem each. The effective dose to the whole body would then also be 1 rem. On the other hand, if the bone surface was to receive 100 rem (1 Sv) and all other organs received none, the effective dose would again be 1 rem, using the ICRP-60 organ weighting factors.⁹²

A term similar to effective dose is committed effective dose (formerly, the committed effective dose equivalent, or CEDE, a term still used), which is the predicted dose from internal exposures over the remaining life of the individual, normally taken to be 50 years for adults, or 70 years for children; it also does not include external exposures. Committed effective dose is thus a subset of effective dose. However, as with equivalent dose compared with committed equivalent dose, confusion has arisen in that some incorrectly use effective dose to refer to only external radiation, because committed effective dose refers only to internal radiation. A new term, total effective dose equivalent (TEDE), is now used to indicate the sum of the external (short-term) and the internal (committed, long-term) effective doses (10 CFR Part 20). TEDE is called the TED in ICRP-60 and current calculations are for TED.

⁹² This example is for illustration only as no accident would give dose to only one internal organ.

Doses arise from both internal and external exposures, as noted above. Per DOE-STD-3009-2014, the only internal exposures of concern consist of inhalation from being immersed in the plume, except when the water pathway could significantly contribute to the overall radiological consequences. The external exposures are from cloudshine, groundshine, and prompt (direct) radiation from a criticality event. These are discussed individually below.

8.2.2 INHALATION (PLUME) DOSE

Inhalation dose from immersion in a plume to a given organ or tissue from a given isotope, *i*, is the product of the amount of respirable radioactive material released, or the source term *ST*, atmospheric dispersion factor χ/Q , breathing rate *BR*, and dose conversion factor *DCF_i*

$$Dose_i = ST_i \times \chi/Q \times BR \times DCF_i$$
 Equation 8-8

assuming the receptor remains exposed for the duration of the plume passage. The total dose to the organ or tissue is the sum over all isotopes inhaled. The source term (ST_i) is the product of the MAR, DR, ARF, RF, and LPF, as discussed in Chapter 5. The χ/Q is discussed in Chapter 6 and the breathing rate and dose conversion factors are discussed below. The breathing rates for the "reference man" for various activities, as have been used in accident analyses for the past several years at many DOE sites, are given in Table 8-3 (ICRP-2 and ICRP-30, *Limits for Intakes of Radionuclides by Workers*). ICRP-66, *Human Respiratory Tract Model for Radiological Protection*, gives revised breathing for the "reference man."⁹³ These are also shown in Table 8-3. Still other breathing rates are appropriate for other individuals, such as infants, the elderly, and the infirm, and for other levels of activity (ICRP-66).

Activity Level	Breathing Rate (m ³ /s)			
ICRP-2, ICPR-30				
Chronic	2.66E-4			
Light	3.33E-4			
Heavy	3.47E-4			
ICRP-66				
Sleep	1.25E-4			
Rest, sitting	1.50E-4			
Light exercise	4.17E-4			
Heavy exercise	8.33E-4			

 Table 8-3. "Reference Man" Breathing Rates for Various Levels of Activity.

DOE-STD-3009-2014, Section 3.2.4.2 requires a breathing rate of 3.3E-4 m³/s. This value was initially developed for "light activity" based on data and methods from ICRP-2 / ICRP-30 DCFs, and is equivalent to "light work" as defined in ICRP-68, *Dose Coefficients for Intakes of Radionuclides by Workers*, using ICRP-66 data. ICRP-68 has revised the 8-hour day breathing rates as follows: light work is defined as 2.5 hr sitting (inhalation rate 0.54 m³/hr [1.5E-4 m³/s], breathing frequency 12/min) and 5.5 hr light exercise (inhalation rate 1.5 m³/hr [4.17E-4 m³/s], breathing frequency 20/min). NNSA SD G 1027, *Hazard Categorization and Accident Analysis Techniques for Compliance with DOE Order 5480.23, Nuclear Safety Analysis Reports to Address Areas in Need of Clarification and Improvement* (Admin

⁹³ The reference man is a male, 30 years old, height 176 cm (5 ft, 9 in.), and weight 73 kg (161 lb). ICRP-89 provides additional data for other factors related to breathing rate, including age, gender, and race.

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Change 1, May 2014) has added significant figures (to bring it to 3.3333E-04 m³/s), although this added precision does not materially change the dose result.

Once radioactive material enters the respiratory tract, it begins to migrate to other parts of the body. A portion is transferred directly to the blood and another portion to the gastrointestinal (GI) tract. Transfer of the material directly from the respiratory tract into the blood depends upon where in the respiratory tract it is deposited and how soluble it is. Material is also cleared from the respiratory tract by means of the body's mucociliary mechanism and then swallowed, thus entering the GI tract. The fraction f_1 of the material that passes from the GI tract into the blood, primarily from the small intestine, depends on the solubility of the material. For some radionuclides, such as iodine, the transfer to the blood is nearly complete ($f_1 = 1.0$). For other radionuclides, such as plutonium, the portion transferred to the blood is much less than 1 percent; the remainder is excreted. Once the material enters the blood, it can be carried to any part of the body. From there, it may preferentially attach to a given organ or tissue, as determined by the chemical properties of the radioactive material and of the organ or tissue. For example, plutonium and americium become preferentially attached to bone surface. The amount of biological damage that radioactive material may inflict on an organ or tissue is given by the DCF mentioned above. For inhalation, this is expressed in units of Sv/Bq (or rem/Ci), which can be converted to Sv/g (or rem/g) by multiplying by the specific activity. An example of tables of DCFs for a large number of radionuclides are given in Federal Guidance Report (FGR)-11 (EPA FGR-11). The DCFs take into account the migration of the radioisotope within the body, the decay of the radioisotope, and the formation of daughter isotopes that may be radioactive.

The residence time of a radioactive particle in the lungs depends in part upon the solubility of the material. Older DSAs use the residence times from ICRP-30 whereas more recent DSAs use the residence times from ICRP-68. Three broad categories for use with ICRP-30 or *Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion* (EPA FGR-11) DCFs have been defined.

- Y: Radionuclides in insoluble compounds remain in the lungs for a long time; these are of Solubility Class Y (for years), also called Lung Clearance Class Y.
- W: Radionuclides in moderately soluble compounds remain in the lungs for weeks; these are of Solubility Class W (for weeks), also called Lung Clearance Class W.
- D: Radionuclides in soluble compounds remain in the lungs for only a short time; these are of Solubility Class D (for days), also called Lung Clearance Class D.

According to EPA FGR-11, plutonium compounds can be Class Y (the oxides⁹⁴) or Class W (all other Pu compounds); there are no Class D Pu compounds. Americium compounds are only Class W. Uranium compounds can be Class Y (UO₂ and U₃O₈), Class W (UO₃, UF₄, and UCl₄), or Class D (UF₆, UO₂F₂, and UO₂(NO₃)₂). Fission products are of all three lung clearance classes.

Should these compounds be involved in a fire, their chemical nature may change. For example, a plutonium salt, as in certain residues, which is Class W, may change to an oxide (Class Y) in a fire. High-fired plutonium oxide is an example of Class Y. However, conversion of a salt in a fire will probably not be complete. Accordingly, it may be appropriate to assume that the resultant chemical form

⁹⁴ Plutonium hydroxides have subsequently been added to Class Y.

is the one that gives the largest dose. In the case of plutonium salts, for example, Class W for plutonium salts may apply.

Newer biokinetic models of the human respiratory system (ICRP-68) give DCFs for plutonium and americium that are notably smaller than those used in ICRP-30. The following differences can be noted between these two databases.

- 1. The DCFs for fission products are similar between the two databases, but those of the actinides are much smaller in ICRP-68 than in ICRP-30.
- 2. The ICRP-68 values do not use the D, W, and Y solubility classes. Instead, they use "F (Fast)," "M (Moderate)," and "S (Slow)," which are broadly equivalent to D, W, and Y.
 - a. "Fast" refers to those compounds that dissolve quickly and are absorbed into the respiratory tissue where they are initially deposited, or directly into the blood, in minutes to hours. There is virtually no time for these compounds to be transported to other respiratory sites.
 - b. "Moderate" refers to those compounds that dissolve more slowly. Only a small portion (modeled as 10 percent) is absorbed directly into respiratory tissue at the initial deposit site, or directly into blood; the remainder is transformed (in a period of weeks) into a more soluble compound. While in this transformed state, it can be transported to other respiratory tissues. It eventually is dissolved into the blood and thus is available for transport to other parts of the body.
 - c. "Slow" refers to those compounds that are essentially insoluble. Almost none of this material is absorbed directly into the tissue at the initial deposit site, or directly into the blood. It is slowly transformed into a more soluble compound (on a time scale of years). While in this transformed state, it can be transported to other respiratory tissues. It eventually is dissolved into the blood and thus is available for transport to other parts of the body.
- 3. The DCFs of ICRP-68 are given for two particulate size distributions, centered at 1 μm and 5 μm. These sizes are referred to as AMAD, the median diameter of a lognormal size distribution. In contrast, the ICRP-30 values were only for one particulate size distribution, 1-μm AMAD.

ICRP-68 recommends that the 5- μ m AMAD DCFs be used unless the analyst can justify the use of the DCFs for the 1- μ m AMAD; such as the case in which the particulates had passed through HEPA filtration. Federal agencies have accepted the use of 1 um AMAD for consequence management response actions (e.g., Federal Radiological Monitoring and Assessment Center Assessment Manual calculations). DCFs generally are larger for smaller particle sizes. HEPA filters are least efficient at about 0.3 - μ m-sized particles for which the DCF would be larger than for either 1 - μ m or 5 - μ m. On the other hand, very small particles tend to agglomerate and stick to surfaces. The DCF chosen for a given scenario needs to be technically justified if other than the value for 1- μ m or 5- μ m. Refer to ICRP-68 Annex F for assigning lung clearance type to different compounds. ICRP-72 has a an even more detailed discussion.

ICRP-68 was developed for assessing potential doses to workers and can be used to evaluate the postulated dose to the CW. For the MOI consequence assessment, the adult dose conversion factors from

ICRP-72, Age-Dependent Doses to Members of the Public from Intake of Radionuclides, Part 5,⁹⁵ is used as described in DOE-STD-3009-2014, Section 3.2.4.2.

8.2.3 CLOUDSHINE DOSE

The amount of gamma radiation (and beta, if appropriate) received by a receptor from a plume of radioactive material depends upon the location of the receptor relative to the plume. The greatest dose would be received by a receptor in the plume centerline and DCFs have been developed for such a receptor. The assumptions made in deriving these DCFs are that (1) the plume is uniform and semi-infinite⁹⁶ and (2) the receptor is standing upright on the ground. The dose received from a given radionuclide is the product of the concentration of the radionuclide and the DCF, integrated over the duration of the plume. The doses from all the radionuclides are then be summed. The DCFs for cloudshine are given in FGR-12, *External Exposure to Radionuclides in air, Water, and Soil*. Information for ordering this report is given in the EPA internet web site http://www.epa.gov/radiation/federal/index.html. Cloudshine DCFs are expressed in units of (Sv-m³)/(Bq-s). FGR-11 also gives DCFs for cloudshine but these have been superseded by those of FGR-12.

The cloudshine doses calculated using the DCFs from FGR-12 are conservative because of the assumptions that the receptor is standing upright in a uniform, semi-infinite cloud. The plume is neither uniform nor semi-infinite, the receptor may not be at the plume centerline, the plume may be elevated, the receptor may be sheltered, and the receptor may not be standing up; each of these factors would tend to reduce the dose. Corrections for finite cloud size and distribution (Gaussian) and for receptor locations off-centerline are included in several computer models of atmospheric dispersion and consequence assessment (see Section 6.12.2). The safety analyst should also consider additional dose reduction factors associated with sheltering.

8.2.4 GROUNDSHINE DOSE

The amount of gamma radiation received by a receptor from radioactive material deposited on the ground through deposition (see Section 6.8.4) depends upon the location of receptor relative to the fallout. The greatest dose would be received by a receptor at the center of the deposition, and DCFs have been developed for such a receptor. The assumptions made in deriving groundshine DCFs are: (1) the material is uniformly distributed on the surface or in the soil for an infinite distance in every horizontal direction azimuth); and (2) the receptor is standing upright on the ground. The dose received from a given radionuclide is the product of the concentration of the radionuclide on, or in, the ground and the DCF, integrated over the duration of the exposure (how long the receptor is present to receive groundshine). The ground shine doses from all the radionuclides are then summed. The concentration to be used in the calculation is either an areal concentration (Bq/m^2), if the material is only on the surface, or a volume concentration (Bq/m^3), if mixed with the soil. The dose rate is the product of the concentration and DCF. Groundshine DCFs are expressed in units of either ($Sv-m^2$)/(Bq-s) for surface contamination, or ($Sv-m^3$)/(Bq-s) for soil contaminated down to a specified depth. The DCFs for groundshine are given in FGR-

⁹⁵ DOE-STD-1196-2011, Appendix A includes dose coefficients for adults consistent with ICRP-72 dose coefficients. DOE has determined that the adult dose coefficients are appropriate for hazard scenario consequence estimates. However, in other situations such as determining collective dose to the public from a release, reference person coefficients from DOE-STD-1196-2011 are more appropriate. That standard includes gender and age weighted dose coefficients that are appropriate for estimating doses to the general public resulting from chronic exposures. These dose coefficients may be appropriate when assessing doses from residual radioactive material over the long-term.

⁹⁶ "Semi" because the plume extends upward from the ground, but not downward.

12. The depths of soil contamination considered in these tables are for 1-cm, 5-cm, 15-cm, and an infinite depth. Groundshine DCFs for other depths of soil contamination can be found by interpolation among these tables.

The groundshine doses calculated using the DCFs from FGR-12 are conservative because of the assumptions that the receptor is standing upright on a uniformly contaminated, infinite plane. The deposition is neither uniform nor infinite and the receptor may not be the middle of it. Furthermore, surface morphology irregularities (uneven terrain) tend to shield the receptor, the receptor may be sheltered, and the receptor may be elevated or more distant from the groundshine; each of these factors would reduce the dose. The safety analyst may also wish to consider additional dose reduction factors associated with sheltering or surface roughness/unevenness.

In calculating groundshine doses, the time variation of the ground concentration at the receptor's location is considered. In the early stages of plume passage, the ground concentration is increasing; the concentration reaching a peak at the end of plume passage. Resuspension (see Section 6.8.4) of the particulates then erodes the amount of contamination. The DOE-STD-3009-2014 recommended exposure duration is up to 8 hours. In calculating groundshine doses, the time variation of the ground concentration at the receptor's location is considered. In the early stages of plume passage, the ground concentration is increasing; the concentration reaching a peak at the end of plume passage. Refer to the toolbox code manuals for details of how each code treats this.

8.2.5 PROMPT (DIRECT) DOSE

Prompt doses from criticality accidents arise exclusively from neutrons and gamma rays from fissions and fission products and capture gamma rays from fission neutrons (see Appendix B). The prompt dose depends directly upon the number of fissions in the criticality accident, the distance to the receptor, and the amount of intervening shielding material, such as steel, concrete, or water. NUREG/CR-6504, *An Updated Nuclear Criticality Slide Rule,* gives curves of unshielded dose as a function of distance, number of fissions, and time after the criticality accident.

Shielding is expressed in terms of the amount of intervening concrete or the equivalent if other shielding materials are involved. Shielding dose reduction factors may be determined from the following relationships, which are taken from NUREG/CR-6504.

Steel Dose Reduction Factor:	neutrons = exp (-0.256 × steel thickness in inches) gammas = exp (-0.386 × steel thickness in inches)
Concrete Dose Reduction Factor:	neutrons, = exp (-0.240 × concrete thickness in inches) gammas = exp (-0.147 × concrete thickness in inches)
Water Dose Reduction Factor:	neutrons = exp (-0.277 × water thickness in inches) gammas = exp (-0.092 × water thickness in inches)

Prompt doses from criticality accidents need to be compared with the Safety Significant (SS) Structure, System, and Component (SSC) guidelines for the FW (Chapters 2 and 10). These guidelines state that "prompt death" or "serious injury" is a high consequence. These refer to deterministic health effects, not cancer. A prompt dose of 450-rad from a criticality accident is considered lethal to 50% of the people within 30 days, a dose labeled $LD_{50/30}$. A dose of about half of this would cause serious injury but not death to most individuals. It is recommended that if the prompt dose exceeds 400 rad it be considered lethal (prompt fatality or "high consequence"). A prompt dose between 200 and 400 rad would cause

serious injury (also a "high consequence") and a prompt dose below 200 rad would not be a serious injury for a healthy worker. See Section 8.3. For a criticality event producing 1E+17 fissions first spike, a dose of 400 rad would be received by an unshielded worker about three meters from the accident.

The total radiation dose from a criticality accident, including inhalation, cloudshine, and from prompt exposure, is included in the assessment of consequences to the CW. However, the prompt dose may be determined to not be significant based on distance and/or shielding, and not included in the total dose estimate. The unmitigated analysis may credit shielding from passive design features such as concrete walls, and their safety significance evaluated per the DOE-STD-3009-2014 guidance on ICs.

8.2.6 PLUTONIUM EQUIVALENT CURIES

For simplification of accident analysis calculations it is beneficial to introduce the concept of surrogate compositions of MAR, based on isotopic-specific DCFs. For example, the concept can be used to establish a common inventory or tracking basis for a dose calculation. It can provide a process for accepting new material while remaining within the bounds of the accident analyses, thus allowing operational flexibility while complying with the safety basis and source strength administrative control limits.

This is commonly done for materials composed of several isotopes of plutonium. For accident analysis purposes and safety system classifications, EGs are in units of TED, which is indifferent to the dose pathway or the kinds of radionuclides involved. The dose equivalent curie concept effectively converts radiological consequences for individual isotopes or mixes of isotopes to the same consequences from a corresponding amount of a base isotope. For example, for Pu-239, a plutonium equivalent curie (PE-Ci) is defined as the summation of the curies of each isotope multiplied by its dose equivalence factor:

$$PE-Ci = \Sigma (dose \ equivalence \ factor)_n \times (curies)_n$$
 Equation 8-9

where *n* is the index for the isotopes included in the mix. In the case of Pu-239, dose equivalence is a method of normalizing the radiotoxicity of various radionuclides to Pu-239 for use in determining relative hazard of radioactive materials. The normalization is often based on the inhalation pathway only. It is derived from the ratio of the inhalation committed effective dose for each radionuclide to that of Pu-239. The inhalation DCFs are based on ICRP-72 for the public receptor and are usually more conservative than ICRP-68 DCFs which were developed for facility worker dose commitments. This ratio is the dose equivalence factor of the isotope per curie of isotope. This approach should not be used for radionuclides that can pose a non-negligible external dose.

8.3 HEALTH RISKS

Although not required for the DSA accident analysis, radiological doses may be converted to health risks for other special assessments, such as comparison to the DOE Safety Goal in DOE P 420.1. For regulatory decision-making, the linear, no threshold (LNT) risk model provides a starting point for calculating stochastic risk factors for low-dose LET radiation. These risk factors do not apply to high doses and have great uncertainty at low doses (less than a few Rad) and low dose rates. This may be done by multiplying doses by stochastic risk factors for comparative purposes. However, the preferred approach is to apply risk coefficients from FGR-13, *Cancer Risk Coefficients for Environmental Exposure to Radionuclides*, directly to the radionuclide intake or exposure (DOE/EH-412/0015/0802; ISCORS Tech. Report 1; EPA FGR-13). Latent cancer fatalities (LCFs) are the (chronic) health risks of

most interest. The term "latent" indicates that the estimated cancer fatalities would occur sometime in the future, within the next 50 years for adults, or the next 70 years for the general population, which includes children. One can also estimate latent cancer occurrences (fatal plus non-fatal) or genetic effects, but these are not normally evaluated in safety analyses. The stochastic risk factor depends upon the type of radiation and the organ considered. The following subsections address health risks from high-LET radiation (alpha particles) and low-LET (beta particles and gamma rays) radiation.

8.3.1 HIGH-LET RADIATION

In the case of alpha emitters, such as plutonium and uranium, the only organs of importance for cancer risk are the lungs, liver, and bone surface as discussed in NUREG/CR-4214, *Health Effects Models for Nuclear Power Plant Accident Consequence Analysis, Modification of Models Resulting From Addition of Effects of Exposure to Alpha-Emitting Radionuclides*. The stochastic risk factors for cancer fatalities for these organs are shown in Table 8-4. For these three organs, the stochastic risk factors are linear and continuous. Earlier models, based on ICRP-26, used a linear-quadratic model. The new model, based on ICRP-60), is linear but may be discontinuous for some radionuclides. The values from NUREG/CR-4214 differ from the earlier ICRP-26 values): the lung factor is about four times larger, the bone skeleton factor is about ten times smaller, and liver factor is about three times smaller than the earlier values. The values in Table 8-4 are for high-LET radiation (alpha particles). Table 8-4 does not give the stochastic risk factor for committed effective dose, as the total cancer risk should be calculated as the sum of the individual organ cancer risk from exposure to alpha radiation and have been ignored.

Organ	Risk Factor (LCF/rem)
Bone surface	6.0E-7
Lungs	8.0E-5
Liver	1.5E-5

Table 8-4.	Stochastic	Risk Facto	ors for Alph	a-Emitters	(NUREG/CR-	4214).
I ubic 0 I.	Stothastic	Ition I uco	oro ror rinpi			

8.3.2 LOW-LET RADIATION

For low-LET radiation (beta and gamma radiation), the latent cancer risk may be estimated for regulatory decisionmaking from the committed effective dose, although the individual organ cancer risks could also be summed. ICRP-60 recommends using a stochastic risk factor of 5.0E-04 LCF/rem (5.0E-02 LCF/Sv) for the whole population,⁹⁷ or 4.0E-04 LCF/rem (4.0E-02 LCF/Sv) for adult workers, based on the committed effective dose.⁹⁸ The stochastic risk factor for the public is higher than for adult workers because the public consists of a mixture of individuals with varying degrees of resistance to hazardous materials, including children, the elderly, and the infirm. This factor includes the cancer risk to all organs, unlike the treatment of alpha radiation, which considers only the three organs of Table 8-4 to be important for cancer risk.

⁹⁷ This ICRP-60 recommendation was adopted by the DOE in 1993 for the evaluations of Environmental Assessments and Environmental Impact Statements, but was increased slightly to 6.0E-04 LCF/rem in the current DOE guidance (DOE/ESH, 2004).

⁹⁸ The ISCORS Technical Report No. 1 (ISCORS, 2002) cites a slightly higher risk factor of 6.0E-2 LCF/Sv (6.0E-4 LCF/rem) without distinguishing between the public and workers.

8.3.3 ACUTE HEALTH RISKS

Doses received in a short time period (acute doses) may cause acute health risks, if large enough. A dose from gamma or neutron radiation, such as from a criticality event, is the primary concern. Table 8-5 (taken from Table 3-2 of EPA-400/R-17/001, *PAG Manual, Protective Action Guides and Planning Guidance for Radiological Incidents*) summarizes the health effects associated with varying levels of gamma radiation.

Feature or Illness	Effects of Whole Body Absorbed Dose from External Radiation or Internal Absorption, by dose range in Rad (Gray)				
	0-100 (0-1 Gy)	100-200 (1-2 Gy)	200-600 (2-6 Gy)	600-800 (6-8 Gy)	>800 (>8 Gy)
Nausea, Vomiting	N	5-50%	50-100%	75-100%	90-100%
Time of onset	- None	3-6 hr	2-4 hr	1-2 hr	< 1 hr to minutes
Duration		< 24 hr	< 24 hr	< 48 hr	< 48 hr
Lymphocyte Count	Unaffected	Minimally Decreased	<1000 at 24 hr	< 500 at 24 hr	Decreases within hours
Central Nervous System Function	No Impairment	No Impairment	Cognitive impairment for 6-20 hr	Cognitive impairment for > 20 hr	Rapid incapacitation
Mortality	None	Minimal	Low with aggressive therapy26	High	Very High: Significant neurological symptoms indicate lethal dose
* Percentage of people receiving whole body doses within a few hours expected to experience acute health effects. Original source as cited in EPA-400/R-17/001: <i>Medical Management of Radiological Casualties</i> , Second Edition, Armed					

Fable 8-5.	Acute Radiation	Effects for	Gamma	Radiation *
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An acute dose from inhalation of plutonium or uranium, the dose received in a few hours or days, is normally very small. All of the isotopes of plutonium and uranium have half-lives of many years; therefore, the inhalation dose received by a person during the first few days following inhalation will only be a tiny fraction of the lifetime committed dose. Accordingly, an acute health effect requires a very large amount of plutonium or uranium to be released. For example, in order for a person at a distance of about 2 km from the release site to get a dose large enough to cause pneumonitis, the first prompt health effect to occur, an airborne release of about 100 kg of respirable plutonium-239 would be required (Peterson, 1993). Such a large release is not physically possible. Therefore, acute health effects to the public need not be considered for releases of plutonium or uranium isotopes.
9 CHEMICAL DISPERSION AND CONSEQUENCE ANALYSIS

9.1 INTRODUCTION

Chapter 6 discussed atmospheric dispersion analysis with its main focus on radiological releases, and Chapter 8 discussed radiological consequence analysis. Many of the atmospheric dispersion principles associated with radiological releases of neutrally-buoyant gases discussed in Chapter 6 are also applicable to neutrally-buoyant toxic chemical releases. Wherever there was commonality between radiological and toxic chemical dispersion and consequence analysis, it was so indicated in that chapter.

There are many types of toxic chemical releases that require a more comprehensive treatment than steadystate releases of neutrally-buoyant gases. These analyses involve more specialized source term phenomenological models and atmospheric dispersion models to address their emission into and redistribution in the atmosphere. In addition, the human health effect metrics of toxic chemicals are far more complex than the metrics associated with radiological health effects. Each of these differences are identified and treated in this chapter.

As discussed in Section 2.3.3, DOE-STD-3009-2014 requires assessment of toxic chemical hazards as part of a DSA hazard evaluation, either qualitatively or quantitatively. This chapter addresses the quantitative analysis of toxic chemical releases applying accident analysis methodologies.

As in Chapter 6, this chapter addresses the evaluation of releases of toxic chemicals and associated concomitant health risks to the facility worker, CW, and the MOI. However, it also discusses the different types of chemical release phenomenology and the factors to consider when estimating the health effects that these toxic chemicals can have on the human body and its target organs. Once the toxic chemical source term phenomenology is established and the appropriate atmospheric dispersion model selected, the resultant health risks associated with each toxic chemical needs to be evaluated at each important receptor and compared to the appropriate chemical health indicators.

NSRD-2015-TD01 concluded:

Similar to calculations for the radiological releases, the chemical release calculations showed that the default χ/Q value is conservative for chemical releases for nearly all cases, except the situations where the building wake cannot be credited or where a building is smaller than that assumed in NUREG-1140. For these situations the default χ/Q value may not provide a conservative estimate of dispersion.

This chapter addresses both the atmospheric dispersion of chemical materials and their consequences in terms of exposure concentrations to meet the requirements of Section 3.2.4.3, Chemical Source Term and Consequence, of DOE-STD-3009-2014, once the source term (ST) either as a release rate (mg/s) or total release quantity (mg) over a release duration (s) is estimated as described in Chapter 5. For safety analysis purposes, the dispersion analysis is used to estimate chemical consequences in terms of a peak air concentration that occurs any time during the duration of the release to the MOI and CW.

The following is the general approach for the atmospheric dispersion and chemical consequence analysis:

- 1. From the accident scenario, as defined by applying Chapter 3 guidance, identify parameters (ground level, buoyant, elevated stack, discharge temperature) relevant to evaluating releases to the environment.
- 2. Select the appropriate dispersion methodology (e.g., DOE Toolbox code, manual spreadsheet calculation).
- 3. Analyze appropriate weather data and convert to a format for the selected methodology.
- 4. Apply the dispersion methodology, justifying input values as affected by the accident scenario, unique site conditions, or recommended default values from the most recent guidance documents, such as those for the DOE Toolbox codes or this chapter.
- 5. Calculate the chemical concentration to the MOI and CW.

This Chapter goes through each of these steps. However, before doing so it begins with some fundamentals of chemical consequence assessment and other topics that support the DSA analysis of chemicals. Specifically this Chapter provides information on:

- Chemical Consequence Assessment Fundamentals;
- Chemical Screening Criteria;
- Chemical Health Effects on the Human Body;
- Toxic Chemical Release Phenomenology and Subsequent Atmospheric Transport And Diffusion;
- Meteorological Parameters Affecting Toxic Chemical Consequence Analysis;
- Toxic Chemical Atmospheric Transport and Diffusion Models;
- Toxic Chemical Consequence Scoping Methodology to Exceed PAC/TEEL Values; and
- Example Toxic Chemical Calculations.

9.2 CHEMICAL CONSEQUENCE ASSESSMENT FUNDAMENTALS

There are a number of ways in which the consequence assessment of toxic chemicals differ from that of radioactive materials; thus requiring more comprehensive treatment. The most fundamental difference is that unlike radiological exposures whose health effects have been normalized to a common scale of rem measurement, each particular toxic chemical insults the human body in its own unique way; enormously complicating the health effects evaluation portion of the assessment process. For a facility with an inventory of many different chemicals, consequence assessment can quickly become a cumbersome process. Accordingly, chemical hazard assessment makes extensive use of a screening process to focus on those chemicals of sufficient quantity and toxicity to present a clear potential threat to the facility worker, CW, MOI, and the public. Without this screening process, the amount of effort to perform chemical consequence assessments would be untenable.

Toxic impacts of most of the chemicals of concern for this handbook are associated with a threshold dose or concentration, usually defined for most toxic chemicals below which no adverse effects are expected. In contrast, the effects elicited by radioactive materials on the human body addressed in this handbook are assumed to occur over a dose continuum. Chemicals that have chronic carcinogenic, mutagenic and teratogenic effects are similar to those of radioactive materials in that they are considered non-threshold events but are only briefly addressed in this accident analysis handbook because those chemicals are not within the scope of 10 CFR § 830.204(b)(3).

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Other consequence assessment differences include the physical and temporal characteristics associated with the release phenomenology, the atmospheric characteristics of the plume, and the nature of the health and environmental effects. For chemicals that have a higher molecular weight than that of the atmosphere (i.e., 28.97 g/mol), density differences can produce dense gas gradients, resulting in airborne plumes that remain near the ground and flow downhill in response to local topography. In addition, liquid pools that are physically much colder than the environment, termed cryogenic, may also exhibit dense gas characteristics. Lastly, the quantity of the release is another important discriminator, as the release has to be sufficiently large to create its own dense gas dispersion environment. The Bulk Richardson number is used by dense gas models (e.g., ALOHA) to determine the nature of the dispersion environment. NRSD-2015-TD01 Section F.6 and Section 7.5.3 of this Handbook present additional discussion on dense gas dispersion. Chemical reactions in contact with air and upon exposure to sunlight and atmospheric moisture can also alter the human toxicity characteristics of a plume by changing its chemical composition and concomitant health effects.

9.3 CHEMICAL SCREENING CRITERIA

The evaluation of toxic chemical hazards often involves the consideration of many chemical substances. The DSA can be simplified with a negligible loss in conservatism and scientific integrity by limiting the chemical hazard evaluation to toxic chemicals that constitute the most significant safety concerns. This simplification can be accomplished through a systematic chemical pre-screening process. DOE-STD-3009-2014, Section A.2, provides the most recent chemical screening guidance for DSA hazard evaluations, such as excluding chemicals that are commonly available and used by the general public, or small-scale use quantities of chemicals. Moreover, SIHs should also be screened out per the guidance presented in Section 2.2.4, Exclusion of Standard Industrial Hazards and Other Hazardous Materials, of this Handbook. The following discussions provide additional clarifications and guidance related to the toxicity guidance addressed in DOE-STD-3009-2014, Section A.2.

The factors that determine the degree of hazard that any given chemical represents include:

- Physicochemical properties that contribute to dispersibility, reactivity, and toxicity;
- Significant quantities of chemicals that may displace oxygen in the air as simple asphyxiants;
- Incompatibility with other chemicals; and,
- Conditions under which the chemical is stored and/or used, including the quantity involved.

Specific questions to determine which chemicals to include in a DSA are presented in Table 9-1 below.

Table 9-1. Identification of Chemicals in the Prescreening Process: Baseline Criteria.

A) Is a particular chemical on any of the following lists? This is the first level of screening in or screening out of any chemical. Note that the TPQ and RQ values should not be used for quantitative screening.
• EPA list of extremely hazardous substances and threshold planning quantities (TPQs) (40 CFR § 355)
• EPA list of hazardous substances and reportable quantities (RQs) (40 CFR § 302)
• OSHA list of highly hazardous chemicals, toxic chemicals and reactive chemicals (29 CFR § 1910.119 Appendix A)
• EPA list of regulated substances and thresholds for accidental release prevention Threshold Quantities (40 CFR Part 68)
B) Is there any indication that the particular chemical exhibits significant toxic properties in Safety Data Sheets (SDSs), required by OSHA Hazards Communication, 29 CFR § 1910.1200?
C) Have any short-term acute exposure limits been derived for a particular chemical?
• EPA Acute Exposure Guideline Limits (AEGLs)
• AIHA Emergency Response Planning Guidelines (ERPGs)
• DOE/NA-41 PAC/TEELs
 D) Does a particular chemical have a National Fire Protection Association Health Hazard Rating of 2, 3 or 4? See DOE-STD-3009-2014, Section A.2.
E) Is a particular chemical extremely reactive or flammable?
F) Is a particular chemical in close physical proximity to other incompatible chemicals, which could result in the release of toxic reaction products in an accident?
G) Is a particular chemical readily volatilized (i.e., having a high vapor pressure) upon release to the atmosphere?

- H) Does a particular chemical generate toxic combustion products?
- Does a particular chemical act as a simple asphyxiant which reduces the available oxygen below 19.5 percent, per OSHA 29 CFR 1926.55 Appendix A? Additional simple asphyxiant guidance is provided in ANSI Z88.2-1992 and DOE-HDBK-1046-2016.

SDSs are required from chemical manufacturers to meet hazard communications requirements in OSHA's rule 29 CFR § 1910.1200. These SDSs also provide valuable chemical exposure health effects information relative to chemical screening, as follows:

- Section 2: Hazards identification inclusive of target organs, routes of entry, acute effects, chronic health effects, carcinogenic, mutagenic and teratogenic effects
- Section 10: Stability and reactivity
- Section 11: Toxicological information

All chemicals that are not screened out are evaluated in the DSA hazard evaluation as discussed in Section 2.3.2.

9.4 CHEMICAL HEALTH EFFECTS ON THE HUMAN BODY

The following subsections address chemical concentration, exposure modes and exposure time, and the various PAC/TEELs⁹⁹ to establish acute human health effects from toxic chemicals. Toxicity is defined as the degree to which a chemical substance or a particular mixture of substances can damage an organism. DSAs only require the assessment of the acute effects of toxic chemicals. Therefore, chronic chemical exposure effects are only briefly addressed in Section 9.4.5.

9.4.1 CHEMICAL CONCENTRATIONS AND EXPOSURE TIME

9.4.1.1 CHEMICAL EXPOSURE TIME

Chemical exposure concentrations may be expressed in either units of mg/m^3 or parts per million volume (ppmV). The latter represents a volume ratio of parts of toxic chemical per million parts of clean air, while mg/m^3 units are commonly used for aerosol (i.e., particulates or droplets of non-volatile liquid) release evaluations. For releases involving gases or vapors from volatile liquids, units of mg/m^3 can be used but ppmV units are more commonly used. Equation 9-1, which is based on the equation of state of an ideal gas, can be used to convert concentrations in units of mg/m^3 to units of ppmV, assuming a standard pressure of one atmosphere (101,325 N/m²) and an ambient temperature of 25°C; the latter recommended in 40 CFR § 68.22.

$$C[ppm] = C[mg/m^3(air)] \times 10^6 [m^3(air)/10^6 m^3(air)] \times \left\{\frac{R \times T}{MW \times P \times 1000}\right\} [m^3/mg] \quad \text{Equation 9-1}$$

Where,

 10^6 = ppmV conversion factor [units of m³(air)/10⁶·m³(air)]

⁹⁹ PAC/TEEL values for emergency planning for chemical release events are based on the following exposure limits, given in terms of airborne concentration, expressed as ppm or mg/m³:

^{1.} AEGL values published by the EPA.

^{2.} ERPG values produced by AIHA.

^{3.} TEEL values developed by the DOE Subcommittee on Consequence Assessment and Protective Actions (SCAPA).

AEGLs, ERPGs, and TEELs have three common benchmark values for each chemical (i.e., PAC/TEEL-1, -2, and -3).

Each successive benchmark is associated with an increasingly severe effect that involves a higher level of exposure. The DOE policy for its facilities and activities established irreversible health effects (the "-2" level) as the protective action criterion benchmark for chemical releases in Table 1 of DOE-STD-3009-2014. ERPGs refer to exposure durations of 1 hour (with shorter periods for some chemicals). While AEGLs are developed for five time periods the PAC database includes the AEGL one-hour value. TEELs have been standardized to one-hour. PAC values are developed to take into account all factors potentially causing a human health affect caused by exposure to the defined chemical. Refer to https://sp.eota.energy.gov/pac/.

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R	=	Universal gas constant [8.314 N·m/gmol·K]
MW	=	Molecular weight [g/gmol]
Р	=	Standard atmospheric pressure [101,325 N/m ²]
Т	=	Temperature [K]
1000	=	Mass conversion factor [units of "mg/g"]

The term enclosed by the large brackets represents the specific volume (reciprocal of density) of the chemical, which is directly proportional to ambient temperature.

Chemical health impacts are based on total exposure, which is a function of both the chemical concentration at the receptor and the exposure time at this concentration. Ten Berge, et al., (1986) developed a technique to account for exposure time on dose, and the ALOHA toolbox code has an algorithm that calculates dose as a function of exposure time using Ten Berge's equations. According to Ten Berge, if the concentration varies during the exposure period, this dose factor may be expressed as $[c(t)]^n dt]$, where c(t) is the concentration as a function of time during exposure and n is a chemical-specific dimensionless exponent:

$$[c(t)]^n dt$$
 Equation 9-2

Ten Berge presents values of the exponent, n, for 20 specific chemicals. For n=1, the effects are assumed to be a function of dose. The developers of AEGL values, which vary from 10-minute to 8-hour exposure times, used empirical data to evaluate the exponent n.

For toxic chemical aerosols and gases with a density approximately that of air, standard Gaussian atmospheric dispersion may be used to estimate chemical consequences. If the toxic material is released at some average rate over some period of time, the peak concentration at the receptor is obtained directly from the definition of the steady state χ/Q

Equation 9-3

 $C = Q'\left(\frac{\chi}{Q'}\right)$

Where,

C = peak concentration (mg/m³) Q' = toxic material release rate (mg/s) χ/Q = relative concentration (s/m³)

Note that in plume dispersion modeling, χ represents the concentration in the atmosphere, while for determining health effects, C denotes concentration of the chemical species.

Equation 9-3 represents a single, steady-state concentration that can be compared to the PAC/TEEL values presented in Section 9.4.1.2. In some cases, the release rate may be temporally variant, and needs to be evaluated as changing over time throughout the duration of the accident. This will result in concentrations at the receptor changing over time, creating a need to modify the time-varying concentration into a single value so it can be compared to the PAC/TEEL values. This can be accomplished using the time weighted average (TWA) concept. The toxicity characteristics of the toxic

chemical and duration of the plume exposure both factor into the time basis for the TWA as discussed in Section A.2 of DOE-STD-3009-2014. The plume exposure duration is generally assumed to be the same as the release duration of the source term.

Some consequence assessment dispersion codes will calculate the desired maximum 15-minute average concentration directly by allowing the analyst to specify the averaging period. To determine the average concentration manually, the following equation may be used:

$$TWA = \frac{C_1 T_1 + C_2 T_2 + \dots + C_n T_n}{T_1 + T_2 + \dots + T_n}$$

Equation 9-4

Where:

C = Concentration (ppmV or mg/m³)T = Time period of exposure (min)

n = Number of time segments

For short-duration releases (e.g., less than 15 minutes), the concentration at the receptor may be calculated as the TWA over the release period, but for no less than 1 minute. Since concentration varies with time due to the time-dependent release rate (Q') and long-wave atmospheric turbulence (i.e., plume meander), concentrations based on one-minute segments do not credit plume-meander; consistent with the concept of determining a peak TWA that is not smeared by time averaging effects.

For release durations longer than 15 minutes, the peak 15-minute average concentration during the duration of the release is used. For the peak 15-minute TWA, the 15-minute period of maximum exposure (concentration) is selected and input as 15, one-minute segments, into Equation 9-4. For exposure periods of less than 15 minutes, the product of C_xT_x may equal zero during the exposure period. Individual time intervals less than one minute are not appropriate for use in the numerator of the above formula for calculating the TWA. This assumption is conservative for "instantaneous" types of releases (e.g., container puncture of powders, over-pressurization of container). However, the use of a shorter averaging duration than 15 minutes, such as the actual exposure period but not less than one minute, may be warranted depending on the acute toxicity of the chemical of interest and the peak concentration observed.

If sufficient physiochemical information is available, the release rate of a toxic chemical can be directly calculated based on the phenomenology of the release and the properties of the chemical. For example, the rate of evaporation from a pool of a spilled chemical may be directly estimated, as discussed in Sections 9.5.4, 9.8.2, 9.9.3 and 9.9.4 of this handbook.

9.4.1.2 PROTECTIVE ACTION CRITERIA FOR RELEASES OF A SINGLE CHEMICAL

Section A.2 of DOE-STD-3009-2014 establishes the need for chemical PACs. Exposure to an air concentration greater than the toxic chemical PAC/TEEL criteria for safety SS control selection is assumed to confer a certain health detriment to the exposed individual. Although a duration of exposure is implicit in the PAC/TEEL definitions, shorter exposures to higher concentrations of some chemicals can have comparable effects. Accordingly, averaging the concentration from a short-duration release over 30 or 60 minutes may significantly under-predict the hazard. On the other hand, averaging over a very short time (e.g., a minute or two) represents the peak concentration more conservatively; however, the validity of any comparison between the calculated "peak" concentration PAC/TEEL value is questionable. It is therefore useful to calculate a TWA concentration at the results can be viewed

as having relevance to the criteria.

To address both concerns, TWA concentration at the receptor location is usually calculated for some period less than that implied by the PAC/TEEL definition, but long enough that the results can be accepted as having some relevance to the criteria. For example, EPA-550-B-99-009 which specifies ERPG-2 values (one of the human health criteria for establishing the PAC/TEEL-2) as primary toxic endpoints for their evaluation, assumes a 10-minute release averaging time in its determination of distance to the endpoint for worst-case analyses of toxic chemicals even though the ERPG-2 values are based on 60 minutes.

The DOE PAC/TEEL concentrations are based on different durations as defined by their concentration limit definitions from EPA or the chemical industry. To standardize releases from gases, liquids, and particulates, the hazard evaluation and/or accident analysis may assume a peak 15-minute, TWA chemical concentration for comparison to the PAC/TEEL values for SS control designation. There is no adjustment of the PAC/TEEL value or the calculated concentration to account for differences between the recommended 15-minute exposure time and the exposure time implicit in the definition of the PAC/TEELs.

9.4.1.3 PROTECTIVE ACTION CRITERIA FOR RELEASES OF MULTIPLE CHEMICALS

For chemical mixtures and concurrent releases of different substances, consequences are assessed using the (CMM) "Hazard Index" approach recommended by the DOE Office of Emergency Management, SCAPA Chemical Mixtures Working Group.¹⁰⁰ A brief explanation of this approach and the published journal article are available on the SCAPA website, <u>https://sp.eota.energy.gov/EM/SitePages/SCAPA-CMM.aspx</u>, under Health Code Numbers. The link also provides access to the CMM Wizard that automates the implementation of the approach for up to 30 chemicals. Although not in the Central Registry toolbox, this capability has undergone a rigorous SQA process. Even so, the analyst should check that this modeling tool is acceptable for use on a particular project by checking the approved software list for that project, or determine what site-specific QA requirements may apply.

Concurrent releases should be analyzed if a plausible scenario exists by which quantities of different substances could be released from the same location at the same time. Concurrent releases of dissimilar substances that, because of separation by distance or physical barriers, could result only from catastrophic events (such as major fires, aircraft crashes, severe NPHs) should be analyzed in accordance with the guidance for DBA scenarios. Concurrent releases of dissimilar substances caused by extreme malevolent acts need not be analyzed.

9.4.2 MODES OF EXPOSURE AND ROUTES OF ENTRY OF TOXIC CHEMICALS THAT RESULT IN HEALTH EFFECTS

Acute health effects from short-term exposures to toxic chemicals differ with respect to mode of exposure or route of entry into the human body. Since the inhalation pathway is also considered the most impactful for toxic chemical exposures, most toxic chemical consequence assessments focus on inhalation exposures. Other chemical exposure pathways (e.g., skin absorption) generally result in less severe health effects than the inhalation pathway. Accordingly, for aerosol-type releases, an inhalation only analysis should be adequate using conservative parameters; thus precluding any unnecessary analyses of alternate

¹⁰⁰ SCAPA: DOE Subcommittee on Consequence Assessment and Protective Actions. SCAPA has several working groups, which include the Chemical Exposures Working Group that developed the PAC/TEELs, and the Chemical Mixtures Working Group that developed the CMM.

pathway exposure. Impacts from chemical ingestion are generally chronic in nature and can be prevented by water and food interdiction management measures or mitigated by chelation processes.

DOE-HDBK-1046-2016, *Temporary Emergency Exposure Limits for Chemicals: Method and Practice*, provides an excellent discussion on all modes of exposure and routes of entry and also discusses each pathway inclusive of inhalation, skin absorption, inter-peritoneal, and ingestion, associated with acute effects of chemicals on human health. These form the toxicological basis for the PAC/TEELs. This Handbook also provides an excellent discussion on which organs are targeted by specific chemicals from the Health Indices and Health Code Numbers of the CMM. The CMM can be used if the analysis involves the release of up to 30 different chemicals.

9.4.3 TOXIC CHEMICAL ACUTE EXPOSURE LIMITS

There are three types of PACs available to the analyst:

- (1) AEGLs for five different exposure periods developed by EPA for about 300 specific chemicals;
- (2) ERPGs for about 150 chemicals for an approximate one-hour exposure period developed by the AIHA; and
- (3) PAC/TEELs developed by the DOE Office of Emergency Response and Policy Implementation (DOE/NA-41) for 3386 specific chemicals.

The following briefly discusses each of these toxic chemical human health criteria.

9.4.3.1 EPA ACUTE EXPOSURE GUIDELINE LEVELS

EPA's Office of Prevention, Pesticides and Toxic Substances established the National Advisory Committee for Acute Exposure Guideline Levels (NAC/AEGL) for hazardous substances to develop AEGLs. They are intended to assist Federal and State Agencies and private sector organizations with their needs for short-term hazardous chemical exposure information.

Final and interim AEGLs for about 300 chemicals have been published by EPA and are essentially comparable to ERPGs. Unlike ERPGs, AEGLs are calculated for five relatively short exposure periods (10 minutes, 30 minutes, one hour, four hours, and eight hours) dictated by the severity of the toxic effects caused by the exposure, with all levels based above which it is predicted that the general population could experience, including susceptible individuals. The levels are based on the following health effects resulting from exposure to a chemical substance:

- AEGL-1: Notable discomfort, irritation, or certain asymptomatic non-sensory effects. However, the effects are not disabling and are transient and reversible upon cessation of exposure.
- AEGL-2: Irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.
- AEGL-3: Life-threatening health effects or death.

The principle advantage of AEGLs is that they have been established for eight exposure times ranging from 10 minutes to 8 hours. AEGLs have a high technical pedigree, since the AEGL process involves an exhaustive search for data, careful analysis, thorough documentation, and expert review. The disadvantage is that they are available for only a limited number of chemical substances. It should be noted that only the one-hour AEGL is used in accident analysis.

9.4.3.2 AIHA EMERGENCY RESPONSE PLANNING GUIDELINES

The AIHA began developing ERPGs for use in evaluating the health effects of accidental chemical releases on the general public. These ERPGs are developed and published annually through a rigorous peer review process conducted by the AIHA Emergency Response Planning (ERP) Committee. The ERPG development process results in high-quality community exposure limits that are recognized and used both nationally and internationally.

For specific chemicals, ERPGs are estimates of concentration ranges above which acute exposure would be expected to lead to adverse effects.

- ERPG-1: The maximum airborne concentration below which it is believed that nearly all individuals could be exposed for up to 1 hour without experiencing other than mild transient adverse health effects or perceiving a clearly defined objectionable odor.
- ERPG-2: The maximum airborne concentration below which it is believed that nearly all individuals could be exposed for up to 1 hour without experiencing or developing irreversible or other serious health effects or symptoms that could impair their abilities to take protective action.
- ERPG-3: The maximum airborne concentration below which it is believed that nearly all individuals could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.

9.4.3.3 DOE PAC/TEELS

Many of the toxic chemicals of interest at DOE/NNSA sites lack ERPGs and AEGLs. In response to this need, the DOE Office of Emergency Response and Policy Implementation developed a TEEL methodology in 1992 to provide interim guidance for chemicals of interest. TEELs estimate the concentrations at which most people will begin to experience health effects if they are exposed to a hazardous airborne chemical for a given duration. TEELs are used for emergency management in similar situations as the one-hour AEGLs and one-hour ERPGs.

TEEL-1, TEEL-2, and TEEL-3 have similar definitions as the equivalent ERPGs and one-hour AEGLs. A chemical may have up to three TEEL values, each of which corresponds to a specific tier of health effects. The three TEEL tiers are defined as follows (PAC, 2016):

- TEEL-1 is the airborne concentration (expressed as ppm or mg/m3) of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience notable discomfort, irritation, or certain asymptomatic, non-sensory effects. However, these effects are not disabling and are transient and reversible upon cessation of exposure.
- TEEL-2 is the airborne concentration (expressed as ppm or mg/m3) of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience irreversible or other serious, long-lasting, adverse health effects or an impaired ability to escape.
- TEEL-3 is the airborne concentration (expressed as ppm or mg/m3) of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience life-threatening adverse health effects or death.

The methodology for assigning TEELs was originally based on hierarchies of commonly available published and documented concentration-limit parameters, particularly occupational exposure limits, later expanded to include other published concentration limits and then further expanded to include the use of

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published toxicity parameters. The current TEEL hierarchy, taken from Table 3.1 of DOE-HDBK-1046-2016 and presented in Table 9-2 is based on 9 concentration exposure indicators and 6 toxicity indicators from 11 technical sources. DOE-HDBK-1046-2016 not only documents the process of how the PAC/TEELs were developed, but provides insights as to how the analyst should apply them to chemical consequence assessments.

TEEL-i	TEEL Data	Data Source
TEEL-3	EEGL (30-min)	NRC
	IDLH (1990 values)	NIOSH
	Other	Various
	LC50	HSDB/SAX/RTECS
	LCLO	HSDB/SAX/RTECS
	LD50	HSDB/SAX/RTECS
	LDLO	HSDB/SAX/RTECS
TEEL-2	EEGL (60-min)	NRC
	LOC	EPA
	TLV-C	ACGIH
	WEEL-C	AIHA
	PEL-C	OSHA
	REL-C	CDC
	MAK-C	GRF
	Other	Various
	TCLO	HSDB/SAX/RTECS
	TDLO	HSDB/SAX/RTECS
TEEL-1	TLV-STEL	ACGIH
	WEEL-STEL	AIHA
	PEL-STEL	OSHA
	REL-STEL	CDC
	MAK-STEL	GRF
	Other	Various

Table 9-2. TEEL Data Selection Hierarchy.

TEEL Toxicity Ind	dicators	
LC50 - Lethal Con		
LC ₅₀ - Lethal Concentration that kills 50% of population LC _{LO} – Lowest reported lethal concentration LD ₅₀ - Lethal Dose that kills 50% of population LD _{LO} – Lowest reported lethal dose TC _{LO} – Toxic Concentration Lowest TD _{LO} – Toxic Dose Lowest		
łygienists alth		
	.Cs0 - Lethal Con .CLO – Lowest rej .D50 - Lethal Doso .DLO – Lowest rej 'CLO – Toxic Cond 'DLO – Toxic Doso 'DLO – Toxic Doso	

As can be seen from ubiquity of Table 9-2, the PAC/TEELs represent the current most comprehensive compendium of acute exposure guidelines. Revision 29 (PAC, 2016), issued in May 2016 can be accessed at http://sp.eota.energy.gov/pac. ERPG values for various substances are revised annually by the AIHA ERP Committee. The newly published ERPG values for a particular chemical will replace its PAC/TEEL values. EPA is no longer developing AEGLs. If EPA resumes its AEGL development effort, when an AEGL value for a particular chemical is newly published, it will replace ERPG or TEEL values. Accordingly, the PAC/TEEL database will be periodically updated and presented in a subsequent revision which can be accessed in the aforementioned link. Safety analysts are encouraged to consult that link prior to completing their chemical consequence analyses to ensure that they use the latest PAC/TEEL values.

For chemicals that are not toxic, but can act as simple asphyxiants at high concentrations that reduce ambient oxygen to levels where human health can be compromised, the PAC/TEELs for that chemical establishes concentrations that will result in various levels of human health insult and incapacitation:

- PAC/TEEL-1 represents a concentration where oxygen levels are reduced to 19.5%; the OSHA limit for respiratory protection.
- PAC/TEEL-2 represents a concentration where oxygen levels are reduced to 16%. At this level, a threshold is reached for the onset of impaired coordination, perception, and judgment; sufficient to compromise a person's ability of self-protection and escape.
- PAC/TEEL-3 represents a concentration where oxygen levels are reduced to 12.5%, the threshold for causing very poor judgment and coordination, followed by unconsciousness and death.

Elemental uranium and its compounds are radiological hazards that are evaluated for radiological consequences using the techniques in Section 6. However, elemental uranium and its compounds also pose a significant toxicological risk to the MOI, CW, facility worker and the public and accordingly, its chemical consequences are also evaluated. In some cases, uranium toxicological risks exceed its

radiological risks. Table 9-3 presents the Revision 29 PAC/TEELs for uranium and its compounds that are the health endpoints an analyst should be informed of when performing a uranium toxic chemical consequence assessment.

Chemical	CASRN#		PACs (mg/m ³)
Sodium uranium oxide monohydrate; (Sodium urinate (VI) monohydrate)	10135-92-9	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		0.82	6.8	41
Uranium	7440-61-1	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		0.6	5	30
Uranium hexafluoride; (Uranium fluoride)	7783-81-5	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		3.6	9.6	36
Uranium hydride; (Uranium (III) hydride)	13598-56-6	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		0.61	5	30
Uranium oxide; (Triuranium octaoxide)	1344-59-8	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		0.71	10	50
Uranium telluride	12138-37-3	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		1.2	10	62
Uranium telluride (U3Te4)	12138-37-3a	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		1	8.5	51
Uranium trioxide	1344-58-7	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		0.045	0.5	3
Uranium dioxide; (Uranium(IV) oxide)	1344-57-6	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		0.68	10	30
Uranyl acetate; (Uranium oxyacetate)	541-09-3	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		0.98	5.5	33
Uranyl fluoride; (Uranium oxyfluoride)	13536-84-0	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		0.78	4.3	26

Table 9-3. Uranium Compound PAC/TEELs.

Chemical	CASRN#	I	PACs (mg/m ³)
Uranyl nitrate (solid); (Bis(nitrato-O,O') dioxouranium)	10102-06-4	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		0.99	5.5	33
Uranyl nitrate (yellow salt)	36478-76-9	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		0.99	5.5	33
Uranyl nitrate hexahydrate	13520-83-7	PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
		1.3	7	42

9.4.4 CHEMICAL MIXTURE METHODOLOGY

Effects from exposure to multiple chemicals can be addressed by using the CMM, also developed by the DOE Office of Emergency Response and Policy Implementation. The CMM approach determines whether effects of multiple chemicals are synergistic or antagonistic on various target organs.

The CMM provides recommended default emergency exposure guidelines for mixtures of chemicals. The CMM makes extensive use of HCNs to examine the additive impact that each chemical component in a chemical mixture may have on specific target organs. The CMM is a more realistic predictor of potential human health impacts than can be obtained using the:

- (1) Non-conservative method of separately analyzing the consequences of each chemical component; or
- (2) Overly-conservative method of adding the exposures from each chemical together regardless of the human organ targeted by the chemical.

The CMM is recommended for potential use in emergency planning hazards assessments, DSAs, and in emergency response circumstances. The CMM and its workbook can be downloaded from https://sp.eota.energy.gov/EM/SitePages/SCAPA-CMM.aspx .

The CMM approach that involves adding all exposures from each chemical, regardless of the target-organ effects of the chemicals, tends to overestimate impacts and therefore be over-conservative. The health impacts from chemicals that target different organs are often not simply additive to all target organs.

When using the CMM, a hazard index (HI) is calculated for each component of a chemical mixture at the chosen receptor point. The "HI_i" is the concentration of chemical "i" (Conc_i) divided by the concentration limit for chemical "i" (Limit_i), as shown in Equation 9-5:

$HI_i = Conc_i / Limit_i$

Equation 9-5

A $HI_i < 1$ means that the limit for that single chemical "i" has not been exceeded. However, if the hazard indices for all chemicals in a mixture are summed, and the cumulative HI is greater than one, then an unacceptable condition may exist and mitigating strategies may need to be considered. Unless the health effects of the components are known to be independent, the toxic consequences of all components should,

306 ENGINEERING-PDH.COM | SAF-143 | as an initial step in an assessment, be considered to be additive. This represents the most conservative upper-bound approach for assessing exposures to mixtures. If this upper-bound approach produces unacceptable results, the next step is to classify the chemicals in the mixture according to their toxic consequences. The toxicological classification of specific chemicals can be accomplished using the HCNs established for each chemical.

HCNs are used in the CMM to identify the target-organ effects of each chemical in the mixture. Any chemicals that targets the same or similar organs or operates by the same acute or chronic mode of toxicity should be considered additive to that target organ or by that same mode of toxicity. Target-organ effects and modes of toxicity are considered simply as target organ effects.

HCNs are similar to medical diagnostic codes in that they are code numbers that identify a particular target organ or health effect to enable classification of chemicals by target organ toxicity. Summation of HIs for all chemicals in a mixture having the same toxic consequences (same or similar HCNs) enables determination of the acceptability or unacceptability of exposure to any specific mixture of chemicals using this more realistic approach.

HCNs also offer a convenient way of performing this exposure addition by numerically "binning" identical or similar target organ effects. All of the individual exposure HIs that are binned into the same or similar HCN bin are added together to yield an "HI sum" for that target organ bin. Any of the individual HI sums that exceed a value of 1.0 indicate that the exposure limit has been exceeded and that some kind of mitigating action should be taken to reduce the exposure to that specific target organ below the applicable limit.

The latest version of the CMM Workbook, which can process up to 30 chemicals in a given mixture, is in CMM Revision 29.

9.4.5 CHRONIC HEALTH EFFECTS OF TOXIC CHEMICALS ON THE HUMAN BODY: CARCINOGENICITY, MUTAGENICITY, AND TERATOGENICITY

Although DOE has a few large inventories of carcinogenic chemicals, DOE DSAs do not evaluate carcinogenic effects but focus on documenting consequences of chemicals with acute exposure effects. The evaluation of cancer effects from chemical releases is not required by DOE-STD-3009-2014 or DOE-STD-1189-2016. The DOE Safety Goal related to LCFs for radiological releases is with respect to 50-mile radius population doses and not to the facility worker, CW, or MOI. There is no analogous DOE Safety Goal associated with carcinogenic chemicals. The following provides some information on where to obtain chronic chemical health effect information should there be a need for a qualitative evaluation.

Dose-response curves for non-carcinogenic chemicals are characterized by the existence of threshold exposure levels below which no toxic effects will be observed. Due to a fundamental difference in the mechanism of action, the dose-response curves for carcinogens are considered as LNT representations.

Known or suspected human carcinogens are identified in the EPA data bases Integrated Risk Information System and Health Effects Assessment Summary Tables, the National Institute for Occupational Safety and Health Pocket Guide to Chemical Hazards, and International Agency for Cancer Research publications.

Per 1986 EPA guidance, confirmed or suspected human carcinogens are treated differently from those compounds eliciting only acute toxic effects. Incremental cancer risk (ICR) can be calculated using the

Integrated Risk Information System database values for the chemical-specific slope factor.

9.5 TOXIC CHEMICAL RELEASE PHENOMENOLOGY AND SUBSEQUENT ATMOSPHERIC TRANSPORT AND DIFFUSION

Unlike radiological releases, which are generally assumed to be continuous and of the same magnitude throughout the accident sequence, there are a large number of variables that need to be accounted for to characterize toxic chemical releases and their effects on the facility worker, CW, and the MOI. Although most chemical releases are associated with complex phenomenology, some of them are continuous steady-state and thus chemical health effects can be determined by simple atmospheric dispersion models. It should be noted that radiological releases can also be subjected to the same phenomenology, but in practice, analysts do not commonly take this into consideration. Phenomenological releases, as described in Chapter 5, and special atmospheric transport and diffusion considerations that are specific to the release of toxic chemicals include, but are not limited to:

- Temperature, pressure, and state of the chemical in its storage container;
- Type of storage container (tank, vessel, pipe);
- Density, temperature and quantity of the substance released that determines whether it will disperse as a positively-buoyant gas, neutrally-buoyant gas, or a dense/heavy gas;
- Phenomenology of release (e.g., guillotine pipe break, small hole);
- Speed of chemical leaving its container through an orifice relative to the speed of the sound (choked flow versus non-choked flow);
- Energy associated with the release, such as thermal energy of a fire;
- Chemical transformations resulting from the effects of fire or reaction with water vapor in the atmosphere (e.g., uranium hexafluoride release into a humid atmosphere); and
- Synergistic and antagonistic effects of a multiple chemical release and the cumulative effects on target organs (see Section 7.4.4).

The following subsections present a discussion on toxic chemical release phenomenology.

9.5.1 PRESSURIZED LIQUIDS: TWO-PHASE FLOW TOXIC CHEMICAL RELEASE

Pressurized liquid releases are the most complex of non-energetic single chemical releases, as two-phase flow needs to be accounted for. The initial portion of the liquid release flashes to a gas, due to its rapid depressurization at the point that it encounters the atmosphere. The flashed portion of this type of release is usually of short duration (a puff) which requires a three-dimensional Gaussian puff model to determine its fate and transport.

The remaining chemical that does not flash forms a liquid puddle, or gaseous area source for a sublimating chemical (e.g., carbon dioxide). The liquid puddle evaporates as a non-pressurized sub-cooled liquid release behind the puff requiring a conventional two-dimensional Gaussian code similar to what would be used on a liquid release that evaporates. This evaluation may also need to be performed in an iterative manner since the source term varies with time.

Pressurized liquid releases from a tank through a pipe adds one additional level of complexity as the rapid depressurization of the chemical when it reaches the atmosphere at the point of the pipe break causes a choked flow condition, discussed in Section 9.5.2, upstream of the pipe. Thus, the flashing of the liquid occurs inside the pipe before discharge, and this choked flow limits the mass release rate. Analysis of this phenomenology is a highly complex time-dependent process as the fluid near the discharge experiences a

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pressure drop and flashes, while the fluid upstream does not sense the break and stays in liquid form. Therefore, an oblique pressure wave travels upstream resulting in a greater fraction of the liquid flashing inside the pipe. For this type of chemical release, the vapor mass fraction needs to be calculated in an iterative manner to determine the time-varying chemical source term. Therefore, the analyst accounts for the phenomenology of pressurized liquid releases using techniques such as those in Section 9.5.1.1.

The Hazard Prediction and Assessment Capability (HPAC) ITRANS source term module provides a comprehensive methodology to establish chemical release quantities; especially for pressurized liquid chemical releases. HPAC has dense gas modeling capabilities, and a sub-code, Second-Order Closure Integrated PUFF (SCIPUFF) (Sykes, 1998), that can also address positively-buoyant gases quantifying its liftoff after release.

The following subsections provide the analyst with some of the complex equations associated with pressurized liquid releases to calculate the flashing fraction and aerosol formation, and for two-phase release of chlorine from a pipe.

9.5.1.1 FLASHING FRACTION AND AEROSOL FORMATION

Section 9.5.1 discusses the complex phenomenology associated with the release of pressurized liquids to the atmosphere. The initial portion of the liquid release flashes to a gas, due to its rapid depressurization at the point that it encounters the atmosphere. The flashing fraction may be calculated by means of a heat balance across the outlet orifice where the decrease in latent heat of vaporization and increase in heat capacity are accounted for as the initial temperature approaches the critical temperature. This fraction is expressed as shown in Equation 9-6.

$$f = 1 - exp^{-2.63} \frac{C_l(T_b)}{L(T_b)} (T_c - T_b) \left\{ 1 - \left[\frac{(T_c - T_l)}{(T_c - T_b)} \right]^{0.38} \right\}$$
 Equation 9-6

Where,

f	=	flashing fraction (dimensionless);
$C_1(T)$	=	liquid heat capacity at temperature T (J/kg °K);
L(T)	=	latent heat of vaporization at temperature T (J/kg);
T _c	=	critical temperature (°K);
T _b	=	liquid boiling temperature at one atmosphere pressure (°K); and,
T_1	=	liquid temperature (°K).

Generally, a superheated liquid jet or spray needs to be present to achieve significant quantities of liquid droplets suspended in the initial cloud. As the discharge pressure decreases, some of the liquid will flash immediately to vapor, while the remaining non-flashed liquid will either be suspended as liquid droplets (i.e., finely distributed aerosols), or fall to the ground forming a pool that will boil or evaporate over time.

The distribution of droplet sizes is required before the rainout fraction can be calculated. Kitamura et al., 1986 and Bettis et al., 1987 have experimentally observed that the droplet sizes are log-normally

distributed, as shown in Equation 9-7.

$$p(d) = \frac{exp^{1/2}\sqrt{[\ln(d) - \ln(\langle d \rangle)]/\ln(\sigma_g)}}{\sqrt{2\pi \ln(\sigma_g)d}}$$
Equation 9-7

Where,

d	=	random droplet diameter (m);
p(d)	=	probability distribution as a function of drop diameter d (dimensionless);
σ_{g}	=	geometric variance (dimensionless) (assume σ_g =1.3; Iannello et al., 1989); and,
<d></d>	=	mean droplet diameter (m).

The mean droplet diameter may be estimated by means of the Nukiyama-Tanasawa equation (see Tilton and Farley, 1990), as shown in Equation 9-8.

$$< d > 585 rac{\sqrt{\sigma_l}}{u_e \sqrt{\rho_l}}$$
 Equation 9-8

Where,

σ_l	=	liquid surface tension (dyne/cm);
ρ_l	=	droplet liquid density (kg/m ³); and,
ue	=	axial spray velocity at end of discharge region (m/s),

where the droplet diameter is μ m units. Using the values for each of the salient parameters germane to anhydrous chlorine yields, a droplet diameter distribution is obtained.

Since an instantaneous release directly into the ambient wind field is postulated for this analysis, the axial spray velocity is assumed identical to the ambient wind speed. The criterion for droplet rainout is satisfied when the inclination of the droplet trajectory, β_d , with respect to the vertical direction is greater than the half angle of jet expansion at the start of entrainment. The subsequent droplet settling velocity (V_d) may be calculated by solving the balance equation expressing the equality between the force of gravity on the droplet and the upward-acting viscous and drag forces, as depicted in Equation 9-9.

$$\frac{\pi}{6}d^3(\rho_l-\rho_g)g=C_d\,\rho_g\frac{v_d^2}{2}\left(\frac{\pi}{4}d^2\right)$$

Equation 9-9

With,

 $\rho_g =$ vapor density after expansion (kg/m³); and, $C_d =$ friction factor including both viscous and drag losses (dimensionless).

Where, Equations 9-10 and 9-11 show:

$$C_d = \frac{24}{Re_d} + \frac{6}{1 + \sqrt{Re_d}} + 0.4$$
Equation 9-10
$$Re_d = \frac{\rho_g V_d d}{Re_d}$$
Equation 9-11

$$Re_d = \frac{\mu_g v_d u}{\mu_g}$$
 Equation 9

Where, μ_g denotes the viscosity of vapor in units of Pa·s.

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Therefore, the final expression, which V_d satisfies, is given by Equation 9-12:

$$3V_d \left[\frac{24\mu_g}{\rho_g V_d d} + \frac{6}{1 + \sqrt{\frac{\rho_g V_d d}{\mu_g}}} + 0.4 \right] - 4d(\rho_d - \rho_g)g = 0$$
 Equation 9-12

The critical droplet diameter (d_c) satisfies the criterion in Equation 9-13:

$$\tan \beta_{d_c} = \frac{V_{d_c}}{U_e} = \tan \beta_e$$
 Equation 9-13

Any droplet trajectory possessing an angle of inclination, β_d , with respect to the horizontal that is greater than the spray half-angle, β_e , will drop out of the vapor-aerosol plume and rainout onto the ground surface to form a pool. Observing that as V_d increases, tan β_d also increases for $u_e > 0$ fixed, and the solution is therefore unique and given by Equations 9-14 and 9-15:

$$V_{d_c} = U_e \tan \beta_e$$
 Equation 9-14

$$f'(d_c) = 3V_{d_c} \left[-\frac{24\,\mu_g}{\rho_g V_{d_c} d_c^2} + \frac{3\sqrt{\rho_g V_{d_c}}}{\sqrt{\mu_g d_c} \left(1 + \sqrt{\frac{\rho_g V_{d_c} d_c}{\mu_g}}\right)^2} \right] - 4(\rho_d - \rho_g) - g$$
 Equation 9-15

Finally, the solution to d_c may be obtained using Newton's method by way of the two functional relationships in Equation 9-16:

$$f(d_c) = 3V_{d_c} \left[-\frac{24\,\mu_g}{\rho_g V_{d_c} d_c} + \frac{6}{1 + \sqrt{\frac{\rho_g V_{d_c} d_c}{\mu_g}}} + 0.4 \right] - 4d_c (\rho_d - \rho_g)g = 0$$
 Equation 9-16

Using a model for a spherical droplet in laminar flow, which is not to be confused with turbulent jet flow during droplet formation, a critical drop diameter, dc, can be calculated.

Droplets possessing a diameter exceeding this value experience a sufficiently large gravitational force to induce the beginning of rainout. Using a value of $\beta_e=9.1^{\circ}$ (Wheatley, 1987), the critical drop diameter has been determined to be 25 microns. The fraction of liquid that rains out, f, is then calculated implicitly from Equations 9-17 and 9-18.

$$f_p = 1 - \int_{-\infty}^{d_c} \rho(\xi) d\xi = \frac{1}{2} [1 - erf(X_c/2)]$$

Where,

$$X_c = \frac{\ln(d_c) - \ln()}{\ln(\sigma_g)};$$
$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-\xi^2} d\xi$$

Equation 9-18

In this case, since $f_p=0.05$, essentially all of the aerosol component remains airborne and evaporates right above the pool as the aerosol particles are transported downwind.

It should be noted that a great deal of uncertainty lies in the estimate of exactly how much of the nonflashed liquid is entrained into the air as a suspended aerosol. Large-scale experiments indicate that the mass of aerosol produced is very roughly equal to the mass of superheated liquid which immediately flashed to vapor when the flashing fraction is less than one-third (Lees, 1996). Since the flashing fraction is below one-third for the chlorine release, the initial aerosol mass is assumed to be equal to the mass of liquid flashed to vapor.

When the release initially results in a dense gas slumping cloud, note that the dispersing medium within the dense gas cloud consists only of the sub-cooled vapor (i.e., vapor evaporated from the pool) component. No clear causal relationship exists between the dense cloud and droplets of liquid raining out of the cloud. Therefore, the model treats these two phenomena separately; specifically the mass fraction of the release which remains suspended as aerosol, and that which falls onto the ground to form a boiling or evaporating pool. A portion of the remaining liquid will either be suspended as liquid droplets or finely distributed aerosol. Any liquid entrained into the vapor cloud as a suspended aerosol is characterized in terms of the liquid mass evaporation rate and temperature as a function of time.

The suspended liquid aerosol droplets evaporate as the ambient air flows past them. The computational model of Papadourakis et al., 1991, is applied to determine the rate at which a droplet of 1000-micron diameter would evaporate in an ambient wind of 5 mph (2.22 m/s) and a temperature of 100°F (37.8°C), using an initial spray velocity of approximately 12 m/sec. A 1,000-micron diameter particle was selected since it represents a 95 percent confidence bound on aerosol particulate size. Only five percent of aerosol droplets formed are expected to have a diameter greater than 1,000 microns for a typical droplet spectrum.

Details of the underlying equations in the model describing the conservation of mass, energy, and momentum are not included in this discussion as they are beyond the scope of this discussion. The final numerical results demonstrate that the entire droplet mass undergoes complete evaporation within 12.25 m of the liquid release point. Therefore, as a conservative and bounding simplifying assumption, the analyst can assume that all-aerosol component evaporates in the near vicinity of the residual liquid pool with no initial dilution and the mass of vapor is then added to the vapor source term.

9.5.1.2 TWO-PHASE RELEASE OF CHLORINE FROM A PIPE

In this specific example, there is conversion of some of the chlorine liquid to vapor within the pipe itself. This change in upstream composition subsequently causes a reduction in the mass release rate and an

increase in outflow velocity.

The variation in these release parameters can be calculated from Equation 9-19, which is the Fauske equation found in *Loss Prevention in the Process Industries* (Lees, 1996):

$$G = A_e \left[\frac{-k}{T_1 + T_2 + T_3} \right]^{1/2}$$
 Equation 9-19

Where,

$$T_{1} = (1 - x + kx)xdv_{g}/dP$$
Equation 9-20
$$T_{2} = \left[v_{g}(1 + 2kx - 2x) + v_{l}(2kx - 2k - 2xk^{2} + k^{2})\right]dx/dP$$
Equation 9-21
$$T_{2} = \left[v_{g}(1 + x(k - 2)) + v_{l}(2kx - 2k - 2xk^{2} + k^{2})\right]dx/dP$$
Equation 9-21

$$T_3 = k[1 + x(k-2) - x^2(k-1)]av_1/aP$$
 Equation 9-22

$$dx/dP = -(dh_f/dP + xdh_{fg}/dP)/h_{fg}$$
 Equation 9-23

Where,

= release rate (kg/s);
= effective area of the orifice (m^2) ;
= mass fraction of vapor in the mixture (dimensionless);
= specific volume of the gas (m^3/kg) ;
= specific volume of the liquid (m^3/kg) ;
$= (v_g/v_l)^{1/2}$
= saturation pressure (Pa);
= enthalpy of the saturated liquid (cal/g); and,

 h_{fg} = latent heat of vaporization (cal/g).

The equation was evaluated using an Antoine equation (Antoine, 1888) for saturated vapor pressure and ideal gas conditions were assumed. Table 9-4 presents the results, which show the percentage of gas mass fraction. The percentage of liquid mass fraction is defined as 1 - gas mass fraction.

Gas Mass Fraction	Mass Release Rate (kg/s)	Release Velocity (m/s)	Initialization Temperature (degrees K)	Density (kg/m ³)	Effective Droplet Diameter (mm)
0.1	81.8	71	239	11.8	0.352
0.2	63.3	101	239	9.2	0.295
0.3	51.8	120	239	7.5	0.270
0.4	43.8	134	239	6.3	0.256
0.5	38.0	144	239	5.5	0.247
0.6	33.6	152	239	4.8	0.241
0.7	30.1	158	239	4.3	0.236
0.8	27.3	163	243	3.9	0.233
0.9	24.9	167	243	3.6	0.231

Table 9-4. Calculated Variation of Chlorine Jet Release Parameters as a Function of Upstream Gas Mass Fraction (Mills And Paine, 1990).

The table shows that the mass release rate is inversely proportional to the gas mass fraction and the release velocity is proportional to the gas mass fraction. As the fraction of the fluid in the pipe that flashes from liquid to gas at the outlet increases, choked flow upstream in the pipe results, and the resultant mass release rate decreases. This is a very interesting case where pressurized liquid two-phase flow from a pipe also exhibits pressurized gas choked flow characteristics.

The aforementioned equations in Sections 9.5.1.1 and 9.5.1.2 are limited to the assumptions in their derivation and/or the conditions under which they were developed. Prior to employing these equations to determine the phenomenology of a specific system or process, the analyst should demonstrate that the application domain of the equations is not exceeded.

9.5.2 PRESSURIZED GASES: CHOKED FLOW TOXIC CHEMICAL RELEASE

The release of pressurized gases is either under choked flow or non-choked flow depending on the internal pressure and the size of the orifice; both of which affect the speed at which the gas escapes through the orifice.

Pressurized gaseous non-energetic single chemical releases (e.g., hole in a cylinder containing gas stored at several atmospheres pressure) also cannot be addressed by steady-state Gaussian models since the source term is never steady-state; always varying with time. This is the result of the internal pressure decreasing with time as the gas escapes through the orifice and the remaining unreleased gas undergoing Joule-Thompson cooling, which affects its temperature and volume. As the internal pressure decreases with time, the release rate will decrease accordingly.

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For highly-pressurized gases that are released through a very small orifice, additional complexities associated with choked flow need to be accounted for. Choked flow occurs when the released gas attempts to exit its storage container at a rate that exceeds the speed the sound, which itself is a function of ambient temperature. Accordingly, a gas cannot travel outside of its containment at a speed greater than the speed of sound, which is a physically limiting factor. Therefore, the analyst needs to account for choked flow until the internal pressure is reduced to a subsonic level, where the flow becomes and remains non-choked. Pressurized gases escaping through an orifice at speeds less than the speed of sound will do so under non-choked flow.

ALOHA Version 5.4.6 incorporates LEAKR algorithms (Belore and Buist 1986) to establish the release rate of gases from orifices, holes and short pipes. It initially determines whether gas flow will be supersonic (choked) or subsonic (unchoked) from the ratio of tank to atmospheric pressure, ratio of hole width to tank length, and critical pressure ratio for sonic flow. Should the pressure difference be large enough, ALOHA models flow as supersonic until the pressure drops to the point at which flow reaches subsonic speeds. From that point onward, ALOHA computes a subsonic release rate tank pressure, which has been reduced to atmospheric pressure. The estimated rate of gas release gets smaller over time since tank or pipe pressure is expected to drop as gas exits and adiabatic expansion from Joule-Thomson cooling, cools the tank contents, further reducing pressure. To account for the phenomenology of pressurized gas releases, use techniques such as those presented in Sections 9.5.2.1 through 9.5.2.5.

The following subsections provide the analyst with some of the complex equations associated with pressurized gas releases to calculate vapor outflow from a pipeline, spherical tank, cylindrical tank, and other type of vessel. Guidance provided by the EPA (EPA-550-B-99-005, Section 8.1.1, Equation 11) offers a method for estimating the maximum emission rate for an unmitigated release of gas from a vessel.). The expression does not account for the decrease in the release rate as the pressure in the tank decreases. A method for determining the time-dependent mass release rate from a pressure vessel is presented in Section 9.5.2.1.

9.5.2.1 TIME-DEPENDENT VESSEL GAS BLOW DOWN MODEL

In the case where the onset of gas release occurs under choked, or sonic, flow conditions, the timedependent mass release rate is given by

$$w(t) = w_o[F(t)]^{(\gamma+1)/(\gamma-1)}$$

Where,

t time [s];

w sonic mass release rate [kg/s];

 w_0 is the initial sonic mass release rate [kg/s] given by

$$w_o = C_d A_d \sqrt{\gamma \rho_o P_o [2/(\gamma+1)]^{(\gamma+1)/(\gamma-1)}}$$

- $C_{\rm d}$ coefficient of discharge [dimensionless];
- A_d outlet (orifice) area [m²];
- g specific heat ratio [dimensionless];
- r_o initial fluid density inside the vessel [kg/m³];
- $P_{\rm o}$ initial fluid pressure inside the vessel [Pa].

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The time dependent function in the relationship, F(t), is given by Equation 9-26, below:

$$F(t) = 1/(1+At)$$
 Equation 9-26

Where.

$$A = w_o(\gamma - 1)/2m_o$$

and.

 m_0 represents the initial mass inside the vessel (kg).

Equation 9-26 is valid only for the conditions of choked (sonic) flow, namely when the internal system pressure, P_0 , exceeds a physical constant referred to the critical pressure $P_{critical}$ defined as:

$$P_{critical} = P_{ambient} \left(\frac{\gamma+1}{2}\right)^{\gamma/(\gamma+1)}$$
Equation 9-28

Where, $P_{ambient}$ is the ambient pressure outside of the vessel.¹⁰¹

Although most of the tank inventory will be discharged in sonic flow, it is possible to calculate the time at which the flow becomes subsonic or unchoked. Assuming ideal gas behavior, the initial mass release rate from the vessel under unchoked (sub-sonic/sub-critical) flow conditions when $P_o \leq P_{critical}$ is given by Equation 9-29, taken from Perry's Chemical Engineers' Handbook (Eighth Edition) (Green and Perry, 2007):

$$m_r(0) = A_d C_d \left\{ 2 \frac{P_{ambient}^{2/\gamma}}{P_o^{1-2/\gamma}} \rho_v \frac{\gamma}{\gamma+1} \left[1 - \left(\frac{P_{ambient}}{P_o}\right)^{(\gamma-1)/\gamma} \right] \right\}^{1/2}$$
Equation 9-2

Where,

 $m_r(0)$ = gas mass release rate at time zero [kg/s]; M_w = gas molecular weight [kg/kg·mole]; and, P_o = gas pressure upstream of the orifice [Pa].

Where, r_{v} denotes the vapor density [kg/m³] at standard temperature and pressure. Again, Equation 9-29, just as in the case of w_0 appearing in Equation 9-26, is an expression of the maximum mass release rate under their respective release regimes.

Alternatively, the following time-dependent expression for the mass outflow may be used to obtain the average mass release rate:

$$m_r(t) = \frac{A_o C_o P_o}{Z R T_o} \left[1 + \tau \left(\frac{\gamma - 1}{2}\right) \left(\frac{2}{\gamma + 1}\right)^{\frac{\gamma + 1}{2(\gamma - 1)}} \right]^{2\gamma/(1 - \gamma)}$$

 101 P_{critical} should not be confused with the critical pressure, P_c, associated with the critical point on a temperaturevolume diagram for a particular substance.

Equation 9-30

9

Where,

$$\boldsymbol{\tau} = \frac{A_o}{V} (\boldsymbol{\gamma} \, \boldsymbol{R} \, \boldsymbol{T}_o)^{1/2} \boldsymbol{t}$$

and,

t = time following the beginning of unchoked flow [s],

- *Z* = compressibility factor [dimensionless];
- R = gas constant [8314.39 N/m·kg-mole·K];
- $T_o =$ gas temperature upstream of the orifice [K];
- V = internal tank volume [m³].

The *average* vapor release rate, $E \{m_r(t)\}$ in the time period [0,T] is then computed by evaluating Equation 9-32.

$$E\{m_{r}(t)\} = \frac{1}{T} \int_{0}^{T} m_{r}(t) dt = \frac{2 A_{o} C_{o} P_{o}}{Z R(1+\gamma) T_{o}} \left\{ 1 - \left[1 + \frac{A_{o}}{V} (\gamma R T_{o})^{1/2} T\left(\frac{\gamma-1}{2}\right) \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}} \right]^{2\gamma/(1-\gamma)} \right\}$$

The expressions presented above for the vapor mass rate of outflow are applicable only to tanks where the inner diameter is much greater than the diameter of the outlet orifice. If the analysis involves leakage from a length of process pipe, then the model described below should be used to estimate the vapor mass outflow rate.

9.5.2.2 VAPOR OUTFLOW FROM BREACH OF A PIPELINE

$$m_r(t) = \frac{m_r(0)}{1+\alpha_P} e^{-\frac{t}{(\alpha_P^2\beta_P)}} + \frac{W_o}{\beta_P} e^{-\frac{t}{\beta_P}}$$
Equation 9-33

The time-varying release rate of gas or vapor from a pipeline rupture is estimated using the following expression (Bell, 1978; Wilson and Angle, 1979): Where,

 $m_r(t) =$ gas mass release rate at time t [kg/sec]; t = time since the pipeline rupture [sec]; $W_o =$ total mass of gas in the pipe length [kg]; and, $b_p =$ a constant expressed as

$$\beta_P = 2(\gamma f)^{1/2} L^{3/2} / 3 \nu_o D^{1/2}$$

f	=	pipe friction factor [dimensionless];
D	=	pipe diameter [m];
L	=	pipe length [m]; and,
v_o	=	speed of sound in the pipeline gas [m/s]

 $v_o = \left(\gamma R T_f / M_w\right)^{1/2}$

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Equation 9-35

Equation 9-31

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 T_f = final temperature of gas release just after leaving the orifice [°K];

 a_p = dimensionless parameter given as:

$$\alpha_p = W_o / \left[\beta_p m_r(0) \right]$$
 Equation 9-36

Equation 9-37

 $W_o =$ total initial mass of gas [kg] given by

$$W_o = \pi D^2 P_o L M_w / (4 R T_o)$$

The variable T_f represents the final temperature of the gas as it first accelerates towards the sonic velocity at the orifice, and then decelerates after passing into the atmosphere. If the gas is assumed to exhibit ideal behavior, there will be no Joule-Thompson cooling; hence $T_f = T_o$.

To calculate the *average* vapor release rate, $E \{m_r(t)\}$, in the time period [0,*T*], use Eq. 9-38 below.

$$E\{m_{r}(t)\} = \frac{1}{T} \int_{0}^{T} m_{r}(t) dt = \frac{m_{r}(0)\alpha_{p}^{2}\beta_{p}}{T(1+\alpha_{p})} \left(1 - e^{-\frac{T}{(\alpha_{p}^{2}\beta_{p})}}\right) + \frac{W_{o}}{T} \left(1 - e^{-\frac{T}{\beta_{p}}}\right)$$
Equation 9-38

When loss of liquid containment results from a localized breach in a self-contained storage vessel, the mass flow rate of liquid out of the orifice may be computed as a function of the upstream pressure. This time-dependent pressure term, in turn, depends on:

- Vapor partial pressure;
- Hydrostatic head above the leak; and
- Pressure head induced externally by a mechanical device such as a compressor.

Assuming that the system pressure input to the code, P_{sys} , reflects the pressure head from the compressor, the first two pressure terms may be calculated. An upper bound on the release duration may be obtained by neglecting terms (1) and (3), which permits some reasonable values for the time intervals to be established.

9.5.2.3 OUTFLOW FROM A CYLINDRICAL TANK

The time-dependent mass flow rate of an incompressible fluid out of an upright cylindrical tank can be derived. Beginning with the Bernoulli equation expressed in the form:

$$\frac{\Delta u_b^2}{2} + g\Delta z + \frac{\Delta p}{\rho} = \mathbf{0}$$
 Equation 9-39

Where, in the MKS system, g_c becomes $(kg)(m)/(N)(sec^2)$ or $g_c \equiv 1$, and g denotes the local value for the acceleration of gravity. The variables u_b , z, r, and P represent the fluid bulk speed, fluid free surface elevation above ground level, fluid density, and pressure experienced at the orifice centerline, respectively.

<u>Note:</u> Δz denotes the distance between the fluid free surface level within the tank and the orifice elevation above ground, and by the convention chosen, the D operator represents the difference in going from the interior of the vessel to the outer ambient environment. For the sake of simplicity, it is assumed that internal and external pressure terms remain constant throughout the release duration. Therefore:

$$egin{aligned} \Delta u_b &= u_{b_{inside}} - u_{b_{outside}} \ \Delta z &= z - z_o \ \Delta p &= p_{inside} - p_{outside} = p_{system} + p_{vapor} - p_{ambient} \end{aligned}$$

Equations 9-40 through 9-42

with the orifice elevation denoted by z_o and the system pressure, saturated vapor pressure, and ambient pressure represented by P_{system} , P_{vapor} , and $P_{ambient}$, respectively.

Further assuming that u_b within the tank as well as all pressure terms are constant with respect to time, Equations 9-40 through 9-42 may be cast into a differential form with respect to time *t*:

$$-u_b \frac{d_{u_b}}{dt} + g \frac{dz}{dt} = \mathbf{0}$$
 Equation 9-43

Where, u_b now represents the bulk fluid outflow speed.

$$\frac{dm_o}{dt} = \rho A_o u_b - \frac{du_b}{dt} = \frac{1}{\rho A_o} \frac{d^2 m_o}{dt^2}$$
Equation 9-44

The quantity of greatest interest is the total mass outflow m_o as a function of time. In order to recast the equation as a differential equation in m_o , the first step is to recognize that the mass release rate dm_o/dt may be expressed in terms of the instantaneous flow velocity, as shown in Equation 9-44, with A_o representing the cross-sectional area of the orifice. Once an expression is obtained for dz/dt in terms of differentials of m_o , the form of an ordinary differential equation.

Equation 9-45 represents the formula for computing the volume of liquid inventory remaining in the tank at time t:

$$V_l(t) = \frac{\pi D^2 z_l(t)}{4} = \frac{m_l}{\rho} - \frac{dz_l}{dt} = -\frac{4}{\rho \pi D^2} \frac{dm_l}{dt} = \frac{4}{\rho \pi D^2} \frac{dm_o}{dt}$$
 Equation 9-45

Where, $V_l(t)$ and $m_l(t)$ represent the volume and mass inventory of liquid remaining inside the tank, respectively, at time *t* while r and D denote the liquid density and diameter of the tank. Substituting this last expression obtains:

$\frac{1}{\rho A_o^2} \frac{dm_o}{dt} \frac{d^2m_o}{dt^2} - \frac{4g}{\pi D^2} \frac{dm_o}{dt} = 0$	Equation 9-46
$\frac{d^2m_o}{dt^2} = \frac{-4g\rhoA_o^2}{\pi D^2}$	Equation 9-47

Final reconfiguration of this equation yields Equation 9-47.

In order to solve the above second order differential equation, two initial conditions are required. One condition is that at time zero, $m_o(t=0) = 0$. The other condition is derived by solving the Bernoulli equation directly for the special case at time zero since $z(t=0) = z_i$ representing the initial liquid level above the outlet centerline axis is given, yielding:

$$\frac{dm_o(t)}{dt}\Big|_{t=0} = \rho A_o \sqrt{2\left[g(z_i - z_o) - \frac{\Delta p}{\rho}\right]}$$
 Equation 9-48

Now that the two initial conditions to the second order linear ordinary differential equation are known, the unique solution is given by Equations 9-49 and 9-50.

$$\frac{dm_o(t)}{dt} = -\frac{4g\,\rho\,A_o^2}{\pi D^2}t + \rho\,A_o\sqrt{2\left[g(z_i - z_o) - \frac{\Delta p}{\rho}\right]}$$
Equation 9-49

$$m_{o}(t) = -\frac{2g \rho A_{o}^{2}}{\pi D^{2}} t^{2} + \rho A_{o} \sqrt{2 \left[g(z_{i} - z_{o}) - \frac{\Delta p}{\rho} \right]} t$$
 Equation 9-50

Only times for which $dm_o/dt>0$ are physically relevant, and since dm_o/dt is monotone decreasing we have the duration of the release given by $t=t_{max}$ satisfying

$$\frac{dm_o(t)}{dt}\Big|_{t=t_{max}} = \mathbf{0}$$
 Equation 9-51

Solving for t_{max} in the Equation above yields:

$$t_{max} = \frac{\pi D^2}{4 g A_o} \sqrt{2 \left[g(z_i - z_o) - \frac{\Delta p}{\rho} \right]}$$
 Equation 9-52

9.5.2.4 OUTFLOW FROM A SPHERICAL TANK

Although a spherical tank is a seemingly benign perturbation away from a simple cylindrical tank, this particular geometry results in a much more complicated expression for the mass flow rate of liquid out of the vessel. The volume of liquid inventory as a function of liquid free surface elevation is given by:

$$V_l(t) = \frac{2}{3}\pi R^3 \int_0^\alpha \sin\varphi \, d\varphi + \frac{1}{3}\pi d^2(z-R) = \frac{2}{3}\pi R^2 z + \pi z (2R-z)(z-R)$$
 Equation 9-53

Where

$$\begin{aligned} \alpha &= \cos^{-1}(1 - z/R) \\ (0 &\le \cos^{-1}(x) \le \pi) \forall x \end{aligned}$$
 Equation 9-54

and R, z, and d represent the tank radius, elevation of the liquid free surface above the bottom of the tank, and one half the chord length of the liquid free surface, or

$$d = \sqrt{R^2 - (R - z)^2} = \sqrt{z(2R - z)}$$
 Equation 9-55

The change in liquid level, z, can be related to the mass outflow rate using the time derivative of Equation 9-53:

$$\frac{dV_l(t)}{dt} = -\frac{1}{\rho}\frac{dm_o}{dt} = -\pi \left\{ 3z^2 - 6Rz + \frac{4}{3}R^2 \right\} \frac{dz}{dt}$$
 Equation 9-56

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$$\frac{dz}{dt} = \left[\pi\rho\left(3z^2 - 6Rz + \frac{4}{3}R^2\right)\right]^{-1}\frac{dm_o(t)}{dt}$$
Equation 9-57

Finally, substituting Equation 9-57 and Equation 9-44 into Equation 9-43, yields

$$\frac{1}{\rho A_o^2} \frac{d^2 m_o}{dt^2} - \frac{g}{\pi \left(3z^2 - 6Rz + \frac{4}{3}R^2\right)} = \mathbf{0}$$
 Equation 9-58

By noting that the mass of outflow at time *t* is expressed as $m_o=m_{tot} - rV_l(t)$ where m_{tot} is the total mass of liquid inventory inside the vessel at time *t*=0 and inspecting the form of the expression for $V_l(t)$ given in Equation 9-53, m_o is a cubic polynomial in the variable z and hence a closed-form analytic solution exists for z as a function of m_o .

Therefore, Equation 9-58 can be recast into an ordinary differential equation in the one dependent variable, m_o . The resulting equation, however, is complicated, highly nonlinear in m_o , and does not lend itself to a solution without the use of rather involved numerical techniques.

An alternate approach is to compute an average flow rate by simply taking the total mass of liquid that can flow out of the vessel and divide by the time t_{max} required for the liquid level to fall from the initial elevation z_i to the elevation of the discharge orifice, z_o . This time is expressed in Equation 9-59.

$$t_{max} = \frac{\pi}{15C_o A_o} \sqrt{\frac{2(z_i - z_o)}{g}} \left(5D \, z_i + 10D \, z_o - 3z_i^2 - 4_{z_i z_o} - 8z_o^2 \right)$$
 Equation 9-59

See Hart and Sommerfeld (1993) for additional details of this derivation.

The aforementioned equations in Sections 9.5.2.1 through 9.5.2.4 are limited to the assumptions in their derivation and/or the conditions under which they were developed. Prior to employing these equations to determine the phenomenology of a specific system or process, the analyst should demonstrate that the application domain of the equations is not exceeded.

9.5.2.5 OUTFLOW FROM PROCESS VESSELS OF OTHER VARIOUS SHAPES

Equations for the drainage time of vessels for other geometrical shapes are presented in Lee and Sommerfeld (1994). This is a starting point for safety analysts in establishing techniques for this type of problem.

9.5.3 DENSE GAS TOXIC CHEMICAL RELEASE AND DISPERSION

Toxic chemical releases are dense or heavy gas releases when their molecular weight is greater than that of air (28.97 g/mol for dry air), or the gas is cryogenic or very cold. Dense gas releases can potentially also occur with gases that have sufficient aerosol content. However, a gas with a molecular weight greater than that of air and/or exhibiting cryogenic properties does not always result in dense gas behavior. To exhibit dense gas behavior, the dense gas blanket needs to be of a sufficient volume to generate its own turbulence field. Therefore, the determination of whether a released material establishes a dense gas flow pattern requires the knowledge of a key parameter, the calculated Bulk Richardson number, which is a relative measure of the potential energy of the cloud with respect to the mechanical

turbulent energy of the atmosphere. The Bulk Richardson number is the critical parameter that provides the benchmark for dense gas behavior. The criterion for dense gas dispersion is that the Bulk Richardson number has to be greater than 50; which is a function of volume, temperature and molecular weight of the gas relative to the gases in the atmosphere.

Initially, a dense gas cloud of material will be undiluted (not mixed with air) and will drop to the ground and flow along the topography downhill or in the direction of the wind, for the most part, although a small part of it may flow uphill or upwind as well, because of gravitational slumping. For this reason, an accurate depiction of the near-field local topography is extremely important to ensure meaningful results from dense gas modeling. Vertical dispersion will be severely restricted for a dense gas, due to gravitational effects, and ambient air will be entrained through the sides of the plume. Thus, the plume shape will take on a pancake-like appearance; further distorted by local topographic anomalies.

Early models of heavy or dense gas dispersion used the Gaussian Line Source model, in which the material was assumed to spread out from a line-source (i.e., formed into a plume), with a Gaussian distribution in the vertical and horizontal directions. The σ_y and σ_z values were assumed the same as given above. These models ignored many important physical phenomena, were generally unsatisfactory, and quickly fell into disuse. More modern models (e.g., DEGADIS, SLAB, HPAC, and HGSYSTEM) took into account phenomena that were not included in the Gaussian Line Source model. These phenomena include:

- Gravitational slumping of the heavy or dense gas and accompanying lateral spreading;
- Stratification of the heavy or dense gas, which tends to dampen turbulence and air entrainment; and
- Heat exchange between the cloud of gas and the ground, which may also cause phase changes.

A more exhaustive discussion of the equations describing the heavy gas model and their use is beyond the scope of this Handbook. Due to the complexity of dense gas dispersion, these codes should not be used as a "black box" without a thorough understanding of the phenomena governing dense gas flows.

The analyst is recommended to use one of the standard computer codes for evaluation of heavy gas dispersion, inclusive of ALOHA Version 5.4.6. The dense gas dispersion calculations used in ALOHA are based on the DEGADIS model (Havens and Spicer 1985, EPA-450/4-89-019). DEGADIS, in turn, is an adaptation of the Shell HEGADIS model described by Colenbrander (Colenbrander 1980, Colenbrander and Puttock 1983). It also incorporates some techniques used by van Ulden (van Ulden 1974, 1983). ALOHA incorporates a decision algorithm to choose between the dense gas and neutrallybuoyant Gaussian models, using the critical Richardson Number as the criterion for distinguishing between passive or non-passive dispersion. The critical Richardson Number is a function of the density of the pollutant, the wind speed, and the release rate. Therefore, the release needs to be of significant magnitude to exhibit dense gas characteristics. As the dense gas plume is dispersed downwind, neutrallybuoyant ambient air begins to mix in, and when the critical Richardson Number decreases to below 50, the plume begins dispersing as a neutrally buoyant gas; that is, entrainment of ambient air as the plume is transported downwind leads to the dense gas plume becoming a neutrally buoyant plume. ALOHA then switches to the neutrally-buoyant Gaussian model. Since the entrainment of air in the sides of the plume generates significant turbulence, dense gas dispersion is actually greater than neutrally buoyant dispersion at 95-percentile meteorological conditions of F stability and 1 meter/second. This is discussed in more detail in the Technical Report NRSD-15-TC01. Section F.8 of this report presented the following conclusions relative to the CW:

- 1. The ALOHA χ/Q values, considering the building wake effects, are consistent with the default radiological χ/Q value specified in DOE-STD-1189-2008.
- 2. The aerodynamic effect of buildings on dispersion is approximately an order of magnitude larger, and is much larger than the dry deposition effect;
- 3. The dispersion from negatively-buoyant, dense gas releases under light wind stable meteorological conditions is greater than neutrally-buoyant releases; and
- 4. The default χ/Q value is not sensitive to release durations.

Some dense gas models (e.g., HGSYSTEM, HPAC) can be used for area sources (e.g., pools) as well as line source applications.

9.5.4 NON-PRESSURIZED LIQUID RELEASE

Source term determinants from liquid releases (e.g., evaporation rate, aerosolization rate) have been addressed in detail in Chapter 3 and Chapter 5. For non-pressurized, non-energetic liquid chemical releases, it can be reasonably assumed that all aerosols immediately liquefy into a sub-cooled liquid puddle. For cryogenic non-pressurized liquids, dense gas dispersion principles still apply. The non-varying source term is commonly based on an evaporation rate, which is a function of wind speed, ambient temperature, solar insolation and an assumed puddle depth of 1 cm. This puddle depth is used in all chemical transport and diffusion codes that have evaporation algorithms and is considered a reasonable assumption by the technical community. Thus, the puddle surface area determines the amount of chemical available to be evaporated for subsequent atmospheric transport and diffusion, and this release continues until the puddle is totally evaporated.

Controls can be used to reduce the source term from this type of release. Impoundment basins allow the chemical depth to increase, thus reducing the surface area of the puddle and subsequent evaporation rate. Floating balls in such impoundment basins have also been used to further reduce the puddle surface area.

Non-pressurized, non-energetic liquid chemical releases with varying release rates cannot be as easily addressed by conventional Gaussian models since the source term can vary with time as the parameters that control evaporation may vary. However, an iterative technique can be applied through successive time steps to account for varying evaporation rates while keeping the atmospheric conditions that affect transport and diffusion constant.

ALOHA Version 5.4.6 has the capacity to calculate toxic chemical consequences from non-pressurized liquid releases, employing one of two methods for finding the evaporation rate depending upon whether or not the puddle is close to its boiling point. It applies Brighton's formulation (Brighton 1985) when the average puddle temperature is sufficiently below its boiling point, and an energy balance method when the puddle approaches its boiling point. ALOHA also allows puddles to transition from boiling to non-boiling, or non-boiling to boiling. It constantly compares the evaporation rate calculated with the boiling puddle model with the evaporation rate calculated with Brighton's model at its temperature limit, and then selects the method that yields the larger evaporation rate.

ALOHA calculates the magnitude of six energy sources to establish puddle temperature. These include:

• Net short wave solar flux into the puddle;

- Long wave radiation flux down from the atmosphere;
- Long wave radiation flux upward into the atmosphere;
- Heat exchanged with the substrate by thermal conduction;
- Sensible heat flux from the atmosphere; and,
- Heat lost from the puddle by evaporative cooling.

An example scenario for a tank release is provided in the ALOHA technical documentation (Example 1, Part 1, ALOHA, August 2013).

Section 9.5.1 discusses the complex phenomenology associated with the release of pressurized liquids to the atmosphere and this section discusses non-pressurized liquid releases. Both phenomenologies involve the evaporation of liquid from a pool. In the event of a boiling liquid pool, two simple expressions for obtaining a first-order conservative approximation to the mass evaporation rate are presented, namely, convective boiling and conductive boiling.

The following subsections provide the analyst with some of the complex equations to account for the phenomenology of the evaporation of a puddle formed by pressurized and non-pressurized liquid releases. In addition, various evaporation rate calculations are presented for nitric acid and carbon tetrachloride to emphasize the complexities of accurately assessing evaporation rates.

9.5.4.1 CONVECTIVE BOILING

Equation 9-60 presents a technique to calculate the mass evaporation rate (m_v) due to convective boiling:

$$m_{\nu} = k_{air} \frac{A_p}{L_p} N u_L \frac{(T_{air} - T_b)}{H_{\nu}}$$
 Equation 9-60

Where,

$m_{\rm v}$	=	mass evaporation rate (kg/m ^{2} s);
k _{air}	=	thermal conductivity of air (kJ/m °K);
A _p	=	pool surface area (m ²);
L _p	=	pool effective diameter in the wind direction (m);
Pr	=	$\mu_{air}c_{p_{air}}/k_{air}$
$\mu_{ m air}$	=	viscosity of air at ambient temperature (poise);
c _{pair}	=	heat capacity of air at constant pressure (kJ/kg $^{\circ}$ K);
T_{air}	=	air temperature (°K);
T_b	=	liquid ambient boiling temperature (°K); and,
H_{v}	=	liquid latent heat of vaporization (kJ/kg).

and,

$$Nu_{L} = \left\{ \begin{array}{c} 0.664 \ Pr^{1/3} Re_{L}^{1/2} for \ Re_{L} \leq 320,000 \\ 0.037 \ Pr^{1/3} \ (Re_{L}^{0.8} - 15200) for \ Re_{L} > 320,000 \end{array} \right\}$$
Equation 9-61

9.5.4.2 CONDUCTIVE BOILING

Equation 9-62 presents a technique to calculate the mass evaporation rate (m_v) due to conductive boiling:

$$m_{v} = \frac{k_{s}A_{p}(T_{air}-T_{b})}{H_{v}\sqrt{\pi\varepsilon t}}$$
 Equation 9-62

Where,

ks	=	thermal conductivity of ground surface (kJ/m °K);
A _p	=	pool surface area (m ²);
t	=	time s;
T_{air}	=	air temperature (°K);
T_b	=	liquid ambient boiling temperature (°K); and,
Tg	=	ground surface temperature (°K);
3	=	$k_s/(\rho_s c_{p_s})$
ρ_s	=	density of ground surface (kg/m ³);
c _{ps}	=	heat capacity of ground surface at constant pressure (kJ/kg °K); and
H_v	=	liquid latent heat of vaporization (kJ/kg).

Conductive boiling, or conductive heat transfer from the ground, is generally the dominant driving mechanism for boiling in the case of most chemical liquids. However, in the case of some cryogenic releases (e.g., sub-cooled anhydrous ammonia, chlorine), the ground conduction is dramatically reduced if there is moisture present in the substrate since a layer of ice has a thermal conductivity much lower than that of most ground surface substances and it quickly forms at the base of the pool. Furthermore, a thin vapor film frequently forms at the interface between the ground surface and the pool, which further reduces the effective conductivity in that region and limits the amount of heat transfer into the pool. Therefore, Equation 9-62 is generally quite conservative during the majority of the boiling regime and most accurately reflects true vaporization conditions at the first instant that the liquid comes into contact with the ground surface. Conversely, Equation 9-60 is more representative of the steady-state vaporization of a pool once the ground surface temperature drops below the boiling temperature of the liquid.

9.5.4.3 NITRIC ACID AND CARBON TETRACHLORIDE POOL EVAPORATION RATES

An alternative correlation that is commonly used in estimating pool evaporation rates and that has been demonstrated to provide lower estimates of pool evaporation rate for a nitric acid and carbon tetrachloride spill is presented. Furthermore, example hand calculations have been provided for the same two releases

based on simple models of heat and mass transfer and compared to the experimental correlations to obtain even a less conservative estimate for the pool evaporation rate.

The following calculations employ a relatively simple means of assessing the accuracy of the pool evaporation source term calculations. Illustrative examples are given that assume liquid nitric acid and liquid carbon tetrachloride spill onto the ground surface and form a pool that will be subject to evaporative sub-cooling. The mass evaporation rate is determined by the following factors:

- 1. Molecular diffusion and mass transport;
- 2. Conductive heat transfer;
- 3. Radiative heat transfer;
- 4. Convective heat transfer;
- 5. Bulk liquid heat transfer; and
- 6. Internal heat content.

The following detailed source term calculations treat provide an upper bound on the potential impact of an evaporating pool in the case that all six evaporation source term factors were considered.

9.5.4.3.1 Nitric Acid Pool Evaporation

Vapor is entrained by air flowing over the surface of the pool. The rate of mass transfer is expressed in Equation 9-63:

$$m_{v} = -\frac{k_{m} P_{t} M_{w}}{RT_{s}} ln \left[1 - \frac{P_{v}}{P_{t}}\right]$$
 Equation 9-63

Where,

k_{m}	=	mass transfer coefficient (m/s);
Pt	=	sum of atmospheric pressure and partial pressure of chemical vapor (Pa);
$M_{\rm w}$	=	molecular weight of chemical (kg/mole);
R	=	ideal gas constant = 8.31424 J/mole·K;
Ts	=	pool surface temperature (K);
$\mathbf{P}_{\mathbf{v}}$	=	chemical vapor pressure at temperature T _s (Pa).

Kulmala (1988) and Barrett and Clement (1988) provide detailed derivations of this expression and Studer et al., 1988 provide a technique for practical use of this expression in the context of pool evaporation.

Equation 9-63 is a specific instance of the mass transfer due to diffusion through a transpired boundary layer. A more general form is presented in Kays and Crawford (1987). While the transpired boundary layer model is not needed for the low vapor pressure associated with HNO₃, CCl₄ evaporates much more rapidly and therefore the transpired boundary layer model is necessary. This will be shown in Section 9.5.4.3.2. It is convenient, then, to operate with the single model for CCl₄ and apply it to HNO₃ as a degenerate case. Mass evaporation equations are part of standard diffusion boundary layer literature and

can be found in numerous texts (see Kays and Crawford, 1987; Bergman et al., 2001).

The mass transfer coefficient may be related to the Sherwood number (Sh), coefficient of diffusivity of the chemical in air (D_{ba}) and the effective path length of air flowing over the pool, which is usually the effective diameter of the pool (L), as shown in Equation 9-64:

$$k_m = Sh \frac{D_{ba}}{L}$$
 Equation 9-64

The diffusion coefficient may be approximated by a group contribution method attributed to Fuller et al. (Reid et al., 1987), as shown in Equation 9-65:

$$D_{ba} = \frac{10^{-3} T_a^{1.75} M_{w_{ab}}}{P_a \left[(\Sigma v)_a^{1/3} + (\Sigma v)_b^{1/3} \right]^2}$$
Equation 9-65

where, the sums apply to the atomic diffusion volumes for each component in the chemical molecule and,

$$M_{w_{ab}} = \frac{M_{w_a} + M_{w_b}}{M_{w_a} M_{w_b}}$$
Equation 9-66

The subscripts b and a, refer to the chemical species and air, respectively. In particular, M_{wb} and M_{wa} denotes the molecular weight of nitric acid and air, respectively.

Assuming the air temperature is 40 degrees °C (313.15 °K) and M_{wb}=63.02 g/mole, M_{wa}=28.97 g/mole, $(\sum v)a = 20.1$ and,

$$(\sum \nu)_b = \nu(H) + \nu(N) + 3\nu(0) = 1.98 + 5.69 + 3(5.48) = 24.11$$
 Equation 9-67

and substituting the above values into Equation 9-65 yields Equation 9-68 for the diffusion coefficient and Equation 9-69 for the maximum pool length.

$$D_{ba} = 1.64 \times 10^{-6} \ m^2/s$$
Equation 9-68
$$L_{max} = \sqrt{\frac{4x(pool\,area)}{\pi}}$$
Equation 9-69

Instead of using the effective length (L), conservatively take L to be the diameter of the pool and assume a pool area of 91 m²; L_{max} becomes 10.8 m.

The Sherwood number may be expressed as in Equation 9-70:

$$Sh = 0.037(Re_L^{0.8} - 15200)Sc^{1/3}$$
 Equation 9-70

Where, the Schmidt number (Sc), and the Reynolds number (Re_L) are expressed in Equations 9-71 and 9-72:

$$Sc = \frac{\mu_v}{\rho_v D_{ba}}$$
 Equation 9-71

Equation 9-72

 $Re_L = \frac{\rho_\infty u_\infty L}{u_\infty}$

With,

$ ho_\infty$	=	main stream density (kg/m ³);
u∞	=	main stream ambient wind speed (m/s); and,
μ_{∞}	=	main stream viscosity (poise).

The Schmidt number arises when considering a laminar boundary layer on a flat plate in which the diffusion was occurring as a result of some mass-transfer condition at the surface. The concentration and velocity profiles will have the same shape when the dynamic viscosity $v_{\infty} = \mu_{\infty}/\rho_{\infty}$ satisfies $v_{\infty}=D_{ba}$ or $v_{\infty}/D_{ba}=1$.

The Schmidt and Reynolds numbers are many times calculated with the fluid properties at infinity in boundary layer coordinates rather than vapor properties (see Bergman et al., 2011). Occasionally one will find the fluid properties calculated at the average of the infinity and wall values. Using the outer fluid properties will significantly affect the resultant value for the Sherwood number in the case of cryogenic spills, for instance, where the thermodynamic properties are sensitive to small changes in ambient conditions.

The above correlation for the Sherwood number in Equation 9-70 only holds true for Re>15,200. Furthermore, the mixed boundary layer, the Sherwood number correlation is not valid for Sc<0.6 (see Bergman et al., 2011). Although Equation 9-70 expression for the Sherwood number is commonly quoted in analyses studying the evaporation of liquids, it was derived from studying the heat transfer coefficient of a dry body. Therefore an alternative, and presumably more appropriate empirical technique to express for the Sherwood number in the event of a liquid spill based on the work of Smolsky and Sergeyev in the area of heat and mass transfer from free surfaces of liquids into a heated turbulent stream is shown in Equation 9-73:

$$Sh = 0.094 Re^{0.8}Sc^{0.33}Gu^{0.2}$$

Where,

$$Gu = \frac{T_{\infty} - T_{w}}{T_{\infty}}$$
 Equation 9-74

Gu denotes the Guhmann number with T_∞ and T_w denoting the mainstream and liquid surface temperature, respectively.

This expression is based on experimental studies of the heat and mass transfer from the free surfaces of various liquids into a heated turbulent air stream. Equation 9-74 is therefore recommended as the more appropriate estimate of the Sherwood number in the case of an evaporating pool. However, estimates of the Guhmann number are vulnerable to high degrees of uncertainty. In an effort to circumvent this issue, the Sherwood number should be estimated using Equation 9-70 with the dynamic viscosity evaluated as the average of the main steam (i.e., air) and boundary layer vapor (i.e., chemical) dynamic viscosities in the definitions of the Schmidt (Sc) and Reynolds (Re) numbers, as depicted in Equations 9-75 through 9-77:

$$\overline{Re}_{L} = \frac{u_{\infty}L}{\overline{v}}$$
Equation 9-75
$$\overline{Sc} = \frac{\overline{v}}{D_{ab}}$$
Equation 9-76
$$\overline{v} = \frac{1}{2} (v_{air} + v_{vapor})$$
Equation 9-77

Applying a nitric acid vapor density of 2.18 kg/m³, u_{∞} =5 m/s and, due to limited data on HNO₃, approximating the vapor viscosity by the gas viscosity for nitrous oxide at the pool surface temperature of 20°C given to be 1.46E-2 c_p or 1.46E-5 kg/m·s yields v_{vapor} = 6.7E-6 m²/s. The outer fluid properties make use of v_{air} =1.72E-5 m²/s, for air at 313K and standard atmospheric pressure, and the pool diameter length scale L_{max} = 10.8 m, the averaged Schmidt (Sc) and Reynolds (Re) numbers are recalculated as shown in Equation 9-78.

$$\overline{v} = 1.19 \times 10^{-5}$$

 $\overline{Sc} = 7.29$
 $\overline{Re}_L = 4.52 \times 10^6$ Equation 9-78

Finally, substituting all the above intermediate results into Equation 9-70 obtains:

$$Sh = 1.4 \times 10^4$$
 Equation 9-79

The mass transfer coefficient therefore becomes the following from Equation 9-64.

$$k_m = 2.13 \times 10^{-3} m/s$$
 Equation 9-80

Therefore, the mass transfer rate is estimated to be the following value as calculated from Equation 9-81:

$$m_{tran} = \frac{-(2.11 \times 10^{-3} m/s)(101325 Pa + 413.2 Pa)(0.06302 kg/mole)}{(8.314 J/mole °K)(293.15°K)} ln \left[1 - \frac{413.2 Pa}{101325 Pa}\right]$$

= 2.29 × 10⁻⁵ kg/m²s
= 0.0229g/m²s Equa

The total mass transfer rate is simply the product of m_{tran} and the pool area of 91 m², as shown in Equation 9-82:

$$m_v(HNO_3) = 2.08g/s$$

9.5.4.3.2 CARBON TETRACHLORIDE POOL EVAPORATION

The diffusion coefficient can be estimated by means of the group contribution method detailed above, with

 $M_{w_b}=153.83$ g/mole, $M_{w_a}=28.9$ g/mole, $(\Sigma v)_a=20.1$ and

$$(\sum v)_b = v(C) + 4v(Cl) = 16.5 + 4(19.5) = 94.5$$
 Equation 9-83

Finally, substituting the above values into Equation 9-65 yields Equation 9-84.

$$D_{ba} = 8.93 \times 10^{-6} m/s$$

Equation 9-84

Equation 9-81

Equation 9-82

Assuming a pool area of 73 m², the length scale L_{max} becomes 9.64 m from Equation 9-69. Assuming a CCl₄ vapor density of 5.32 kg/m³, u_{∞} =5 m/s, and the vapor viscosity at the pool surface temperature of 20°C determined to be 9.66E-3 c_p or 9.66E-6 kg/m·s yields $v_{vapor}=1.82E-6 \text{ m}^2/\text{s}$.

The outer fluid properties, $v_{air}=1.72E-5$ m²/s for air at 313K and standard atmospheric pressure, the averaged fluid properties Schmidt (Sc) and Reynolds (Re) numbers are calculated to be what is shown in Equation 9-85.

$$\overline{v} = 9.51 \times 10^{-6}$$

$$\overline{Sc} = 1.06$$

$$\overline{Re}_L = 5.07 \times 10^6$$
Equation 9-85

Substituting all the above intermediate results into Equation 9-70 yields:

$$Sh = 8.15 \times 10^3$$
 Equation 9-86

The mass transfer coefficient therefore becomes:

$$k_m = 7.55 \times 10^{-3} m/s$$
 Equation 9-87

Therefore, the mass transfer rate is estimated to be what is shown in Equation 9-88.

$$m_{tran} = \frac{-(7.5 \times 10^{-3} m/s)(101325 Pa + 2 \times 10^{4} Pa)(0.15383 kg/mole)}{(8.314 J/mole °K)(293.15°K)} ln \left[1 - \frac{2 \times 10^{4} Pa}{101325 Pa}\right] = 1.27 \times 10^{-2} kg/m^{2} s$$

= 12.7g/m²s Equation 9-88

Using a pool area of 73 m², the total mass transfer rate is simply the product of m_{tran} and the pool area, as shown in Equation 9-89:

$$m_v(CCl_4) = 0.928kg/s$$
 Equation 9-8

In contrast to nitric acid, the boiling temperature of CCl₄ is closer to that of ambient temperature and the effects of bulk liquid heat transfer and internal heat content play a more important role in the overall mass evaporation rate. Both of these factors serve to mitigate the release rate to some extent. However, because of the greater volatility of CCl₄, solar radiation and convective heat transfer have a significant effect in terms of increasing overall mass evaporation rate.

No simple correlation has the capabilities of accurately incorporating all the various thermal phenomena taking place in the event of a volatile liquid release. However, a simple correlation can provide a reasonable conservative estimate of the true evaporation rate.

Compare the evaporation correlation used in the CEI guidelines (TNO, 1979), as shown in Equation 9-90.

$$\dot{m} = 9 \times 10^{-4} A_p^{0.95} \frac{(MW)P_v}{T+273}$$

Where,

Equation 9-90

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 $\dot{m} = pool evaporation rate (kg/hr);$

 $A_p = pool area (m^2);$

MW = chemical molecular weight (g/mole);

 P_v = vapor pressure of the chemical at the characteristic temperature (kPa); and

T = characteristic pool temperature (°C).

with a similar closed-form expression described by Clewell (1983), as shown in Equation 9-91:

$$\dot{m} = 8 \times 10^{-2} u^{3/4} A_p Z (1 + 4.3 \times 10^{-3} T^2)$$
 Equation 9-91

Where, Z is the volatility factor of species x with respect to hydrazine expressed as such in Equation 9-92.

$$Z = \frac{(MW)_x P_{v_x}}{(MW)_{hydrazine} P_{v_{hydrazine}}}$$
Equation 9-92

Predicted evaporation rates for nitric acid and carbon tetrachloride at various ambient temperatures with a fixed pool surface area of 1 m^2 and an ambient wind speed of 5 m/s are provided in Figure 9-1 and Figure 9-2, respectively.

In the turbulent boundary layer, the mass transfer coefficient is proportional to $u^{0.8}$ and $L^{1.8}$, while in the TNO correlation, the mass transfer coefficient is proportional to $u^{0.8}$ and $L^{1.9}$. Accordingly, the TNO expression will be become progressively more conservative as the pool area increases and as the laminar region, where Sh is proportional to Re^{1/2}, increases.

As for the additional modes of heat transfer, evaporative cooling offsets heating effects due to ground conduction and solar radiation. For volatile liquids such as CCl₄, Clewell suggests a pool temperature decrease of 10-20 °C is not unreasonable due to evaporative cooling (Clewell, 1983). By setting the pool temperature equal to the air temperature, a conservative evaporation rate is maintained. This is equivalent to assuming a very large convective heat transfer coefficient between the pool and the air.

The standard turbulent boundary layer calculation also suffers from lack of data as the diffusion coefficients for CCl₄ vapor is calculated based on the chlorine diffusion volume, which, according to Perry's *Chemical Engineers' Handbook* (2008), is based on very little data. No data was found to directly compare to the calculated diffusion coefficients for HNO₃ as well.

Table 9-5 compares the results for the hand calculations, the TNO model, and the Clewell model in the case of the nitric acid and carbon tetrachloride evaporation rates. Although there is relatively good comparison among all three models in the case of nitric acid, there is a disparity among results in the case of carbon tetrachloride. The hand calculation is in itself conservative, but even after allowing for pool cooling and other mitigating features, the question as to whether simple correlations can be relied upon to yield conservative results for a wide class of chemicals remains unanswered.

The aforementioned equations in Sections 9.5.4.1 through 9.5.4.3 are limited to the assumptions in their derivation and/or the conditions under which they were developed. Prior to employing these equations to determine the phenomenology of a specific system or process, the analyst should demonstrate that the application domain of the equations is not exceeded.

These examples were chosen to dramatize the point that one should never blindly place faith in experimental correlations based on limited data.

as Applied to HNO ₃ and CCl ₄ .			
Model	HNO ₃ Evaporation Rate (g/sec)	CCl ₄ Evaporation Rate (g/sec)	
Hand Calculation	2.08	928	
TNO	1.53	342	
Clewell	2.82	606	

Table 9-5. Comparison of Results for Three Evaporation Models as Applied to HNO3 and CCl4.

HNO3 Pool Evaporation Rates

Wind Speed = 5 m/s, Pool Area Normalized to 1 m²



Figure 9-1. Comparison of Evaporation Rate Predictions for 60 Percent Solution of Nitric Acid with a 1 m² Pool Surface Area.



Wind Speed = 5 m/s, Pool Area Normalized to 1 m²



Figure 9-2. Comparison of Evaporation Rate Predictions for Carbon Tetrachloride with a 1 m² Pool Surface Area.

9.5.5 ENERGETIC EVENTS: FIRES, DEFLAGRATIONS, DETONATIONS, DELAYED IGNITION EXPLOSIONS, AND BLEVES

For toxic chemical dispersion and consequence energetic events analysis, the initial phase of such an event releases a volume of hot gases under high pressure. Hot gases rise through its' own buoyancy and expand rapidly until reaching equilibrium with atmospheric pressure, determining the plume initial dimensions and effective height of release. After reaching equilibrium with the ambient atmosphere, conventional atmospheric redistribution processes act on this plume, carrying it downwind as it continues to expand through turbulent diffusion in the horizontal and vertical planes.

Energy associated with the release, which includes a fire, deflagration, detonation, delayed ignition detonation, and BLEVE, require special analytical treatment. A BLEVE occurs during a fire event where the contained liquid in a vessel expands due to the sensible heat transfer to the inside of the vessel and eventually reaches a point where the internal pressure from the expanding vapor in the vessel exceeds the vessel's structural integrity and a violent explosion occurs.

Few atmospheric dispersion codes in common use at DOE facilities model atmospheric dispersion from energetic events. ERAD, applicable to radionuclide releases from HE, has been discussed in Chapter 6.

Special techniques and codes have been developed to determine the radiant heat and other impacts resulting from fires, deflagrations, and detonations. Deflagrations differ from detonations in that for deflagrations the pressure wave expands at less than the speed of sound. When chemical fires propagate at a speed that exceeds the speed of the sound, the propagation causes an overpressure in the atmosphere, which essentially moves the ambient atmosphere at a faster speed to a point downwind than it would normally move causing a compression wave, or overpressure. The detonation overpressure, which is measured in atmospheres, can be quite destructive. Detonations can be an immediate phenomenon, or can result hours after the release of a flammable gas when the chemical disperses to a concentration between its upper and LFLs and encounters an ignition source. The effects of overpressures on the CW, MOI and the public from either a delayed ignition detonation or immediate detonation are a function of its overpressure magnitude, the distance from the detonation (i.e., attenuation), and other mitigating factors (e.g., shielding from buildings).

Hydrogen is a by-product of radiolysis, and build-up of this lighter-than-air gas can lead to either deflagrations or detonations. Given this complexity, determination of the physics underlying hydrogen deflagrations or detonations has undergone much research. Table 4-2 and Section 4.3 provide some guidance on determining whether the hydrogen-air mixture is explosive, whether the propagation speed is sufficient to become a detonation, calculation of its energy and peak Chapman-Jouget pressure, and the consequences of a hydrogen detonation on SSC integrity and the health and safety of the facility worker, CW and the public. MELCOR and FLUENT codes can be employed to establish initial conditions and gas distribution of the detonation calculations.

ALOHA Version 5.4.6 and other peer-reviewed techniques and codes are required to determine the overpressures from a delayed ignition detonation, an immediate detonation, or a BLEVE. This version of ALOHA is in the DOE Central Registry and is capable of addressing the energetic events discussed in this subsection. It has the capacity to calculate toxic chemical consequences from pool fires, BLEVEs, flash fires or vapor cloud explosions, and jet fires.

ALOHA Version 5.4.6 only models combustion reactions and estimates the blast wave from unconfined vapor cloud explosions (e.g., fast deflagrations, detonations). Confined vapor cloud explosions generally

produce more damaging blast waves than unconfined or partially confined explosions.

The overpressure calculation utilizes the Baker-Strehlow-Tang (BST) model (Pierorazio et al. 2005), employing non-dimensional, empirically-derived blast curves to establish overpressure. Overpressure magnitude is a function of the flame front propagation speed and the mass of fuel involved in the reaction.

ALOHA Version 5.4.6 also models flame hazards associated with the combustion of liquids and gases. However, fire scenarios involving chemicals with flashpoints exceeding 300°F cannot be modeled. Two types of combustion are addressed in ALOHA: (1) a fuel mixed with air to form a cloud with concentrations within the flammability range; and (2) an overly-rich core of fuel that burns at its outer edges. Different methodologies are applied for estimating the threat zones for these two types of combustion events. ALOHA Version 5.4.6 employs solid flame models to compute thermal radiation hazards from fireballs, jet fires, and pool fires, where the flux of thermal radiation emitted from the surface of the flame is computed and the radiation impinging upon a distant target is determined.

ALOHA Version 5.4.6 has a BLEVE-fireball model based on studies of fireballs resulting from BLEVEs (CCPS, 1994). A fire thermally stresses a vessel causing the internal pressure to rise beyond the capacity of pressure relief valves, leading to a tank explosion. The tank contents are rapidly released and quickly flash boil as they depressurize, and both liquid droplets and gas ignite. Since the substance is too rich to burn; a fire burns at the surface where sufficient air can mix with the fuel resulting in a fireball that burns for tens of seconds. The flux of thermal radiation emitted from the burning surface is computed, and the radiation impinging upon a distant target is determined.

Example scenarios for pool fires (Example 1 Part 2), BLEVEs (Example 2 Part 1), flash fires or vapor cloud explosions (Example 2 Part 2), and jet fires (Example 2 Part 3) are provided in ALOHA Example Scenarios.

If a small quantity of chemical is spilled or released in a fire or explosion, the resultant plume can be approximated with the Gaussian plume model, as long as the additional plume buoyancy and explosion overpressures are addressed in other codes. EPIcode has an explosion sub-model that addresses this type of release, calculating a virtual point of release in three-dimensional space before applying Gaussian modeling techniques.

Other complicating factors, such as chemical reactions and chemical transformations within the plume, should be addressed on a case-by-case basis using the dispersion modeling protocol in Section 6.1.9. See Section 4.3 on explosions for additional information on energetic release phenomenology, chemical reactions, and chemical transformations.

Section A.2 of DOE-STD-3009-2014 states that the DSA does not evaluate decomposition of chemicals from accidental fires, nor establishes SSCs or SACs based on the hazards of these toxic products. Accordingly, this technical area is not included in this Handbook.

9.6 METEOROLOGICAL PARAMETERS AFFECTING TOXIC CHEMICAL CONSEQUENCE ANALYSIS

The discussions in Section 6 on the meteorological parameters of wind speed, wind direction, sigma theta, temperature, and precipitation are also applicable to toxic chemical releases. For these meteorological variables, the atmosphere does not operate any differently whether the release is a radionuclide or toxic

chemical, or a combination of both. Turbulence typing for chemical dispersion and consequence analysis is the same as for radiological releases that was also described in Section 6. In calculating plume concentrations, both "typical" and "unfavorable" dispersion conditions are of special interest in accident analyses.

Several meteorological variables, namely temperature and humidity, are specific to analyzing the consequences of toxic chemical releases. A brief discussion on each follows.

9.6.1 TEMPERATURE EFFECTS

The atmospheric variables of temperature and moisture (e.g., relative humidity, wet-bulb temperature) do not directly affect the magnitudes of the atmospheric dilution and diffusion for radionuclide release evaluations. However, for releases of toxic chemicals, these variables play a significant role in determining the thermodynamics in establishing rates of flashing, aerosolization, and puddle evaporation.

Section 9.5.4 provides a discussion of puddle evaporation algorithms and heat balance including conduction from the ground surface. It also provides a discussion of impoundment basins and how they limit the surface area of the puddle and therefore reduce evaporation rate.

9.6.2 RELATIVE HUMIDITY EFFECTS

Uranyl hexafluoride (UF₆) is a special case due to its disassociation into hydrofluoric acid (HF) and uranyl fluoride (UO₂F₂) in a humid environment. A special code developed by Hanna in the 1980s, HGSYSTEM-UF6, and a recent version of the NRC code, RASCAL, has an algorithm to model the conversion rate of UF₆ to UO₂F₂ and HF over time and subsequently disperses both compounds.

Some chemical releases are also sensitive to ambient relative humidity; especially chemicals that are deliquescent and absorb water. An interesting situation is the release of ammonia (NH_3) in a dry environment, where it remains as a positively buoyant gas; while in a humid environment it becomes ammonium hydroxide (NH_4OH) , which behaves as a dense gas.

The release of elemental tritium is also very sensitive to the amount of water vapor in the atmosphere at the time of release as it will convert to tritium oxide rapidly in a moist environment. There are significant differences in the DCFs between elemental tritium and tritium oxide.

9.7 TOXIC CHEMICAL ATMOSPHERIC TRANSPORT AND DIFFUSION MODELS

Many codes are available for evaluating toxic chemical releases, atmospheric dispersion, and concomitant consequences to the CW, MOI, and the public. It has been estimated that in the 1980s, there were as many as 250 atmospheric dispersion modeling codes available both internationally and within the private and public sectors of the United States. However, codes need to be maintained and improved in order to remain viable, so this number has decreased with time.

In 1995, SCAPA published "*Atmospheric Transport Modeling Resources*" (Mazzola and Addis, 1995), in which information about various aspects of 94 distinct atmospheric transport models were catalogued and presented in an easy-to-use format. In March 1999, the Office of the Federal Coordinator for Meteorological Services and Supporting Research (OFCM) published a much more comprehensive version of this document for 64 frequently used atmospheric dispersion models. This latter work is available electronically by accessing the technical documents section of the OFCM web page (<u>www.ofcm.gov</u>). In addition, the APAC Methodology Evaluation Program analyzed 15 radiological

dispersion models (Working Group 5) (APAC5, 2003) and 25 chemical dispersion models (Working Group 6) (APAC6, 1997) in significant detail.

Some models have undergone extensive SQA inclusive of verification and validation. Other codes are available and may be more appropriate for some applications but were not included in those summaries because they are not commonly accessible or require specialized knowledge for their proper use.

DOE-STD-3009-2014, Section 3.2.4.3 states: "Atmospheric dispersion for hazardous chemicals may be modeled in a manner similar to radioactive material dispersion where the material transport characteristics are similar." As indicated in Section 6.1.10, three options are given in DOE-STD-3009-2014 to evaluate atmospheric dispersion and the resulting χ/Q :

- Option 1: Follow a process based on NRC Regulatory Guide 1.145;
- Option 2: Use a DOE-approved toolbox code and apply the conservative parameters; or
- Option 3: Use site-specific methods and parameters as defined in a site/facility specific DOE-approved modeling protocol.

Since Option 1 is only applicable to radiological consequences, for toxic chemical releases, use either Options 2 or 3. The Section 6.11 dispersion modeling protocol is applicable to both radiological and toxic chemical releases.

9.7.1 NEUTRALLY-BUOYANT GAUSSIAN MODELS

Gaussian models, due to their relative simplicity and ease of application, are the most common atmospheric dispersion models employed by analysts to determine consequences from toxic chemical releases. There are two chemical dispersion models (e.g., ALOHA, EPIcode) in the DOE CR, ALOHA meets all DOE O 414.1D and DOE G 414.1-4A SQA guidance, and although EPIcode does not, it is still determined to be adequate for safety analysis. The codes and their latest version in the CR are listed below.

- Areal Locations of Hazardous Atmospheres (ALOHA) Version 5.4.6, an EPA and National Oceanic and Atmospheric Administration (NOAA)-sponsored code (ALOHA, 2013); and,
- Emergency Prediction Information code (EPIcode), Version 8.0.2 (EPIcode, 2015).

ALOHA is the more versatile of the two toolbox codes as it contains both dense-gas and neutrallybuoyant dispersion models, and it can address various chemical release phenomenology and energetic events. During an ALOHA neutrally-buoyant dispersion model execution, the code selects one model based on the environment in which the release is occurring, the nature of the release, the toxic chemical being analyzed and the source-receptor distance of interest. For dense gas releases, ALOHA calculates the dispersion within the dense gas "blanket" and with each succeeding time step, evaluates whether the plume, which is gradually entraining ambient neutrally-buoyant air, still will disperse as a dense gas. Once the plume parameters no longer support the definition of a dense gas as it moves further downwind, ALOHA switches to the neutrally-buoyant Gaussian model. In contrast, EPIcode is based only on the neutrally-buoyant atmospheric dispersion model, but allows the user to vary the release time and deposition velocity, as well as implement a building wake effect model.

9.7.1.1 ALOHA

The ALOHA code was jointly developed by EPA and the hazardous materials division of NOAA. It is

part of the Computer-Aided Management of Emergency Operations (CAMEO) suite of codes and is used primarily for emergency response situations and for training. As such, it is user-friendly, allowing easy data input and convenient output of areal maps with contours of concentration of toxic chemicals using the MARPLOT feature. Many of the internal features of the code are hidden from the user in order to make it more user-friendly. The full suite of ALOHA modeling capabilities can be referenced in NOAA Technical Memorandum NOS OR&R 43, ALOHA technical documentation (ALOHA, 2013).

Unlike some radiological dispersion codes (e.g., MACCS2, GENII, Hotspot), ALOHA does not have the capability to incorporate hourly, site-specific meteorological data and calculate 95th percentile levels consequences based on meteorological variability. EPIcode Version 7.0 has been recently upgraded to execute with hourly meteorological data files. For ALOHA applications, a single combination of atmospheric stability and wind speed is input instead of hourly meteorological data files. For dispersion analysis, 40 CFR § 68.22(b) specifies that poor dilution and diffusion conditions of 1.5 m/sec wind speed and F atmospheric stability class should be assumed.¹⁰² Related conditions of ambient temperature and relative humidity, as may be needed, are recommended from the prescription also identified in 40 CFR § 68.22(b).¹⁰³

ALOHA is intended for the evaluations of the consequences of toxic chemical releases. If the chemical released is a heavy gas, a heavy-gas model (i.e., a stripped-down version of DEGADIS) is used; otherwise, a neutrally-buoyant Gaussian model is used. ALOHA computations represent a compromise between accuracy and speed: it has been designed to produce good results quickly enough to be of use to first responders.

ALOHA Version 5.4.4 has the following attributes:

- Since evaporation of volatile chemicals is especially time-variant, ALOHA can calculate the time-dependent evaporation source term and resulting plume concentration;
- It can determine the extent of dense gas behavior and the distance of transition to neutrally buoyant gas behavior;
- It can predict the rates at which chemical vapors may escape into the atmosphere from broken gas pipes, leaking tanks, and evaporating puddles;
- It can address energetic events such as BLEVEs, vapor cloud explosions, detonations, delayed ignition detonations, and radiant heat effects of flash fires and jet fires;
- Its chemical library contains information about the physical properties of about 3,000 common toxic chemicals;

¹⁰² **Wind speed and atmospheric stability class**. "For the worst-case release analysis, the owner or operator shall use a wind speed of 1.5 m per second and F atmospheric stability class. If the owner or operator can demonstrate that local meteorological data applicable to the stationary source show a higher minimum wind speed or less stable atmosphere at all times during the previous three years, these minimums may be used. For analysis of alternative scenarios, the owner or operator may use the typical meteorological conditions for the stationary source" (40 CFR §68.22(b)).

¹⁰³ **Ambient temperature and relative humidity**. "For worst-case release analysis of a regulated toxic substance, the owner or operator shall use the highest daily maximum temperature in the previous 3 years and average humidity for the site, based on temperature/humidity data gathered at the stationary source or at a local meteorological station; an owner or operator using the Risk Management Program Offsite Consequence Analysis Guidance may use 25 °C and 50 percent humidity as values for these variables. For analysis of alternative scenarios, the owner or operator may use typical temperature/humidity data gathered at the stationary source or at a local meteorological station" (40 CFR §68.22(c)).

- It has a Site Acquisition of Meteorology (SAM) option, where an instrumented meteorological tower can provide input directly to the code; and
- It permits changes in the wind direction parameter every fifteen minutes when the SAM component is applied. This is known as the segmented Gaussian plume. When used in this mode, changes in wind direction allow the plume to bend in the downwind direction.

ALOHA Version 5.4.4 has the following limitations:

- It does not calculate plume rise for ground level releases, so it cannot realistically account for the enormous buoyancy effects of fires and energetic releases;
- It only addresses pure chemicals and consequently is not capable of analyzing the complexities of atmospheric chemistry associated with chemical reactions and mixtures of chemicals;
- It does not have any algorithms that account for dry deposition, wet deposition, plume depletion, and resuspension. Therefore, it does not do particularly well for releases that contain particulates;
- It is a segmented Gaussian plume model, which limits its ability to address complex flows associated with topography; and
- Like all Gaussian models that are steady-state by definition, is not reliable for very low wind speeds, for very stable atmospheric conditions, for shifting winds and terrain-steering situations, or for concentration patchiness.

9.7.1.2 EPICODE

EPIcode was originally developed at the Lawrence Livermore National Laboratory (LLNL) to provide emergency response personnel and emergency planners with a software tool to help evaluate downwind concentrations from atmospheric releases of toxic substances. It can also be used for safety analysis planning purposes for facilities handling toxic chemicals.

EPIcode has many similarities to ALOHA, in that it is a straight-line Gaussian model with an extensive chemical library. However, unlike ALOHA, it can only address direct and evaporating puddle chemical release situations since it does not contain pipe and tank sub-models.

The version of EPICode that is in the DOE Central Registry is EPICode Version 7.0. Attributes and limitations of a more recent version are presented below:

EPIcode Version 8.0.2 (EPIcode, 2015) has the following attributes:

- It can assess area releases, fire releases, and explosion releases; but not the energetics associated with these accidents;
- Its chemical library is slightly smaller than that in ALOHA, but it still addresses more than 600 specific chemicals;
- It has algorithms for dry deposition;
- It allows fast estimation and assessment of chemical release scenarios associated with accidents from industry and transportation;
- It is menu-driven and user friendly, requiring minimal user training;
- It contains a good graphics package; and
- Its User Manual also contains 11 case studies showing how the code can assess a wide range of chemical accident scenarios.

EPIcode Version 8.0.2 has the following limitations:

- It has a very simple evaporation rate algorithm.
- It only addresses pure chemicals and consequently is not capable of analyzing the complexities of atmospheric chemistry associated with chemical reactions and mixtures of chemicals;
- It does not have any algorithms that account for wet deposition and resuspension;
- It is a straight-line Gaussian model, which limits its ability to address complex flows associated with topography; and
- Like all Gaussian models that are steady-state by definition, is not reliable for very low wind speeds, for very stable atmospheric conditions, for shifting winds and terrain-steering situations or for concentration patchiness.

9.7.1.3 CHEMICAL DISPERSION ANALYSIS WITH ALOHA AND EPICODE

A parametric study from a very limited data set, provides insight to important sensitivities related to modeling evaporative chemicals with earlier versions of ALOHA and EPIcode and analysis of the concentrations at a 100-m distance (Thoman et al., 2006). This study, summarized in Table 9-6, yielded the following conclusions for ALOHA:

- Class F stability at 1 m/s wind speed for a rural region of transport is bounding relative to urban conditions for both EPIcode and ALOHA. The same conclusion holds for the results comparing the Class D stability at 2 m/s results; and
- ALOHA dense gas results for Class D stability at 2 m/s wind speed bounds the Gaussian neutrally-buoyant gas results for both rural and urban regions of transport, and the rural terrain dense gas results for Class D stability at 2 m/s wind speed are bounding relative to the urban terrain dense gas results.

Chemical Released	Dispersion Model ¹⁰⁴	Region of Transport	Stability class/ wind speed (m/s)	Release rate (g/s)	Concentration at 100 m (mg/m ³)
Nitric Acid	GNB	Rural	F/1	5.3	2.3 E2
	DG	Rural	F/1	5.3	8.8 E1
	GNB	Urban	F/1	5.3	4.8 E1
	DG	Urban	F/1	5.3	6.1 E1
Nitric Acid	GNB	Rural	D/2	9.1	3.2 E1
	DG	Rural	D/2	9.1	7.3 E1
	GNB	Urban	D/2	9.1	1.3 E1
	DG	Urban	D/2	9.1	4.9 E1
Chlorine	GNB	Rural	F/1	2100	2.1 E4
	DG	Rural	F/1	2100	3.0 E3
	GNB	Urban	F/1	2100	4.4 E3
	DG	Urban	F/1	2100	1.5 E3
Chlorine	GNB	Rural	D/2	2800	2.4 E3
	DG	Rural	D/2	2800	2.6 E3
	GNB	Urban	D/2	2800	9.5 E2
	DG	Urban	D/2	2800	1.6 E3
Benzene	GNB	Rural	F/1	9.6	4.3 E2
	DG	Rural	F/1	9.6	1.3 E2
	GNB	Urban	F/1	9.6	9.0 E1
	DG	Urban	F/1	9.6	9.1 E1
Benzene	GNB	Rural	D/2	17	4.9 E1
	DG	Rural	D/2	17	1.1 E2
	GNB	Urban	D/2	17	2.0 E1
	DG	Urban	D/2	17	7.4 E1
Ammonia	GNB	Rural	F/1	400	6.9 E3
	DG	Rural	F/1	400	7.6 E2
	GNB	Urban	F/1	400	1.4 E3
	DG	Urban	F/1	400	6.7 E2
Ammonia	GNB	Rural	D/2	540	8.6 E2
	DG	Rural	D/2	540	1.3 E3
	GNB	Urban	D/2	540	3.5 E2
	DG	Urban	D/2	540	8.7 E2

Table 9-6. ALOHA Results for Evaporative Releases of Four Selected Chemicals.

For the same chemical release under evaporative conditions, the neutrally-buoyant Gaussian model ALOHA results for the F stability conditions and 1 m/s wind speed for a rural region of transport bounds

 $^{^{104}}$ GNB = Gaussian neutrally-buoyant; DG = Dense Gas or heavy gas

all other dense gas results in both rural and urban regions of transport and all other neutrally-buoyant Gaussian model results. For example, the Gaussian neutrally-buoyant nitric acid result of 230 mg/m³ for F stability and 1 m/s wind speed bounds the other seven chlorine results obtained using the ALOHA model. Chemical release concentrations for the three other toxic chemicals also showed the same bounding value for Class F stability conditions and 1 m/s wind speed for a rural region of transport.

Both EPIcode and ALOHA allow the evaporative source term and dispersion calculations to be coupled such that the plume exposure time reflects the time over which the evaporation release occurs. For EPIcode, an evaporation rate that is constant with time is modeled. ALOHA calculates a time–varying evaporative release rate that is reflected in downwind concentrations that are observed to vary with time as shown in Figure 9-3.



Figure 9-3. Example of ALOHA concentration output from an evaporative pool of hydrogen chloride.

It should be emphasized that this parametric study is based on a limited data base and its results should not be overly generalized.

9.7.2 DENSE GAS DISPERSION MODELS

Practically all of the hazardous chemicals that are stored and/or used at DOE facilities have densities greater than dry air. Some exceptions include anhydrous ammonia, nitric oxide and carbon monoxide.

Several heavy gas or dense gas codes have been developed to analyze the slumping effects of an accidental release of a dense gas. Each of these codes has been recommended for application in a broad range of safety basis documentation by APAC Working Group 6 (APAC6, 1997).

9.7.2.1 ALOHA

ALOHA can also be executed in heavy gas mode, if not bypassed by the user, for a release of a chemical with a molecular weight of greater than the molecular weight of dry air (28.97 g/mol) given that the critical Bulk Richardson number criterion is fulfilled during release conditions. ALOHA contains a stripped down version of the DEGADIS code to address the effects of heavy gases.

ALOHA can be run in Gaussian mode or dense gas mode. For dense gas applications, the dense gas model operates until the critical Bulk Richardson number is reached as the dense gas plume gradually entrains ambient air into the blanket. Once sufficient ambient air is within the dense gas blanket, it becomes neutrally-buoyant and ALOHA switches to the Gaussian model.

NSRD-2015-TD01 concluded:

The ALOHA neutrally-buoyant Gaussian model results for a rural region of transport bounds all other dense gas results in both rural and urban regions of transport, as well as all other neutrally-buoyant Gaussian model results.

This is applicable to ground-level chemical releases and the health impact at a CW at 100 m for meteorological conditions of 1.0 m/s and F stability class.

9.7.2.2 DEGADIS

Version 1 of the Dense Gas Dispersion (DEGADIS) model was developed by the University of Arkansas for the United States Coast Guard and the Gas Research Institute in 1985. In 1988, Havens (1988) interfaced Ooms' 1974 jet model to develop Version 2.0. The present Version 2.1 was established in 1989 through the work of Spicer and Havens (EPA-450/4-89-019).

EPA lists DEGADIS as an "Appendix B" refined air quality model that may be considered for individual regulatory applications on a case-by-case basis. It presently manages the maintenance of the model (EPA-450/4-88-006a; EPA-450/4-89-019). Updates can be accessed through the EPA Support Center for Regulatory Atmospheric Modeling bulletin board: <u>http://www.epa.gov/scram001/tt22.htm#degadis</u>.

Although the model is relatively easy to run, the analyst should take special care to fully understand the user options and the data input requirements, for example, distinctions between isothermal and non-isothermal simulations.

DEGADIS has the following attributes:

- It can address the transport and diffusion of many types of dense gas releases and account for a variety of surface roughness elements; and
- It can also simulate atmospheric transport and diffusion of pure chemical releases in passivedispersion flow regimes.

DEGADIS has the following limitations:

• It does not have a front-end chemical library that the ALOHA and EPIcode models have. Correspondingly, the analyst should couple the DEGADIS dispersion results with chemical source terms generated from other models; and • It cannot address buoyant plumes, although it is usually chosen for application for cases where the plume slumps due to its own density.

9.7.2.3 HGSYSTEM

Heavy Gas (HG) SYSTEM was developed for the American Petroleum Institute in 1990. Its current version, 3.0, was released in 1994.

Unlike DEGADIS and SLAB, HGSYSTEM is able to generate its own chemical source terms and therefore does not need to be supplied with an additional modeling technique.

HGSYSTEM has the following attributes:

- It can efficiently handle time-dependent dispersion by an internal automated selection of advection and averaging time; and
- It can also treat multi-component mixtures and vapor-aerosol generation.

HGSYSTEM has the following limitations:

- Proper training is needed. Although not as complex as a research-grade model, the user needs prior experience and familiarity with the code's features since there are a large number of alternative options available that need to be fully understood; and
- It also has had difficulty in appropriately quantifying evaporation under low exit velocity release conditions and very stable low wind speed meteorological conditions.

A specially designed HGSYSTEM-UF₆ model has been developed for use in the accident analysis of Oak Ridge facilities to quantify the chemical consequences from a release of uranium hexafluoride.

9.7.2.4 SLAB

SLAB was developed from basic research involving experiments with chemical releases at China Lake, CA and the Nevada Test Site in the early 1980s (Ermak, 1990).

SLAB has the following attributes:

- It is not only easy to use, but it can be applied to a wide range of chemical release scenarios. These include application to jets released at any angle to evaporative area sources to instantaneous sources.; and
- It also contains a unique averaging time algorithm that allows application of the model to timevarying source emissions.

SLAB has the following limitations:

- Like DEGADIS, it does not have a front-end chemical library that the ALOHA and EPIcode models have;
- The analyst should couple the SLAB transport and diffusion results with chemical source terms generated from other models; and
- SLAB cannot address buoyant plumes.

9.7.3 VARIABLE TRAJECTORY DISPERSION MODELS

The frame of reference of all steady-state two-dimensional Gaussian-type models is Eulerian, meaning that the receptor is on a fixed coordinate system and receives no impact until the plume front reaches it. For sites that are located in regions that experience three-dimensional flows due to complex terrain (such as valley-mountain wind regimes) or due to temperature differences at land-water interfaces (such as sea breezes, lake breezes), the application domain of Eulerian codes is severely limited.

For the evaluation of chemical releases at locations with complex air flows, three-dimensional Lagrangian mass-consistent codes, (e.g., codes developed at NARAC) need to be considered for toxic chemical releases. Since the distance to the CW is sufficiently close enough where airflow trajectory reversals have not yet begun to occur, there is no practical need to be concerned with these complex terrain effects for this application. However, since the public is usually far enough away to experience the effects of airflow trajectory reversals, which are common at some DOE sites (Y-12, ORNL, NNSS, LANL, Hanford, INL), for that evaluation, a three-dimensional Lagrangian mass-consistent variable trajectory model would provide more accurate results than a Gaussian model that provides more bounding results. Several models have been developed to characterize atmospheric dispersion in regions of complex terrain. A few of these models that can be applied to address the effects of chemical as well as radiological releases in mountain-valley and sea breeze topographic settings include:

- NARAC codes;
- HYSPLIT;
- HYRAD;
- AERMOD; and
- CTDMPLUS.

9.7.4 RESEARCH-GRADE DISPERSION MODELS

Several research grade atmospheric dispersion models are applicable to chemical consequence analysis. The APAC Working Groups reviewed several of these codes, which include:

- HOTMAC/RAPTAD;
- FEM3C;
- SCIPUFF;
- VDI; and
- VLSTRACK.

The analyst is referred to the APAC Working Group 6 (APAC6, 1997) report for further information regarding the applicability of any of these codes to specific problem solving.

9.8 TOXIC CHEMICAL CONSEQUENCE SCOPING METHODOLOGY TO EXCEED PAC/TEEL VALUES

As discussed in Section 2.3.2, Chemical Hazard Evaluation and Section 9.3, Chemical Screening Criteria, chemical hazards are screened for further hazard evaluation by applying criteria such as in Section A.2 of the DOE-STD-3009-2014. For some of those hazards that are not screened out, a qualitative evaluation of toxic chemical consequences is generally sufficient to provide a basis for comparison to the qualitative consequence thresholds in Table 2-8, Consequence Thresholds, of this Handbook. However, for some of those hazards that are not screened out, a quantitative evaluation may be necessary to determine impacts to CWs, the MOI, and the public, when the toxic chemical hazards have the potential to exceed the SS control selection criteria.

This section provides a simplified quantitative scoping methodology for determination of toxic chemical quantities that are sufficient to challenge the screening criteria. This scoping methodology is based on EPA-550-B-99-009 for liquid evaporation, and from a 2007 calculation, "Chemical Threshold Quantities for Safety Basis Categorization," for gas, powder, and solid releases. PAC/TEEL-2 and PAC/TEEL-3 values were adjusted for Revision 29 values (PAC, 2016). Note that this is only one type of methodology receiving a positive review. Other equivalent methodologies may be acceptable.

This scoping methodology is applied to the following toxic chemical releases:

- Gas, powder, and solid release (Section 9.8.1); and
- Evaporation of a liquid release (Section 9.8.2).

Section 9.8.3 compares the scoping methods to applicable PAC/TEEL values for the MOI high consequence case.

9.8.1 GAS, POWDER, AND SOLID RELEASE MODEL

For all of the cases presented, the downwind toxic chemical concentration, C(x), in mg/m³, can be described by Equation 9-93:

$$\boldsymbol{C}(\boldsymbol{x}) = \boldsymbol{Q}' \times \boldsymbol{\chi} / \boldsymbol{Q}(\boldsymbol{x})$$

Equation 9-93

Equation 9-94

Where,

Q' = release rate (mg/s) $\chi/Q(x)$ = atmospheric dispersion factor at receptor of interest distance (x) (s/m³)

The distinction between powders and solids is based on how they are treated in the DOE-HDBK-3010-94, and Chapter 5 of this Handbook. For gas, powder, and solid releases, the model to calculate the release rate, (Q') of a toxic chemical (i.e., MAR) that will exceed applicable PAC/TEEL values is calculated by Equation 9-94:

$$Q' = ST/t$$

Where,

ST = source term released to air (mg) t = release duration (s)

Assume 900 s for 15-min (900 s) TWA as discussed in Section 9.4.1.1, Chemical Exposure Time.

The five-factor ST formula from Equation 5-1 can be reduced to ST = MARxARF based on a conservative assumption for the unmitigated analysis that all of the MAR is released or spilled (DR = 1.0), all released MAR is of respirable size (RF = 1.0)¹⁰⁵, and all of the airborne release within a facility is released to the environment (LPF = 1.0)¹⁰⁶. Combining this conservative ST equation with Equations 9-

 $^{^{105}}$ EPA-550-B-99-009 allows <100 μm fraction with 1.0 ARF for powders released over 10 minutes. However, this is not used in this screening calculation

 $^{^{106}}$ EPA-550-B-99-009 allows a LPF = 0.55 for in-facility deposition. However, this is not used in this screening calculation.

93 and 9-94, the MAR quantity released or spilled is presented as a function of the concentration, release duration, ARF, and atmospheric dispersion factor in Equation 9-95:

$$MAR = [C(x) \times t] / [ARF \times \chi / Q(x)]$$

Equation 9-95

For this scoping calculation, estimates of ARF based on a similar logic applied for nuclear hazard categorization determinations, are assumed to be bounding for particular chemical and potential accident stresses being evaluated as follows:

 $\begin{array}{ll} ARF &= 1.0 \text{ for a gas} \\ ARF &= 0.01 \text{ for a powder} \\ ARF &= 0.001 \text{ for a solid}^{107} \end{array}$

9.8.2 LIQUID EVAPORATION SCOPING CALCULATION MODEL

This EPA technique is for a 15-minute average evaporation rate. Should the analyst need to address timevarying evaporation, this technique is not recommended, as the application domain of the EPA model is insufficient. More comprehensive techniques which were presented in Section 9.5.4 are recommended.

For sub-cooled liquids, where no heated correction factor is required, the evaporation model used to calculate the release rate, Q', is from EPA-550-B-99-009, Equation D-1 (see the EPA reference for its derivation and English to metric unit conversions that are reflected in the constants in the Equation 9-96), which is based on surface area and volume of the spill, density, vapor pressure, and molecular weight of the liquid; and wind speed; as shown in Equation 9-96:

$$Q' = \left[0.284 \times u^{0.78} \times MW^{2/3} \times A \times VP\right] / \left[82.05 \times T\right]$$
 Equation 9-96

Where,

Q' = release rate (lb/min)

U = wind speed
$$(m/s)$$

Assume U = 1.0 m/s, Class F Stability to be consistent with 95th percentile χ/Q .

MW	= molecular weight
А	= V/h = unconfined surface area of pool (1 cm depth per EPA-550-B-99-005),
	converted to ft)
h	= dike height for confined pool (ft)
V	= MAR/ ρ = volume of liquid spilled (ft ³)
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 ρ = density of liquid = specific gravity × 1.0 g/cm³ VP = vapor pressure at ambient temperature (mm Hg)

 $VP = [VP_{data}/T_{data}] \times 298^{\circ}K [25^{\circ}C]$

Equation 9-97

T = liquid temperature (K)

¹⁰⁷ EPA-550-B-99-009 evaluates powder in solution, or solids in molten form, with different methods.

Equation 9-97 is based on the method from the calculation that adjusts the VP for temperatures other than 25°C¹⁰⁸ by the Ideal Gas Law.¹⁰⁹ VP is the most sensitive parameter for application of Equation 9-96, and can be obtained from the PAC/TEEL website for pure chemicals, or for lesser concentrations, can be obtained from chemical references such as Green and Perry (2007). As an alternate method to Equation 9-96, Figure 9-4 illustrates how the vapor pressure varies as a function of the liquid temperature for a 70 wt% nitric acid water solution. The vapor pressure data are from Table 3-16 of the Chemical Engineers' Handbook (Green and Perry, 2007), and from EPIcode predictions from a site-specific evaluation.



Figure 9-4. Comparison of Vapor Pressure Data vs. EPIcode Fit for 70 wt% Nitric Acid.

A recommended release rate correction factor (CF) to account for liquids with high vapor pressure at ambient T of 298°K (25°C) is shown in Eq. 9-98.

$$CF = -[P_a/VP] \times [ln(1 - VP/P_a)]$$

Equation 9-98

¹⁰⁸ That calculation was based on 20°C, which has been revised to 25°C per the EPA methodology used for this scoping calculation.

¹⁰⁹ According to the linear function from zero at 0° K to the tabulated vapor pressure and temperature from a chemical reference.

Where,

 $P_a = 760 \text{ mm}$ Hg ambient pressure @ Standard Temperature and Pressure, or local ambient P_a

For liquids with high vapor pressures, the corrected release rate (mg/s) becomes:

$$Q''/A = CF \times [0.284 \times u^{0.78} \times MW^{2/3} \times VP]/[82.05 \times T]$$
 Equation 9-99

The spill temperature, *T*, should be selected considering the range of possible liquid temperatures, consistent with the storage/operating temperature or the temperature of the environment. For common operational spills of liquids, not resulting from fire events, if conditions differ significantly from the default 25°C (77 °F) from EPA-550-B-99-009, the spill temperature should be selected as the greater of: (1) the maximum storage/operating temperature; or, (2) the highest maximum daily temperature for the previous three years (40 CFR § 68.25(d)(2)). The EPA-550-B-99-009 guidance assumes meteorological conditions for the worst-case scenario of Class F (stable atmosphere) and wind speed 1.5 m/s (3.4 mph), which is roughly equivalent to the 95th percentile dispersion condition required by DOE-STD-3009. For this conservative dispersion condition, EPA also allows use of an ambient air temperature of 25 °C (77 °F) for the worst case scenario when applying Equation 9-99, even if the maximum temperature at the site in the last three years is higher. However, an exception is provided if other methods and codes are being used). As an alternative, the analyst could consider whether an ambient temperature for conservative dispersion conditions consistent with their 95th percentile χ/Q calculation is a sufficiently conservative assumption for the spill temperature.

For spills of liquids under fire conditions where the fire is of sufficient size to cause bulk boiling of the spilled liquid, the spill temperature should be selected as the normal boiling point of the spilled material. Otherwise, the spill temperature should be selected as discussed above. Other corrections (such as VP, density) are also required as recommended in EPA-550-B-99-009.

The time to evaporate the entire MAR spilled or released, t_{evap}, is:

$$t_{evap} = [\rho \times h] / [Q''/A]$$

Equation 9-100

Using Equations 9-99 and 9-100 with Equation 9-95, the quantity of toxic chemical MAR to exceed a specified concentration for high vapor pressure liquids, at a downwind distance can be calculated as shown in Equation 9-101:

$$MAR = [C(x) \times \rho \times h] / [Q'' / A \times \chi / Q(x)] \times [900 / minimum (t_{evap}, 900)]$$
 Equation 9-101

Note that the last term of Equation 9-101 adjusts for rapid $t_{evap} < 900$ s, or makes no adjustment for slow evaporation > 900 s. Thus, for evaporation that takes place over a >900 sec period, the last term is unity.

Lastly, the t_{evap} term can be modified by multiplying by % weight fraction of chemical concentration for liquids with impurities using Raoult's Law (Smith, J. M., et al., 2005).

9.8.3 SCREENING METHOD FOR MAXIMALLY-EXPOSED OFFSITE INDIVIDUAL (MOI) HIGH CONSEQUENCE

Since the release is assumed to be at ground-level, the MOI will be at the site boundary. For the MOI, the relevant inputs to Equations 9-95 and 9-101 are:

C (site boundary) =PAC/TEEL-2 (PAC, 2016)

 χ/Q (site boundary) = normalized dispersion at site boundary for MOI (s/m³)

The MOI MAR quantity of toxic chemical to exceed PAC/TEEL-2 is determined for high VP liquid releases and other releases applying Equations 9-102 and 9-103, respectively.

High VP liquid releases:

$$MAR = [PAC/TEEL - 2 \times \rho \times h] / [Q''/A \times \chi/Q(site \ boundry)] \times [900/minimum (t_{evap}, 900)]$$
Equation 9-102

Other liquid releases:

$MAR = [PAC/TEEL - 2 \times t] / [ARF \times \chi/Q(site boundary)]$ Equation 9-103

To estimate the MAR that could exceed the MOI moderate consequence threshold, the high consequence MAR can be multiplied by the PAC/TEEL-1/PAC/TEEL-2 ratio, or alternately, can be scaled by the moderate CW consequence MAR by the χ/Q (100 m)/ χ/Q (site boundary) ratio.

The site-specific overall 95th percentile sector independent χ/Q or 99.5th percentile sector dependent χ/Q as determined by Section 6.1.10 of this Handbook, is applicable. Alternately, the following conservative assumptions can be made using the Tadmor-Gur rural dispersion factors for Class F stability and wind speed of 1 m/s, with a 3 cm surface roughness factor assumed in the modeling protocol. Note that this is the same as the reference value from the original experiments.

For illustration purposes, a minimum distance to the site boundary of 1 km is used in the following equations and in Section 9.9.

$\sigma_z(x) = 0.2 \times x^{0.602} \times (surface roughness/3cm)^{0.2} = 12.79m at 1km$	Equation 9-104
$\sigma_y(x) = 0.0722 \times x^{0.9031} = 36.97m \ at \ 1km$	Equation 9-105
$\chi/Q(x) = \left[\pi \times u \times \sigma_y(x) \times \sigma_z(x)\right]^{-1} = 6.73 E - 4 s/m^3 at 1 km$	Equation 9-106

9.9 EXAMPLE TOXIC CHEMICAL CALCULATIONS

Four example calculations, presented in Sections 9.9.1 through 9.9.4 representing a range of plausible release types and liquid release vapor pressures, are provided in the following subsections:

- Ammonia gas;
- Aluminum oxide powder;
- Liquid 70% nitric acid evaporation (unconfined spill); and
- Liquid 55% hydrofluoric acid evaporation (confined spill into a diked area).

These are based on the CW method, exceeding the PAC/TEEL-3 threshold. As previously indicated, these results can be scaled to estimate the quantity to exceed PAC/TEEL-2 moderate consequence for the CW or to exceed the MOI high PAC/TEEL-2 threshold or moderate PAC/TEEL-1 threshold. The last calculation in Section 9.9.4 looks at unmitigated and mitigated analyses for the CW and MOI for two PAC/TEEL criteria.

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9.9.1 EXAMPLE 1: CALCULATE AMMONIA GAS QUANTITY THAT EXCEEDS PAC/TEEL-3 AT THE CW

Equation 9-103, modified for the CW χ/Q (100m) = 3.5E-3 s/m³, applies to this example with the following inputs and assumptions:

C (100 m)	= PAC/TEEL-3 at 100 m = 770 mg/m ³ [PAC, 2016] for ammonia CASRN 7664-41-7
t	= 900 s [15 min TWA]
ARF	= 1.0 for gaseous release
χ/Q (100m)	$= 3.5 \text{E-3 s/m}^3$
MAR	= $[PAC/TEEL-3 \times t]/[ARF \times 3.5 E-3 s/m^3]$
MAR (100 m)	= $[(770 \text{ mg/m}^3)(900 \text{ s})] / [(1.0)(3.5\text{E}-3 \text{ s/m}^3)] \times [1b/453.6 \text{ g} \times \text{g}/1,000 \text{ mg}]$

Conclusion: MAR = 4.37E+2 lb or greater of ammonia gas, needs to be released to exceed PAC/TEEL-3 at the CW.

9.9.2 EXAMPLE 2: CALCULATE ALUMINUM OXIDE POWDER QUANTITY THAT EXCEEDS PAC/TEEL-3 AT THE CW

Equation 9-103, modified for the CW χ/Q (100m) = 3.5E-3 s/m³, applies to this example with the following inputs and assumptions:

C (100 m) = PAC/TEEL-3 at 100 m = 990 mg/m³ [PAC, 2016] for aluminum oxide, CASRN 1344-28-1

t = 900 s [15 min TWA] ARF = 0.01 for powder release χ/Q (100m) = 3.5E-3 s/m³

MAR = $[PAC/TEEL-3 \times t]/[ARF \times 3.5E-3 \text{ s/m}^3]$ MAR (100 m) = $[(990 \text{ mg/m}^3)(900 \text{ s})] / [(0.01)(3.5E-3 \text{ s/m}^3)] \times [lb/453.6 \text{ g} \times \text{g/1,000 mg}]$

Conclusion: MAR = 5.6E+4 lb or greater of aluminum oxide, needs to be spilled to exceed PAC/TEEL-3 at the CW.

9.9.3 EXAMPLE 3: CALCULATE LIQUID 70% NITRIC ACID QUANTITY THAT EXCEEDS PAC/TEEL VALUES AT 1 KM SITE BOUNDARY

Eq.9-102, modified for the CW χ/Q (100m) = 3.5E-3 s/m³, applies to this example with the following inputs and assumptions: 70% nitric acid is a high vapor pressure release, and spill occurs at sea level under Standard Temperature and Pressure (STP) conditions. Note that ARF is not applicable to a liquid evaporation release, and the duration (t) is the evaporation time if less than the 15-min as used for the TWA calculation. References for the input data are included in [brackets].

PAC/TEEL-3 = 92 ppm = 240 mg/m³ [2.58 mg/m³/ppm from PAC, 2016] for nitric acid, CASRN 7697-37-2.

- MW = 63.01 g/mol
- VP = $4.49 \text{ mm Hg} @ 26.4^{\circ}C (299.4^{\circ}K)$ [data provided by vendor specifications]

 $VP \qquad = [VP_{data} \, / T_{data}] \times 298^\circ K$

VP =
$$(4.49 \text{ mm Hg})/(299.4^{\circ}\text{K}/298^{\circ}\text{K}) = 4.47 \text{ mm Hg} @ 25^{\circ}\text{C} (298^{\circ}\text{K})$$

SpG = $1.4134 @ 20^{\circ}C (293^{\circ}K)$

 ρ = 1.4134 g/cm³

- T = temperature of liquid = ambient 25° C = 298° K
- $P_a = 760 \text{ mm Hg} @ \text{ ambient STP}$

h =
$$1.0$$
 cm; depth of unconfined puddle (EPA-550-B-99-005)

u = 1.0 m/s; wind speed [consistent with χ/Q wind speed assumption for Class F stability]

Q' =
$$[0.284 \times u^{0.78} \times MW^{2/3} \times A \times VP]/[82.05 \times T]$$

$$Q'/A = [0.284 \times u^{0.78} \times MW^{2/3} \times VP]/[82.05 \times T]$$

$$Q'/A = [0.284 \times (1 \text{ m/s})^{0.78} \times (63.01)^{2/3} \times (4.47 \text{ mm Hg})]/[82.05 \times 298\text{K}] = 8.22\text{E}-4 \text{ lb/min/ft}^2$$

$$CF = - [P_a / VP] \times [ln (1 - VP/P_a)]$$

CF = - [(760 mm Hg)/(4.47 mm Hg)] × [ln (1 – (4.47 mm Hg)/(760 mm Hg)] = 1.003

Q''/A = CF × $[0.284 \times u^{0.78} \times MW^{2/3} \times VP]/[82.05 \times T]$

Q''/A = $(1.003)(8.22E-4 \text{ lb/min/ft}^2) = 8.24E-4 \text{ lb/min/ft}^2$

 $Q''/A = (8.24E-4 \text{ lb/min/ft}^2)(453.6 \text{ g/lb})(\text{min/60 s})(0.0328 \text{ ft/cm})^2 = 6.71E-6 \text{ g/s/cm}^2$

 $t_{evap} = [\rho \times h]/[Q''/A]$

 $t_{evap} = [(1.4134 \text{ g/cm}^3) \times (1.0 \text{ cm})]/[(6.71\text{E-6 g/s/cm}^2)] = 2.1\text{E+5 s} (min/60 \text{ s}) = 3.5\text{E+3 min} > 15 \text{ min} (no adjustment = 1).$

MAR = [PAC/TEEL-3 × ρ × h]/[Q''/A × 3.5E-3 s/m³] × [900/minimum (t_{evap}, 900)]

MAR = $[(240 \text{ mg/m}^3)(1.4134 \text{ g/cm}^3)(1.0 \text{ cm})] / [(6.71\text{E-}6 \text{ g/s/cm}^2) \times (3.5\text{E-}3 \text{ s/m}^3)] \times [1] \times (1b/453.6 \text{ g}) \times (g/1,000 \text{ mg})$

Conclusion: MAR = 3.2E+4 lb or greater of 70% nitric acid needs to be spilled, to exceed PAC/TEEL-3 at the CW.

For perspective, a spill of 3.2E+4 lb of 70% nitric acid translates to:

Volume spilled	= 2,666 gal
----------------	-------------

Puddle area $= 81,271 \text{ ft}^2$

Puddle diameter = 322 ft

To exceed High MOI consequences at 1 km, Equation 9-102 applies with the following inputs:

PAC/TEEL-2 = 62 mg/m^3 [PAC, 2016]

 χ/Q (site boundary) = 6.73E-4 s/m³

MAR = [PAC/TEEL-2 × ρ × h]/[Q''/A × χ /Q (site boundary)] × [900/minimum (t_{evap}, 900)]

MAR = $[(62 \text{ mg/m}^3)(1.4134 \text{ g/cm}^3)(1.0 \text{ cm})]/[(6.71\text{E}-6 \text{ g/s/cm}^2)(6.73\text{E}-4 \text{ s/m}^3)] \times [1] \times (1b/453.6 \text{ g}) \times (g/1,000 \text{ mg})$

Conclusion: MAR = 4.28E+4 lb or greater of 70% nitric acid needs to be spilled, to exceed PAC/TEEL-2 at a site boundary distance.

9.9.4 EXAMPLE 4: CALCULATE LIQUID 55% HYDROFLUORIC ACID QUANTITY THAT EXCEEDS PAC/TEEL VALUES AT 1 KM SITE BOUNDARY

Equation 9-102, modified for the CW χ/Q (100m) = 3.5E-3 s/m³, applies to this example with the following inputs and assumptions: 55% hydrofluoric acid is a high vapor pressure release, and spill occurs at sea level under STP conditions. ARF is not applicable to a liquid evaporation release, and the duration (t) is the evaporation time if less than the 15-min as used for the TWA calculation. References for the input data are included in [brackets].

PAC/TEEL-3 = 36 mg/m^3 [PAC, 2016] for hydrofluoric acid, CASRN 7664-39-3.

- MW = 20.01g/mol
- VP = $50 \text{ mm Hg} @ 25^{\circ}C$ [data provided by vendor specifications]

 $VP = [VP_{data} / T_{data}] \times 298^{\circ}K$

- VP = $(50 \text{ mm Hg})/(298^{\circ}\text{K}/298^{\circ}\text{K}) = 50 \text{ mm Hg}$
- $\label{eq:rho} \begin{array}{l} \rho & = 100,000 \mbox{ lb } /1,353 \mbox{ ft}^3 = 73.91 \mbox{ lb/ft}^3 \mbox{ [based on vendor specifications for design of a dike]} \\ = 73.91 \mbox{ lb/ft}^3 \times 453.6 \mbox{ g/lb } / \mbox{ 28,317 cm}^3/\mbox{ ft}^3 = 1.184 \mbox{ g/cm}^3 \end{array}$
- T = temperature of liquid = ambient 25° C = 298° K
- $P_a = 760 \text{ mm Hg} @ \text{ ambient STP}$
- h = 92.7 cm depth in dike [see liquid depth data]
- u = 1.0 m/s wind speed [consistent with χ/Q wind speed assumption for Class F stability]

Q' =
$$[0.284 \times u^{0.78} \times MW^{2/3} \times A \times VP]/[82.05 \times T]$$

$$Q'/A = [0.284 \times u^{0.78} \times MW^{2/3} \times VP] / [82.05 \times T]$$

- $Q'/A = [0.284 \times (1.0 \text{ m/s})^{0.78} \times (20.01)^{2/3} \times (50 \text{ mm Hg})]/[82.05 \times 298\text{K}] = 4.3\text{E-}3 \text{ lb/min/ft}^2$
- $CF \qquad = \text{-} \left[P_a \, / VP \right] \times \left[ln \left(1 VP / P_a \right) \right]$

CF = $-[(760 \text{ mm Hg})/(50 \text{ mm Hg})] \times [\ln (1 - (50 \text{ mm Hg})/(760 \text{ mm Hg})] = 1.034$

Q''/A = CF × $[0.284 \times u^{0.78} \times MW^{2/3} \times VP]/[82.05 \times T]$

Q''/A = (1.034) (4.3E-3 lb/min/ft²) = 4.4E-3 lb/min/ft²

 $Q''/A = (4.4E-3 lb/min/ft^2)(453.6 g/lb)(min/60 s)(0.0328 ft/cm)^2 = 3.6E-5 g/s/cm^2$

 $t_{evap} = [\rho \times h]/[Q''/A]$

- $t_{evap} = [(1.184 \text{ g/cm}^3) \times (92.7 \text{ cm})]/[(3.6\text{E-5 g/s/cm}^2)] = 3.05\text{E+6 s} (\min/60 \text{ s}) = 5.08\text{E+4 min} > 15 \text{ min} (\text{no adjustment =1}).$
- MAR = [PAC/TEEL-3 × ρ × h]/[Q''/A × 3.5E-3 s/m³] × [900/minimum (t_{evap}, 900)]
- $MAR = [(36 \text{ mg/m}^3)(1.184 \text{ g/cm}^3)(92.7 \text{ cm})]/[(3.6\text{E-5 g/s/cm}^2) \times (3.5\text{E-3 s/m}^3)] \times [1] \times (1b/453.6 \text{ g}) \times (g/1,000 \text{ mg})$

Conclusion: MAR = 6.9E+4 lb or greater of 55% hydrofluoric acid, needs to be spilled to exceed PAC/TEEL-3 at the CW.

For perspective, a spill of 6.9E+4 lb of 55% hydrofluoric acid translates to about 7E+3 gal for a density around 74 lb/ft³.

To exceed High MOI consequences at 1 km, Equation 9-102 applies with the following inputs:

- PAC/TEEL-2 = 20 mg/m^3 [PAC, 2016]
- χ/Q (site boundary) = 6.73E-4 s/m³
- MAR = [PAC/TEEL-2 × ρ × h]/[Q''/A × χ /Q (site boundary)] × [900/minimum (t_{evap}, 900)]
- MAR = $[(20 \text{ mg/m}^3)(1.184 \text{ g/cm}^3)(92.7 \text{ cm})]/[(3.6\text{E-5 g/s/cm}^2)(6.73\text{E-4 s/m}^3)] \times [1] \times (1b/453.6 \text{ g}) \times (g/1,000 \text{ mg})$

Conclusion: MAR = 2.0E+5 lb or greater of 55% hydrofluoric acid, needs to be spilled to exceed PAC/TEEL-2 at a 1 km site boundary distance.

10 HAZARD CONTROL SELECTION AND CLASSIFICATION

Hazard controls are those engineered and administrative measures that act to prevent or mitigate hazards to workers, the public, or the environment. The primary purpose of the hazard and accident analysis is to select appropriate hazard controls and classify their importance to safety.

The initial identification of selection of hazard controls typically occurs as part of the HA process and is captured in the hazard evaluation table where potential means for preventing or mitigating the hazardous conditions (or hazard scenarios as described in Chapter 2) are listed. Identification of hazard controls should start during the hazard identification phase and carry through the end of the hazard evaluation or into the accident analysis phase.

Depending on the scope of the HA, hazard controls may be selected from existing controls or proposed as new controls. For design of a planned facility or major modification to an existing facility, the HA may be used to propose controls for the facility. For an existing facility, the HA may be used to evaluate the existing controls for the facility or recommended controls that may be needed.

In DSAs prepared for DOE HC-2 and -3 nuclear facilities, control selection is based on the unmitigated evaluation of hazardous conditions and accidents scenarios¹¹⁰. An unmitigated consequence potential above a predetermined level identifies events for which SS or SC controls may be needed. The mitigated evaluation involves the functioning of designated preventive and/or mitigative hazard controls that reduce consequence, likelihood, or both.

The control selection methodology depends in part on the 10 CFR Part 830 Subpart B "safe harbor" methodology being applied for the development of the DSA or other safety basis document. There are differences between the guidance from DOE-STD-3009-94 CN3, and its successor document, DOE-STD-3009-2014, and these also are different from other safe harbor methods such as the DOE-STD-1120-2016. Also, DOE-STD-5506-2007 identifies preferred and alternate controls for a range of hazardous conditions or DBA/EBAs that exist in many types of facilities that handle or dispose of TRU waste. Nonetheless, the guidance herein is general enough to apply to most control selection applications; where specific guidance from a safe harbor method is invoked, the appropriate reference is provided.

10.1 HAZARD CONTROL SELECTION

10.1.1 HAZARD CONTROL SELECTION PROCESS

The control selection process facilitates selection of those hazard controls that are relied on to prevent or mitigate a potential hazardous condition or accident, based on formal hazards and accident analyses. The process organizes and evaluates the initial identification of hazard controls from the hazard evaluation portion of the HA then provides supplemental or specific controls that are effective in preventing or mitigating postulated accidents from the formal accident analysis. The output is a compilation of controls that are essential for protection of the public, for CWs and facility workers, and for defense in depth.

10.1.1.1 HAZARD AND ACCIDENT ANALYSIS INPUT TO CONTROL SELECTION

The hazard evaluation includes the initial identification of hazard controls that is an integral element of most hazards evaluation techniques (see Section 2.8). There are several types of hazard controls (engineered, administrative) that may be designated as part of the hazard evaluation process and various ways to organize the information.

The potential severity of each hazard or hazardous condition identified in the hazard evaluation is estimated as part of the process. Control selection as described in this section is not necessary for accident scenarios that do not meet the criteria requiring SC or SS controls (i.e., are of low consequence and/or likelihood). For such low-risk events, it is sufficient to confirm that the hazard is adequately addressed by an implemented Safety Management Program, applicable regulatory requirements, and engineering features. After attributing controls to low-risk events, the controls should be reviewed and provided consideration as defense-in-depth or as a major contributor to defense-in-depth.

¹¹⁰ The term "accident" as used in this chapter may include "hazardous conditions" and "hazard scenarios" unless it is specifically referring to DBA/EBA scenarios.

Once the hazard scenarios are identified, the HA team identifies potential controls that are available for these events and to identify candidate controls that are available to prevent or mitigate the postulated accident scenarios. The list below details common practices for organizing information:

- A typical approach is to organize information into the bounding and/or representative hazardous conditions such that a common set of controls may be effective for the conditions defined. The bounding conditions facilitate the level of importance of the control set (e.g., SC); the representative conditions provide a basis for selecting the minimum set of controls that will address a common set of hazardous conditions.
- It is usual that unique conditions exist that are not completely represented by a common hazardous condition. This means that the candidate control set may be inadequate as well. In that case, those unique conditions should be evaluated as single events for which hazard controls will be determined.
- For a broad type of hazardous condition (e.g., fire events), it may be useful to represent different magnitude conditions as separate events. In this case, smaller-scale conditions may be bounding in frequency space, while larger-scale events may be bounding in consequence, or magnitude space. It is appropriate to represent both events, as the candidate controls may be different for each. For example, the smaller event may rely on preventive measures (e.g., ignition source control) to preclude ignition of combustibles, while the larger event may rely on mitigative measures (e.g., fire-rated barriers) to reduce the consequences of a major fire.

From the initial identification of hazard controls and throughout the process, the focus is to determine those controls that are most effective and practicable in controlling a particular hazard in the conditions analyzed. The HA team makes a final selection of controls that are relied on to perform or maintain a safety function, including controls required to protect assumptions. Effective control sets generally follow the recommended hierarchy¹¹¹ from DOE-STD-3009-2014, Appendix A:

- 1. Engineered controls¹¹² that are preventive and passive;
- 2. Engineered controls that are preventive and active;
- 3. Engineered controls that are mitigative and passive;
- 4. Engineered controls that are mitigative and active;
- 5. Administrative controls that are preventive; and
- 6. Administrative controls that are mitigative.

While this hierarchy is preferred, it may be determined that a hazard control lower in the hierarchy is more effective, reliable, or appropriate for the facility in question and for a given scenario. In such cases, a supporting basis should be developed for the selected hazard control.

The identification of hazard controls incorporates a defense-in-depth approach that builds layers of defense against a significant release of radioactive or other hazardous materials such that no single layer of defense is completely relied upon. This does not mean that all identified Safety Management Program or other hazard controls are part of the selected set of hazard controls. The control selection process evaluates the available pool of candidate controls from the hazard and accident analyses by considering the hierarchy of controls described above. Other control selection considerations are further discussed in Section 10.1.2, such as whether they are effective, efficient, reliable, and implementable.

¹¹¹ According to DOE-STD-3009-2014, Section A.8, an exception to this hierarchy is confinement of radioactive materials. In such cases, active confinement ventilation is preferred over passive confinement systems.

¹¹² Engineered controls are described as "structures, systems, and components (SSCs)" in DOE-STD-3009.

Bounding, representative and unique hazardous conditions are candidates for formal accident analysis (see Chapter 3, *Accident Analysis*). The accident analysis evaluates phenomenology associated with the various accident types as they apply to the specific facility or operations being analyzed. Hazard controls from the hazard evaluation are further evaluated in the accident analysis (based on the insights from the quantitative evaluation of accident conditions) to determine their safety classifications, as discussed later in this chapter.

10.1.1.2 HAZARD CONTROL TYPES

Controls selected are passive or active, preventive or mitigative, can be engineered or administrative, or serve to protect initial conditions or crucial assumptions in the analysis. Each is discussed below.

Preventive Control: Prevents an accident scenario or accident from happening or decreases its likelihood (frequency of occurrence). Preventative control approaches may act to prevent the initiation of an accident scenario or to interrupt an accident scenario before it leads to a hazardous condition. Prevention may also involve actions by an operator to shut down a process, close a valve, or take some other protective action. Operator actions should be sparingly relied on as a control strategy, due to inherent risk of inaction or error and overall less reliability than an engineered control. Preventive controls are functional prior to the initiation of an event, but are not required to survive the event provided the preventive function has been performed. The identification of such features is made without regard to any possible pedigree of the feature, such as procurement level or existing safety classification. Note that the elimination of a hazard (e.g., through substitution of a non-hazardous material) is not typically considered a "preventive" measure, but such action falls within the definition of a hazard control, and so should be documented when performed.

Mitigative Control: Decreases the potential consequences of the hazard scenario. It acts to reduce the severity of the hazard scenario or accident by providing barriers to an uncontrolled release of radioactive and other hazardous material or energy, such as confinement or shielding. Mitigation may also involve action by facility workers to self-protect from hazardous conditions by evacuation or sheltering, even though the accident sequence may continue uninterrupted (see Section 2.5.1, Qualitative Consequences, for determination of unmitigated consequences). Note that some hazardous conditions may not provide enough time to permit self-protective actions by workers, even if detection or monitoring capability exists.

Some controls are purely mitigative, others are purely preventative, and still others are both mitigative and preventative. Examples include:

- HEPA filtration is purely mitigative.
- The administrative control of preventing the entry of explosives into a nuclear facility is purely preventive.
- Fire suppression sprinklers can be both preventive and mitigative, but not for the same scenario (unless both functions are evaluated in an event tree analysis):
 - Suppression of the size of the fire and associated radiological or hazardous material reduces the consequence of the event (mitigative);
 - Failure of the sprinkler system may be credited to reduce the likelihood of a large fire (preventive) that has a larger radiological or hazardous material consequence than if it were credited to suppress or control the fire; or
 - Success of the sprinkler system may be credited to prevent any radiological or hazardous material release (preventive).

In practice, sprinklers are often considered preventive, that is, the controls are based on the preventive feature of sprinklers, not the mitigative, and are credited to reduce the scenario likelihood due to the failure of sprinklers, however, this is a site- or facility-specific decision.

In some cases, systems or features can serve different safety functions to different receptors. For example, shield walls are mitigative for the CW but may be preventive to facility workers by keeping them out of a high radiation area.

Engineered Control: SSCs that perform a safety function by preventing or mitigating a postulated hazardous condition or accident sequence. Engineered controls may be active or passive systems designed to function in the postulated accident environment. Active engineered controls may require one or more support systems or utilities to assure performance of their safety function. Failure mechanisms of active controls should be evaluated to identify support systems whose failure could defeat the safety function of the control. If an active control is found to not fail in a safe condition upon the loss of a support system, that support system also becomes a hazard control. Passive design features are generally more reliable than active systems when their design can withstand imposed loads or other environmental conditions postulated by the hazardous condition or accident.

When developing an engineered system, the analyst should be aware of limitations of the system and components taking into account the possibility that the event scenario may disable the functionality of the candidate control. For example, consider the limitations of a detection system. A detection system may be credited to lower a likelihood or consequence under some conditions, such as response to an alarm may be credited to reduce the potential that a small fire may become a large one and thus limit the total inventory involved. The analyst should take into account the possibility that the event scenario may disable the functionality of the candidate detection system. Necessary protective measures to prevent the loss of an engineered control due to the specific accident scenario progression will may also need to be credited as part of the hazard control.

Administrative Controls (ACs): Controls that are dependent on human actions. These controls are identified from the hazard evaluation and are designated as SACs, ACs, or are encompassed in safety management programs as committed to by a general TSR AC requirement. ACs also include (a) site/facility programs such as configuration management, (b) program elements such as control of combustible materials, and (c) safety requirements such as criticality safety limits.

DOE-STD-3009 provides a listing of safety management programs for consideration. SMPs are designed to ensure a facility is operated in a manner that adequately protects workers, the public, and the environment. By definition (10 CFR §830.3), SMPs are programs that cover topics such as quality assurance, maintenance of safety systems, personnel training, conduct of operations, criticality safety, emergency preparedness, fire protection, waste management, and radiological protection of workers, the public, and the environment. Where SMPs are selected as controls, the HA team should identify the most important elements of the program being relied upon (see DOE-STD-3009-2014, Section 4 [7.X.3]). The HA team should also determine if additional safety management programs are required based on the specific hazards present (e.g., explosives).

Depending on the situation, some ACs that perform specific preventive or mitigative functions for accident scenarios may be credited in the hazards evaluation or accident analysis. These are more specific functions than implied by general commitments to SMPs, and they may need to be raised to a higher importance level. Some of these ACs may have critical importance similar to or the same as those that would be classified as SC or SS, if the safety functions or objectives were performed by engineered

safety systems. These are called SACs. SACs are selected to provide a preventive or mitigative function for specific accident scenarios, and having a safety importance equivalent to a safety SSC. A SAC may replace or augment a safety SSC when an engineered feature is not available or not practicable. SACs may also provide a limit or boundary condition for the hazard or accident analysis, such as a radioactive material inventory limit. Refer to DOE-STD-1186-2016, *Specific Administrative Controls*, for discussion of SAC types and examples, and to DOE-STD-3009-2014 discussions in Sections A.11 and A.12 regarding SMPs and SACs, respectively.

ACs and SACs may also protect initial conditions or assumptions made that provide the bounding conditions in which hazard or accident scenarios are evaluated. Initial conditions and assumptions should be explicitly identified in the event one or more of them constitute a hazard control to be further evaluated for safety classification (see Chapters 2 and 3). Controls that protect assumptions are not credited for either frequency or consequence reductions but need to be protected for basic assumptions used in the analysis (e.g., MAR) to remain valid.

10.1.1.3 USE OF RISK MATRICES FOR CONTROL SELECTION

A method to supplement control selection uses a "risk matrix" approach, encouraged by DOE-STD-3009 and DOE-STD-5506-2007. This approach begins with unmitigated risk estimates (frequency and consequences) and follows a risk ranking process to identify higher risk hazardous events and provide a qualitative tool for enhancing the selection of hazard controls. The degree to which a given hazard control is judged to be effective in performing its preventive or mitigative safety function is illustrated in the risk matrix by the movement to lower frequency and/or consequence bins as controls are applied. Although these estimates are judgment-based, consistent application provides a sound basis for comparison.

The risk ranking process bins the results of unmitigated hazard and accident analysis for the public (via the MOI receptor), CWs onsite, and optionally, for the facility workers. Table 10-1 (an adaptation of Table 2-10 from Chapter 2) establishes risk ranking bins that consider the consequence rankings from Chapter 2 Table 2-8 together with the postulated accident likelihoods defined in Table 2-9. Based on these factors, an accident is ranked as Risk Class I through IV.

quence Bins		Beyond Extremely Unlikely	Extremely Unlikely	Unlikely	Anticipated
	High	III	П	Ι	Ι
onse	Moderate	IV	III	П	П
	Low	IV	IV	III	III

Fable 10-1 .	Typical	Risk	Class	Matrix.
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Likelihood Bins

I = Combination of conclusions from risk analysis that identify situations of major concern

II = Combination of conclusions from risk analysis that identify situations of concern

III = Combination of conclusions from risk analysis that identify situations of minor concern

IV = Combination of conclusions from risk analysis that identify situations of minimal concern

Risk Class I events for the public are addressed by hazard controls that are designated as SC SSCs or SACs, and by associated TSRs (see Section 10.2, Safety Classification of Controls) for radiological consequences or SS SSCs or SACs for chemical exposures.¹¹³ Operational accidents resulting in high offsite radiological consequences from the hazard evaluation are moved forward into accident analysis for determination of safety classification, without consideration of likelihood. High consequence NPH DBAs as defined by DOE-STD-1020 and external events with likelihood greater than 1E-6/yr are also moved forward into accident analysis for determination of safety classification. SS controls may also be warranted for protection of the public as discussed in Section 10.2.2.

Risk Class I events for the CW are addressed by hazard controls that are designated as SS, SSCs, SACs, and by associated TSRs. Risk Class II events for all receptors, are addressed by hazard controls for which consideration as SS SSCs, SACs, and by associated TSRs should be made. The consideration of a SS hazard control is based on the effectiveness and feasibility of the controls along with the identified features and layers of defense in depth. Risk Class II events resulting in high offsite radiological consequence are included in subsequent accident analysis for determination of safety classification, without consideration of likelihood.

In essence, controls are considered for any unmitigated Risk Class I/II events. Preventive controls applied to the initial unmitigated Risk Class I/II event may suffice to prevent the event. Mitigative controls applied to the initial unmitigated Risk Class I/II event should reduce the event consequence to an acceptable value below the EG. In some cases, more than one control may be required to reduce the consequence and/or likelihood from Risk Class I/II to Risk Class III or IV depending on its reliability or efficiency.

Risk Class III – Consider defense in depth hazard controls or safety management programs to reduce risk to Risk Class IV. Risk Class III events are generally addressed by SMPs or other Administrative Controls. However, they may require further evaluation of the need for SS controls for high-consequence operational events judged to be beyond extremely unlikely. Use of qualitative risk binning does not negate the need to designate safety SSCs and/or SACs for plausible operational accidents using the consequence thresholds established in DOE-STD-3009. These events may also be considered for defense-in-depth SSCs in unique cases.

Risk Class IV – No additional hazard control measures apply that are explicitly credited with a SC/SS designation as identified in the DSA, but may still be identified in a hazard evaluation table.

As stated above, facility workers may or may not be evaluated for control selection purposes using the risk matrix approach. If included, the above risk guidelines for protection of the CW are applied for selection of controls to protect the facility worker. If the facility worker is not evaluated using the risk matrix approach, facility workers exposed to a high consequence event (as defined on Table 2-8, Consequence Thresholds) may require an SS SSC or SAC. Consequences below high generally are dealt with using an SMP or other administrative control.

When the risk matrix approach is *not* used, the designation of hazard controls as SC, SS, or SACs follow the guidance provided in Section 10.2 without the enhancement of a risk ranking to demonstrate control effectiveness.

¹¹³ Per DOE-STD-3009-2014 Sections 3.3.1 and 3.3.1, SC SSCs, SACs, and TSRs are established for radiological events that exceed or challenge the 25 rem Evaluation Guideline (regardless of frequency).

10.1.2 HAZARD CONTROL SELECTION CONSIDERATIONS

The hazard controls compiled from the hazards and accident analyses form the basis for control selection. Candidate hazard controls should receive specific considerations from operations, engineering, maintenance, and safety basis staff. These considerations should include the following matters.

Effectiveness

- Does the control function in the accident environment postulated? Are specific qualifications needed?
- Is the control most effective in reducing risk?
- How far from the hazard are the controls located? ¹¹⁴?
- Where is the control on the control hierarchy? Is the selection justified?

Efficiency

- Is the control effective for several accidents or hazardous conditions? Does it provide defense in depth or worker safety for multiple events?
- Is the control dependent on support systems or utilities? Are these also qualified for their environment?
- Does the control minimize the number of active or supporting safety features?
- Does the control provide functional diversity or redundancy?
- Is the control cost-effective?

Implementation & Reliability

- Does the control preclude the need for compensating measures or features?
- Is the control simple or straightforward to establish, surveil, and maintain?
- Is the control insensitive to random failure or false indication?
- Does the control provide advance notification of trouble (accident does not initiate upon failure)?
- Does the control incorporate human factors to ensure reliable performance or to facilitate surveillance and maintenance?
- Is implementation of the control practicable in terms of impact on the primary process and the cost of installation and operation?

Functional and environmental requirements should be defined with due consideration of the hazard analysis, accident analysis, and design engineering processes. To develop the performance specifications for equipment relied upon in mitigating or preventing the accident under conditions existing during and following the accident scenario, consider the following.

- The time-dependent temperature and pressure at the location of the equipment during the most severe DBA/EBA.
- The humidity during the accident scenario.
- Chemical effects especially if the composition of the chemicals can be affected by equipment malfunctions.
- The radiation environment associated with the DBA/EBA during which the equipment is required to remain functional.
- Aging of equipment could cause degradation which can have an effect on the functional capability of the equipment.

¹¹⁴ In some scenarios, the closest controls may be more effective.

- Synergistic effects are to be considered when these effects are believed to have a significant effect on equipment performance.
- Interactions of the system with other environmental stresses of the accident environment, such as filter loading or water spray from fire sprinkler activation.

Selected hazard controls should reflect a robust, defense in depth approach to postulated accident scenarios. Redundancy and overlap are encouraged.

10.2 SAFETY CLASSIFICATIONS OF CONTROLS

10.2.1 SAFETY CLASS DESIGNATION

DOE-STD-3009 defines an EG of 25 rem TED to the public and requires designation of SC SSC to mitigate the dose to below the EG. The dose estimates to be compared to it are those received by a hypothetical MOI or public receptor at the site boundary from a DBA or EBA causing an unmitigated release of radioactive material that challenge the EG (see DOE-STD-3009-2014, Section 3.3.1 regarding MOI unmitigated doses exceeding 5 rem TED that may challenge the EG). The control selection process of DOE-STD-3009-2014, Section 8.1 will result in the identification of hazard controls that will prevent or mitigate DBA/EBA consequences to less than the EG. Additional controls to further reduce consequences to well below the EG or to provide defense in depth may be candidates for SS designation as discussed in DOE-STD-3009-2014, Section 8.2.2.

10.2.2 SAFETY SIGNIFICANT DESIGNATION

The designation of SS SSC is based on the criteria from Section 3.3 of DOE-STD-3009-2014 for selecting SS controls are based on four criteria: (1) protecting CWs at 100m that receive an unmitigated dose of 100 rem TED; (2) protection of the public from releases of hazardous chemicals; (3) protecting facility workers from significant injury or fatality, or from exposure to radioactive or hazardous material (not including standard industrial hazards, see Section 2.2.4); or (4) determined to be a major contributor to defense in depth that provides additional protection of the public and the environment. These four criteria are more specific than the criteria of DOE-STD-3009-94, CN3.

10.2.3 CLASSIFICATION OF OTHER HAZARD CONTROLS

The hazard evaluation process could identify preventive or mitigative controls that do not rise to the level of SC or SS controls but still enhance the safety of the facility. These controls are identified in the hazard evaluation table and may be determined to be important to defense in depth or worker safety, but not explicitly credited with a SC or SS designation. See guidance on defense in depth in DOE-STD-3009-2014, and in the DOE Guide DOE G 420.1-1A, *Nonreactor Nuclear Safety Design Guide for Use with DOE O 420.1C, Facility Safety.* Such controls are maintained in accordance with SMPs or other ACs and the Unreviewed Safety Question process (which includes consideration of equipment important to safety as described in the DOE G 424.1B, *Implementation Guide for Use in Addressing Unreviewed Safety Question Requirements*).

Specific controls may be required by DOE in its Safety Evaluation Report. (See DOE-STD-1104-2016, *Review and Approval of Nuclear Facility Safety Basis and Safety Design Basis Documents*, for further guidance.) These controls will be designated SC or SS if so directed in the SER.

10.3 EVALUATION OF EXISTING FACILITIES WITH MITIGATED OFFSITE CONSEQUENCE ESTIMATES OVER THE EVALUATION GUIDELINE

There is a special case if the MOI consequences cannot be prevented or effectively reduced to below the EG. This "Over the EG" evaluation is required for all existing DOE facilities with mitigated offsite consequence estimates over the EG, regardless of the safe harbor used. This "Over the EG" evaluation is expected to be rarely applied. The following additional guidance and methods are provided for effective implementation, when used.

DOE-STD-3009-2014, Section 3.3.1, establishes requirements for existing facilities with mitigated offsite consequence estimates over the EG where the EBA is not prevented. In addition, the DOE review and approval of the DSA includes DOE requirements and guidance for this situation, as described in the DOE-STD-1104-2016, *Review and Approval of Nuclear Facility Safety Basis and Safety Design Basis Documents*, Section 4.9, Existing Facilities with Mitigated Offsite Consequence Estimates over the EG. The requirements and guidance from both standards are summarized on Table 10-2, along with additional clarifications and guidance.

DOE-STD-3009-2014 Section 3.3.1, SC Controls	DOE-STD-1104-2016 Section 4.9, Existing Facilities with Mitigated Offsite Consequence Estimates over the EG	Additional Clarifications and Guidance
In circumstances where no viable control strategy exists in an existing facility to prevent or mitigate the consequence of one or more of the accident scenarios from exceeding the EG, the following information shall be provided in the DSA, or an attachment to the DSA:	This section provides specific approval bases for rare situations where safety class controls are not provided to prevent or mitigate offsite doses below the EG. For proposed changes to an existing facility safety basis where no viable control strategy exists in an existing facility to prevent or mitigate the consequence of one or more of the accident scenarios from exceeding the EG, DOE shall verify that information is included in the proposed safety basis change that addresses the requirements described in Section 3.3.1 of DOE-STD-3009-2014. The following criteria should be used to judge technical adequacy of DSA information:	The DSA Section [3.4.3.X.5], Summary of SC and SS SSCs, SACs, and TSR Controls, may be an appropriate location to document the "Over the EG" evaluation, or depending on its complexity, an appendix may be more suitable that is referenced in this section of the EBA evaluation. An executive summary of this evaluation should be included in the DSA Section [E.6], Safety Analysis Conclusions.
• Identification of the accidents that cannot be mitigated or prevented, including the likelihood of the events and the mitigated consequences associated with the events, based on	• Accidents that cannot be mitigated below the EG or prevented, are explicitly identified, including the likelihood of the event and the mitigated consequences associated with the event.	Accidents that cannot be mitigated below the EG or prevented, are explicitly identified in the DSA accident analysis of the EBA and further evaluated. An example of an EBA that cannot be prevented or mitigated below the EG could be a collapse of the structure from a DOE Order O 420.1C design basis earthquake that has a greater magnitude due to a 10-year

Table 10-2. Over the EG Evaluation.

DOE-STD-3009-2014 Section 3.3.1, SC Controls	DOE-STD-1104-2016 Section 4.9, Existing Facilities with Mitigated Offsite Consequence Estimates over the EG	Additional Clarifications and Guidance
calculations following the methodology described in this Standard.	 Accidents likelihood and consequences are determined in accordance with the DSA safe harbor methodology (e.g., Section 3.2 of DOE-STD- 3009-2014). This includes source term estimates, dispersion analysis methodology, and dose consequence assumptions. 	updated assessment of seismic hazards that is being evaluated for an existing facility. Accident likelihood and consequences are summarized from information that is already part of the DSA accident analysis for the EBA such as Sections [3.4.3.X.1] Scenario Development, [3.4.3.X.2] Source Term Analysis, and [3.4.3.X.3] Consequence Analysis
• A discussion of the credited controls, including their reliability and adequacy, and an analysis	• The reliability and adequacy of credited controls is addressed consistent with DOE-STD- 3009-2014 system evaluation requirements for SC SSCs.	This should include identifying the safety function of the credited control to prevent or mitigate the EBA as described in the DSA Chapter 4 along with a description on how they prevent the event, or reduce its likelihood or consequences. The reliability and adequacy of credited controls should be described, along with discussions of potential failure modes of these credited controls, and any compensatory measures established. This information is already part of the DSA Chapter 4 and is summarized in the "Over the EG" evaluation. Significant contributors to uncertainty in both the likelihood and consequence evaluations associated with the credited controls should be identified and characterized.
 A discussion of the available controls⁶⁰ that could reduce the likelihood and/or consequences of the associated accidents, including their potential failure modes, their potential impact on accident mitigation, any relevant cost/benefit results, and the reasons why they are not selected as credited controls to reduce the consequences to below the EG. ⁶⁰ Controls considered but not identified as SC controls that were not elevated to SC status, as 	• Controls considered (SSCs and SACs) but not identified as SC that could further reduce the likelihood and/or consequences of the associated accidents are described in the DSA. The impact of these controls on accident mitigation, as well as the rationale for not classifying these controls as SC should be presented. Discussions of potential failure modes of SSCs and any relevant cost/benefit results are included.	Footnote 60 clarifies other available or new controls that were considered, which could include additional MAR restriction, operational restrictions, and/or additional compensatory measures. Those existing controls (SSCs and ACs) considered but not identified as SC are identified and described, including their impact on accident mitigation or further reduction in the likelihood. The rationale for not crediting and classifying these controls as SC should be provided. Some examples include lack of reliability of the SSC that cannot be augmented with compensatory measures to provide a SC safety function, effectiveness of the control, human factors considerations to implement the AC as a SAC, and feasibility of implementing a new control. Discussions of potential failure modes of these potentially available controls and any relevant cost/benefit results should be included in the discussion. This section addresses controls that were consider that can be readily
DOE-STD-3009-2014 Section 3.3.1, SC Controls	DOE-STD-1104-2016 Section 4.9, Existing Facilities with Mitigated Offsite Consequence Estimates over the EG	Additional Clarifications and Guidance
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well as new controls that could have been established through changes to the facility or to its operations. This includes controls to reduce the radiological source term. Controls can include SSCs and ACs.		implemented rather than those additional controls that are being committed to and identified in the next section on planned operational or safety improvements.
 A discussion of any planned operational or safety improvements, including potential facility modifications, reductions in MAR, and/or additional compensatory measures, and associated schedules, to further reduce the likelihood and/or mitigate consequences of an accident. Note: Where DOE has accepted a path forward, the path forward may be used to support this discussion. 	• Planned operational or safety improvements are presented and include potential facility modifications, removal of MAR, packaging of MAR into containers, operational restrictions, and/or additional compensatory measures, and associated schedules, to further reduce the likelihood and/or mitigate consequences of an accident.	This section addresses additional measures that are being committed to, including new preventive or mitigative controls that can't be readily implemented, and are identified as planned operational or safety improvements. The STD-1104 guidance identifies some of the potential improvements, and discussion of associated schedules. Where compensatory measures that are not readily implementable will be provided, these should be clearly identified and summarized.
 A discussion of an analysis of the expected likelihood and mitigated offsite consequence estimates of the associated accidents. The analysis should include a discussion of the significant contributors to uncertainties in both the likelihood and consequence evaluations. The analysis should compare the risk (i.e., likelihood and consequences) based on calculations performed per Section 3.2 of this Standard to the risk calculated using 	 Mean or best estimate values used for source-term and dispersion input parameters that are part of comparative analyses (as described in DOE- STD-3009-2014, Section 3.3.1, bullet #2) have a valid technical basis that includes logical assumptions that are based on experiments, tests, or sound engineering judgment. The analysis describes the significant contributors to uncertainties in both the likelihood and consequence evaluations. The mean or best estimate calculation is used to provide perspective regarding the degree of conservatism that is imbedded in the consequence calculation. 	A more realistic risk assessment of the EBA provides an important perspective for the contractor and DOE acceptance of risk associated with not preventing or mitigating the EBA to below the EG. This section should present any quantitative or qualitative evaluations of the risks and document the basis for risk acceptance. DOE Policy 420.1, <i>Nuclear Safety Policy</i> , establishes two goals (not requirements) for public protection: 1) The risk to an average individual in the vicinity of a DOE nuclear facility for prompt fatalities that might result from accidents should not exceed one-tenth of one percent (0.1%) of the sum of prompt fatality risks resulting from other accidents to which members of the population are generally exposed. For evaluation purposes, individuals are assumed to be

DOE-STD-3009-2014 Section 3.3.1, SC Controls	DOE-STD-1104-2016 Section 4.9, Existing Facilities with Mitigated Offsite Consequence Estimates over the EG	Additional Clarifications and Guidance
 mean or best estimate values for source-term and dispersion input parameters (with supporting technical basis). A qualitative or semi- quantitative comparison of the facility risk from the identified scenarios and total facility risk (i.e., cumulative risk estimate for facility accidents) with the quantitative safety objectives provided in DOE Policy 420.1. Discuss the level of risk and the basis why this risk is acceptable, taking into account an evaluation of available alternatives, the benefits to the public of the alternatives. 	 A qualitative or semi- quantitative comparison of the facility risk from identified scenarios and cumulative facility risk (for all facility operations) estimate for facility accidents (including the results in response to the second bullet) is presented along with a comparison to the quantitative safety objectives provided in DOE Policy 420.1. A discussion of the level of risk and the basis why this risk is acceptable is provided, taking into account an evaluation of available alternatives, the benefits to the public of the alternatives, and the costs to the public of the alternatives. 	 located within one mile of the site boundary. 2) The risk to the population in the area of a DOE nuclear facility for cancer fatalities that might result from operations should not exceed one-tenth of one percent (0.1%) of the sum of all cancer fatality risks resulting from all other causes. For evaluation purposes, individuals are assumed to be located within 10 miles of the site boundary Site-specific or locality-specific quantitative data should be used whenever available. For the DOE Policy 420.1 risk perspectives, the risk from the facility includes the full- spectrum of operations, including normal operations, operational accidents, external events, and NPH events. Other accidents/events could be presented for perspective, such as risk of a prompt fatality or latent cancer fatalities from aircraft crashes, dam failures, fires, explosions, chlorine releases, and natural phenomena events as previously evaluated for the nuclear reactor industry.
The level of detail for the analysis above may be implemented on a graded approach that considers the remaining operating life of the facility and the extent of deviation from the EG. For example, where the remaining lifetime of the facility is less than five years, a detailed analysis using mean values and making comparisons to the DOE Policy 420.1 safety goals is not necessary, but a discussion of available controls considered and planned safety improvements and associated schedules is expected.	The level of detail for the analysis above may be graded based on the remaining operating life of the facility and the extent of deviation from the EG. The DOE review should consider the best available mission statements related to facility operations and determine whether there is a high likelihood that projected estimates of remaining operational life are supported and commensurate with details provided in the DSA. Likewise, the extent of deviation from the EG for mitigated consequences estimates should be explicitly addressed by the DOE review team and discussed in the SER as part of the approval basis. Planned operational or safety improvements, including compensatory measures, should be pursued where the deviation	

DOE-STD-3009-2014 Section 3.3.1, SC Controls	DOE-STD-1104-2016 Section 4.9, Existing Facilities with Mitigated Offsite Consequence Estimates over the EG	Additional Clarifications and Guidance
	from the EG is significant (such	
	as where the mitigated offsite	
	dose estimate is more than two to	
	three times greater than the EG),	
	the remaining life is significant	
	(such as more than 1-3 years), and	
	the likelihood is significant (such	
	as more often than 1 in 10^6 years).	
	Compensatory measures should	
	be commensurate with the	
	significance of the deviation from	
	the EG, the likelihood of	
	accidents, and the length of time	
	needed to resolve the condition.	

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APPENDIX A: HAZARD ANALYSIS TABLE DEVELOPMENT

This appendix provides examples of the documentation of hazard analysis (HA) results to support development of a safety design basis document. Although other formats may be used to capture this information, a table format has been selected to capture the requirements. This table is prepared with columns or sections corresponding to the headings of sections A.1 through A.10 of this appendix. Those sections describe the content of the corresponding column of the table for each HA hazard scenario. This format can be used to document the Preliminary Hazard Analysis (PHA) developed during the conceptual design, or the hazard evaluation at the process level developed during the preliminary or final design. It should be updated as the design matures through final design and transition to operations.

As this documentation is a central element of the safety basis, it is maintained after project transition to operations as a basis document for the final Documented Safety Analysis (DSA) or a supporting document for the DSA. Although alternate formats such as a database may be used to capture and retrieve this information, the material identified in this appendix is required to be developed for projects subject to DOE-STD-1189-2016, *Integration of Safety into the Design Process* or its predecessor, DOE-STD-1189-2008. The appropriate HA technique is selected that will be sufficiently detailed to provide a comprehensive examination of the hazards associated with the facility given the complexity of the operation and degree of design maturity and develop the information required by this appendix. See Chapter 2, "Hazard Analysis," for further discussion of the hazard evaluations.

A.1 SCENARIO DESCRIPTION

Describe each postulated hazard scenario that could lead to the release of radioactive and hazardous materials or energy. The description should appropriately describe the mechanisms that lead to the release. Examples include spills, over-pressurization, deflagration, fire, and similar mechanisms. This description should be as complete as possible for the current design stage to facilitate use in developing controls and their functional and design requirements, as well as support unreviewed safety question determinations during operation.

The description should also include an explicit description or reference to the Material at Risk (MAR), chemical or radiological, as appropriate, involved with or potentially affected in the scenario. As appropriate, describe the effect that the initiating event has on the major facility structures, systems, and components (SSCs), primarily those that could release energy or radioactive/hazardous material.

Scenarios identified during the PHA process for conceptual design will be facility-level or major MAR location events for the facility. The objective in conceptual design is to review the release mechanisms for the major MAR inventory locations sufficiently to ensure that high-cost safety functions have been identified and included in the project design and cost estimates.

A.2 INITIATING EVENT FREQUENCY

Provide the conservatively assigned likelihood or frequency of the initiating event of the hazard scenario, where a series of events contribute to a release of material, such as fire events or a natural phenomena hazard (NPH) followed by spill or fire. The goal is to qualitatively bin the event likelihood (Anticipated, Unlikely, Extremely Unlikely, and Beyond Extremely Unlikely) sufficiently to aid in event prevention and mitigation strategy selection. The initiating event frequency should be consistently applied as the initiator frequency.

A.3 UNMITIGATED CONSEQUENCE EVALUATION

Describe the radioactive and hazardous material or energy release with respect to facility workers in each unique location, co-located workers, and offsite public that are affected.

Identify the consequence to each receptor for the event. Although detailed knowledge may not be available, qualitative conservative determinations of dose consequences are needed so that the safety control selection is also conservative. When available, quantitative information should be used as a guide for consequences due to chemical or radioactive material releases based on bounding assumptions. However, binning into defined ranges is preferred and specific values are not required. This is especially true for facility worker consequences, which are intended to be qualitative, but also applies to qualitative estimates of co-located worker and public consequences.

Assumptions established as a part of the consequence determination should be identified, in order to provide the technical basis for parameters of interest. Particularly, the radioactive or hazardous material inventory, airborne release fraction (ARF), and damage ratio (DR) and their bases should be described. Reference appropriate calculations that support the identified consequence, when they have been performed.

While an assessment of the level of hazard scenario consequences is necessary to determine the need and safety classification of SSCs providing protection of facility workers, these assessments should be, at most, "back of the envelope" calculations, to give a sense of the order of magnitude of the doses. In the case of facility worker consequences, especially immediately involved workers, the assumptions that could be made in the course of any more definitive calculations could easily affect the results by orders of magnitude. Thus, such calculations, if used to apply a numerical criterion, would divert attention from good safety decisions to arguments about the calculations and assumptions during the review.

A.4 SAFETY FUNCTIONS

Within an operating facility, or during the preliminary and final design phases of a new facility, controls (SSCs or ACs) are already identified to perform a generic preventive or mitigative safety function. However, during the conceptual design phase of a new facility, generic safety functions are first defined instead of the controls themselves. The next entry in the hazard analysis table is a list of these generic safety functions needed to prevent or mitigate any release event. The safety function is a qualitative statement of a function that prevents an initiating event or release, or that mitigates the outcome. The safety function is the desired result from an SSC or administrative action and should be stated in a general way, while still describing the preventative or mitigative action.

For conceptual design, the safety function in this entry should not specify a SSC or otherwise state how the safety function is satisfied. This has two purposes: (1) it provides flexibility in SSC selections; and (2) it ensures that the specific functional and design attributes for a selected SSC fulfill the defined higher-level safety function identified for the event. Additional considerations in defining safety functions are as follows:

• The safety function statement during the conceptual design phase serves as a link between the HA and the safety SSCs that are later identified to fulfill safety functions, thus defining the overall objective and top-level functional requirements for the SSC. The top-level functional requirements are those performance parameters of special importance because they are specifically relied upon in the safety analysis.

- Safety functions should not be predicated on the SSCs or Specific Administrative Controls (SACs) that may be chosen to provide the function. The opportunity for novel and improved solutions is reduced when the solution drives the requirement.
- The generic safety function statement at this stage should be sufficiently specific to enable assigning appropriate supporting SSCs or SACs to fulfill the needed safety function completely.
- Safety functions should include the following:
 - situations and any general hazard scenario or accident types during which the function is required to be met;
 - o specific functional needs that prevent, detect, or mitigate an event; and
 - sufficient description to enable clear functional requirements and later, design requirements and performance criteria for those SSCs ultimately chosen to meet the top-tier safety function described.

A.5 PREVENTIVE FEATURES (DESIGN AND ADMINISTRATIVE)

List all SSCs and administrative controls (ACs) that have the potential to prevent the release or the event initiator, or reduce the frequency of accident progression. This should be consistent with the approach used to determine the likelihood (see Section A.2 above). In the early stages of the conceptual design process, this listing may include SSCs that are currently not part of the conceptual design; but, if selected, would be added to the conceptual design. Initiating events that cannot be prevented, such as NPH events that lead to a release, should be listed as not applicable (N/A).

This listing will be used to select the suite of safety systems, important to safety systems, and/or defense in depth SSCs for the release events. When complete at Critical Decision-1, only SSCs actually present in the conceptual design should be included.

A.6 METHOD OF DETECTION

Identify all SSCs and administrative functions that could detect the event. This would include SSCs that may or may not be selected, as well as direct observation by the operators. In the early stages of the conceptual design process, this listing may include SSCs that are currently not part of the conceptual design.

A.7 MITIGATIVE FEATURES (DESIGN AND ADMINISTRATIVE)

List all SSCs and ACs that potentially could mitigate the event by limiting the consequences after the event has happened. In early stages of the conceptual design process, this listing may include SSCs that are not currently part of the conceptual design. Consideration of the following mitigative systems and design features should be included:

- Fire suppression/detection;
- Confinement ventilation;
- Emergency power;
- Nuclear criticality design features and/or alarms, consistent with DOE-STD-3007-2017;¹¹⁶
- Seismic design, including addressing level of confinement for primary confinement system (building structure); and

¹¹⁶ If the facility is expected to contain a critical mass of fissionable material.

• Flammable gas controls.

A.8 SSC SAFETY CONTROL SUITE AND SAFETY FUNCTIONS

Summarize the suite of hazard controls, including safety SSCs that will be relied upon to detect, prevent, or mitigate each event. The requirements in DOE O 420.1C, *Facility Safety*, are essential inputs to the identification of the safety control suite selected, the functional classification of selected SSCs, and the NPH requirements.

The hazard controls identified in the conceptual design PHA are preliminary until later safety analysis confirms their need and validates that they are the correct and adequate controls for the event. The identification of the hazard controls should be conservative to establish an appropriate cost and schedule basis for the project. The selection of hazard controls is iterative. If, after selecting one or more of the available controls, the mitigated consequence still exceeds the applicable threshold criteria, additional controls are selected or identified and classified accordingly. In some cases, it may be prudent to use multiple controls where only one may be required to effectively prevent or mitigate the event. Where SACs are included in lieu of an SSC, an explanation should be provided. The final list of selected controls should be provided in the PHA tables.

A.9 MITIGATED CONSEQUENCES

Estimate the consequences for the identified receptor after crediting the hazard controls. During conceptual design, the quantitative results for the unmitigated events may not be known. In this case, the mitigated results are qualitatively estimated based on a reduction factor on the unmitigated consequences. Once the design basis accident (DBA) analysis is performed, this section will be updated with the results of this quantitative analysis. If the preventive controls eliminate the hazard or terminate the hazard or accident scenario and prevent a release of radioactive or other hazardous materials, this result is reported in the mitigated consequence column as "prevented." The result is input to the overall control suite of the safety design basis.

A.10 PLANNED ANALYSES, ASSUMPTIONS AND RISK/OPPORTUNITY IDENTIFICATION

List remaining analysis or assumption validations and risk/opportunities associated with the selected strategies. The bounding events that require further analysis are identified in the PHA. The events selected are grouped into DBAs that are representative of the hazardous conditions and accident categories. The DBAs are defined in such a way as to predict the consequences so as to be bounding for all similar events with the same control suite. Other events, for which the need for hazard controls (or the functional classification or NPH criteria) was not obvious, should also be evaluated in more detail (potentially quantitatively) later in the preliminary design phase. This will ensure that the selection for each safety control has a firm basis and that the assigned functional classifications and design criteria are also based on objective determinations.

Assumptions used in the PHA process need to be verified as the design matures. As an example, the facility MAR used in the hazards analysis may have been based on a highly conservative assessment of tank volumes and concentrations. When the final documents and process and instrumentation drawings are issued in preliminary design, the actual tank volumes should be used in the DBA analyses. Other assumptions concerning the event progression, such as impact to SSCs, are also verified. Remaining evaluations to be performed are identified.

Potential risks and opportunities should be fed into the Risk and Opportunity Assessment as the safety control suite is constructed. The presentation of risks and opportunities associated with the strategies are essential elements of risk-informed decision-making in the authorization for the project to proceed to preliminary design.

A.11 HAZARDS EVALUATION TABLE

Construct the final hazard evaluation table. This table includes the items discussed above and portrays the hazard scenarios associated with the facility and the safety systems that will detect, mitigate, or prevent unacceptable MAR and energetic releases. The table should present the logical binning of events evaluated. In essence, these scenarios are those from which the DBAs for the facility are selected. The table provides valuable information to be included in the risk and opportunities analysis and needed studies to validate fundamental assumptions. This table portrays the functional safety attributes for the facility safety systems that are to be incorporated into the conceptual design and cost estimates. The final table will be used as the foundation for development of the safety basis design documents, which will describe the events evaluated and the safety control suite in a format that can be used as the foundation for a final DSA for the facility.

APPENDIX B: CRITICALITY ACCIDENTS

B.1 INTRODUCTION

The purpose of this appendix is to provide guidance for the quantitative estimate of radiological doses to support the qualitative assignments of consequences for the DSA hazard evaluation as discussed in Section 2.3.2, Nuclear Criticality Hazard Evaluation, of this Handbook. As discussed in Section 2.3.2, criticality hazards are those associated with process operations, not nuclear reactors or sub-categories of nuclear reactors, such as critical experiments. The general approach to evaluate a dose from a criticality accident is:

- 1. Determine the fission yield (i.e., power history).
- 2. Determine the direct (prompt) dose at the appropriate distance.
- 3. Determine fission product quantities.
- 4. Determine the source term for inhalation dose. This includes the determination of nuclides present in the released cloud at the time of exposure, including the effects of decay during transport.
- 5. Determine external beta and gamma doses from the cloudshine and groundshine.

Section B.2 provides a brief overview of current regulatory requirements, recommendations, and guidance. Guidance for the first two these steps is provided in Section B.3 on determining fission yields, and in Section B.4 on direct (prompt) dose. The last three steps are briefly addressed in Section B.5 on the source term analysis of fission product inventories, airborne release fractions (ARFs) and respirable fractions (RFs), and radiological dose assessments.

Criticality accident hazards are unique to nuclear facilities and even then only to a subset of these facilities. This subset has a fissile material inventory that is significant, generally defined as exceeding the single parameter subcritical mass limits given in ANSI/ANS-8.1-2014, *Nuclear Criticality Safety in Operations with Fissionable Materials Outside Reactors*, and requiring specific criticality controls to reduce the likelihood of a criticality accident to an acceptable level. This acceptable level is generally one that results in the accident likelihood being judged to be incredible.

Commonly accepted terminology, as used in the criticality safety discipline, is found in report LA-11627-MS (Paxton, 1989). In particular the following two terms are important to the discussions in this Appendix:

Criticality Accident: The release of energy as a result of accidentally producing a self-sustaining or divergent fission chain reaction.

Criticality Safety: Protection from the consequences of a criticality accident, preferably by prevention of the accident. Encompasses procedures, training, and other precautions in addition to physical protection.

Criticality accidents outside of reactors (such as process criticality accidents) are the subject of this Appendix. Criticality accidents associated with reactors, including critical experiments, are considered and analyzed under the umbrella of Reactor Safety, a separate discipline.

Process criticality accidents have been few, both in the US and worldwide, 7 and 22, respectively; and fatalities have been similarly infrequent, 2 and 9, respectively (LA-13638, McLaughlin et al., 2000). The most recent US criticality accident was in 1978 and worldwide in 1999. No accidents have resulted in

any significant mechanical energy release, and radiation exposure is the only significant hazard. From criticality accidents seen to date, significant doses have only been associated with nearby facility workers, with insignificant exposures to co-located workers (CWs) outside the facility, the public, or the environment.

When criticality accident likelihoods are judged to be non-trivial in a facility, then it is almost always concluded that a criticality accident alarm system is an appropriate safety system for consequence mitigation, in accordance with ANSI/ANS-8.3-1997 (R2012), *Criticality Accident Alarm System*. Competing risks associated with the response to false alarms may rarely modify the decision as to when a criticality accident alarm should be installed.

B.2 REGULATORY REQUIREMENTS, RECOMMENDATIONS AND GUIDANCE

DOE O 420.1C, *Facility Safety*, and 10 CFR Part 830, Subpart B, both address the process analysis requirement from ANSI/ANS-8.1 Section 4.1.2:

Before a new operation with fissionable material is begun, or before an existing operation is changed, it shall be determined that the entire process will be subcritical under both normal and credible abnormal conditions.

Credible accidents, including credible criticality accidents, are analyzed in the Documented Safety Analysis (DSA). It is assumed that controls for the prevention of criticality accidents are, or will be, in place. It is also assumed that the need for criticality alarms will be determined, and alarms installed, if required by the ANSI/ANS-8.3 evaluation. This Appendix also assumes that enough fissionable material is being handled in a manner such that any potential criticality accident is identified by the hazards evaluation. If the fissionable quantities are below the minimum subcritical limits in the appropriate ANSstandard (ANSI/ANS-8.1-2014 or ANSI/ANS-8.15-2014, *Nuclear Criticality Safety Control of Selected Actinide Nuclides*) analysis of a criticality accident may not be needed, and in this instance would not be identified in the hazard evaluation.

In addition to the guidance provided in this Appendix, ANS-8 Standards that are particularly pertinent to accident analysis include ANS-8.1; ANS-8.3; ANS-8.10 and ANS-8.23. Additional DOE guidance is found in DOE-STD-3009-2014 and in DOE-HDBK-3010-94.

B.2.1 UNMITIGATED ANALYSIS

DOE-STD-3009 provides guidance on unmitigated accident analysis. In essence, unmitigated analysis means that controls intended to prevent or mitigate an accident are assumed not to function. In the case of a criticality accident, this means, in part, that the accident is assumed to happen with no mitigative features taken into account. An exception to this is that passive safety features that can be shown to survive the initiating event may be considered in the analysis. For example, if a seismic event causes a criticality accident in a shielded area (including building walls), and the shield can be shown to survive the event, then the effectiveness of the shield in mitigating worker accident doses can be accounted for in the unmitigated analysis. Passive features assumed to perform their safety functions are evaluated per DOE-STD-3009 for designation as safety class or SS SSCs and protection as TSR controls.

For the analysis of criticality accidents that have the potential for lasting longer than an initial pulse, the accident duration should be limited to two (2) hours, except for scenarios that are slow to develop and complete. In those cases, the accident duration should be limited to eight hours (based on guidance from DOE-STD-3009). These analyses should be based on bounding scenarios. If able to be estimated, the dose integration time should be based on the power history of the postulated accident scenario.

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DOE-STD-3009 requires the analysis of unmitigated accidents to determine the class of needed controls, that is, safety class or SS. For purposes of this Appendix, the need for safety class controls is based on the unmitigated consequences to the public at the site boundary, and the need for SS controls is based on the unmitigated consequences to the co-located worker. The co-located worker is 100 meters from the criticality accident for direct exposure calculations. For atmospheric dispersion, the co-located worker is 100 m from the building emission point. DOE-STD-3009 also has requirements related to selecting SS controls based on other criteria; however, these criteria are not addressed in this Appendix. In general terms, if the dose to the public at the site boundary is less than 0.05 Sv (5 rem), safety class controls are not needed, and if the unmitigated dose exceeds 0.25 Sv (25 rem) then safety class controls are not needed. If the dose to the co-located worker at 100 meters is less than 1 Sv (100 rem), SS controls are not needed.

For the analysis of criticality accidents, Chapter 6 of DOE-HDBK-3010-94, Change Notice 1, provides values for fission yields, and is a recognized source for other accident analysis parameters. ANSI/ANS-8.23 requires evaluation of bounding, operational-specific accidents, including locations, yields, and dose determinations. Further, for solution or solution-like criticality accidents, Appendix C of ANSI/ANS-8.23 presents data directly useful for estimating bounding first-spike and time-integrated fission yields. As with any accident parameter, fission yields should be justified and shown to be applicable to the accident situation.

A bounding criticality accident that requires further evaluation in the DSA hazard evaluation is one that would be expected to have the highest unmitigated potential radiological consequences to the co-located worker or public, and is selected from similar types of criticality accidents evaluated in the criticality safety evaluations. For example, the bounding solution criticality accident would generally involve the largest volume in a hydrogenous, liquid environment coupled with making the conservative assumption that the system reaches the prompt critical state such that the information in Figure B-1 as discussed in Section B.3.1 would be applicable. This would lead to the largest number of fissions and thus be "bounding," which is viewed as the maximum "credible or plausible" accident yield rather than the most probable yield. Rare, extenuating circumstances such as larger accidents that are more remote or in shielded areas may result in a "bounding" accident that does not coincide with the largest number of fissions.

For both existing and new facilities the DSA or safety design basis document should provide information as to planned operations and facility layouts and features such as wall compositions and thicknesses. This information should be used with the techniques discussed in Section B.3 to estimate bounding, unmitigated fission yields.

B.3 ACCIDENT FISSION YIELDS

As with many known hazards, the understanding of, and thus the control of, the criticality accident hazard has improved dramatically since this hazard was first introduced in the 1940s with the advent of the production of significant quantities of plutonium and enriched uranium. Both the causes, largely human factors, and the personnel effects, localized to within a few to several meters of the accident location, are now well understood. Nevertheless, risks will never vanish and a thorough hazards analysis (in this case, a criticality safety evaluation) should always be performed. For operations with credible criticality accident likelihoods, fission yield determination, and, as needed, follow-on consequence analysis should be conducted.

B.3.1 FISSION YIELDS OF SOLUTION AND SOLUTION-LIKE SYSTEMS

History has shown that process criticality accidents have occurred almost exclusively in (hydrogenous) liquid media. The most common medium was fissile material in nitric acid, followed by organic solutions

and then suspensions/slurries. The hydrogenous nature of the medium results in relatively slow fission excursions and insignificant likelihoods of mechanical (destructive) energy releases. The liquid nature of the medium results in a combination of instantaneous bubble generation and thermal expansion as the major feedback mechanisms for limiting the first-spike yield (fissions) of the excursion. Flooded solids such as metal fines and powders also fall into this category since the water is the dominant factor in determining the fission yield (although they have not been associated with any known criticality accidents).

ANSI/ANS-8.23, Appendix C, provides a comprehensive summary of data from criticality accident simulations in controlled environments and the application of this data to estimating accident yields, both the first spike and the steady-state fission rate should the accident not immediately self-terminate. The data cover broad ranges of important parameters, most importantly the solution volume and the reactivity insertion rate.

Two figures from reference documents, reproduced in ANSI/ANS-8.23, Appendix C, are also reproduced here. Figure B-1 shows the variation in the specific yield of the first spike for prompt critical excursions from the literature data. As is shown, for all but very rapid excursions the specific, first-spike fission yield is $\sim 1 \times 10^{15}$ fissions/liter.

Some of the process criticality accidents did not even reach the prompt critical state and thus had much smaller specific yields. However, this value of ~1 x 10^{15} /liter is judged to be a practical upper bound for a first spike yield for the purpose of accident analysis. None of the process accidents exhibited specific yields statistically greater than this value. The data in the figure for the very short period excursions, <10 ms, that do show larger specific yields resulted from reactivity insertion rates that are likely not credible during process accident conditions. During the accident analysis for postulated accidents the scenario development will necessarily include information that enables estimates of the reactivity insertion rate and the related reactor period.

Figure B-2 shows a curve judged to be a practical bounding envelope of the integrated specific fissions during the first 10 minutes subsequent to a prompt critical excursion that is neither self-terminating nor otherwise terminated. Application of the information in Figures B-1 and B-2 enables a conservative upper estimate to be made of both the first-spike and the integrated total number of fissions from a postulated process accident. It also enables the analyst to estimate the dose rate at various locations in order to make decisions as to immediate evacuation zone boundaries and appropriate muster locations. Finally, if this 10-minute time window is consistent with site emergency plans and procedures, then the fission yield curve in Figure B-2 would be appropriate for determining bounding co-located worker and public exposures prior to possible further personnel relocations/evacuations. To take credit for emergency response actions being a mitigating factor, a SAC may be required per DOE-STD-3009.



Figure B-1 – Specific fissions in first spike as a function of reactor period. Reactor period is the time required for power to increase by Euler's number (Napier's constant) (Extracted from Figure C.1 of American National Standard ANSI/ANS-8.23-2007 (R2012) with permission of the publisher, the American Nuclear Society)



from criticality solution excursions in CRAC and Silene

DOE-HDBK-1224-2018

(Extracted from Figure C.2 of American National Standard ANSI/ANS-8.23-2007 (R2012) with permission of the publisher, the American Nuclear Society)

For an unmitigated accident with an 8-hour duration there is scant data upon which to base total fission/liter estimates. The Hanford (1962), Novosibirsk (1997) and Tokai-Mura (1999) accidents are the only reported process accidents to have continued fissioning for at least 8 hours. No accident simulations, such as the CRAC series, were allowed to run for more than minutes. Based on these three accidents and the reality that the fission rate is (theoretically) expected to decrease over time, and did in these three accidents, one can only estimate the ratio of the 8-hour fissions to first-spike fissions as perhaps a factor of 30.

The information contained in Figure B-2 has also been incorporated into the Nuclear Criticality Slide Rule that may also be used to estimate bounding fission yields (NUREG/CR-6504). Similar results will be attained.

B.3.2 FISSION YIELDS OF NON-SOLUTION-LIKE SYSTEMS

As the world-wide accident history shows, non-solution accidents are rare. From a review of the circumstances leading up to the one reported non-solution accident, it is apparent that this accident was enabled by a long-standing working environment that condoned significant procedural violations in the interest of expediency. It also had, as a contributing factor, a significant, negative human factors aspect. This human error situation was that the container in which the accident occurred could both accommodate a larger than critical volume/mass of metal and the contents could not be readily seen by the operator. The following should assure that similar breakdowns of operational discipline at DOE facilities be quite rare.

- 1. Application of DOE O 420.1C, Chg.1, Facility Safety, requirements;
- 2. A well-considered implementation of ANSI/ANS nuclear criticality safety standards; and
- 3. Effective oversight by both the contractor and DOE.

With well-developed Conduct of Operations programs in DOE facilities, criticality accidents in nonsolution environments, be they metals, compounds/powders, or storage operations, will be rare events and may well be shown as not credible per a comprehensive application of ANSI/ANS-8.1 and DOE-STD-3007-2017, *Preparing Criticality Safety Evaluations at Department of Energy Nonreactor Nuclear Facilities*.

The non-solution fissile material types and forms discussed in the following paragraphs are those mentioned in DOE-HDBK-3010-94, Section 6.2.3, and originally documented by Woodcock, 1966. The fission yields discussed in DOE-HDBK-3010-94 are based exclusively on critical experiment experience and Woodcock's professional judgments for operations at his facility more than 50 years ago in England. In summary, the fission yields that are presented as "judged or considered to be bounding" in DOE-HDBK-3010-94, Section 6.2.3, have no technical basis when applied to process operations.

B.3.2.1 METALS/SOLIDS - ONE OR A FEW LARGE PIECES

Bounding first-spike yields with uranium or plutonium in metal/alloy form consistent with known accidents, are 1×10^{18} and 1×10^{16} fissions, respectively. For these large, judged to be bounding, first-spike yields prompt shutdown due to mechanical shock would be expected. For lesser first-spike yields a delayed-critical fission reaction is bounding and judged to produce maximum 8-hour yields of 1×10^{19} and 1×10^{18} fissions respectively. Radiation exposures from metal critical experiment accidents are known to be essentially all from direct neutrons and gamma rays with insignificant fission product

releases. For fissile material operations conducted inside typical facilities with thick concrete walls that can be credited as passive design features if protected by Technical Safety Requirements (TSRs) as discussed in Section B.2.1, there would be minimal exposures to co-located workers or the MOI from these bounding fission sources.

B.3.2.2 DRY, UNMODERATED SOLIDS – NUMEROUS SMALL PIECES, AND LARGE ARRAYS

There is no accident history associated with either process or critical experiments for systems such as these (e.g., metal fines, loose oxide powders) that would be dominated by fast neutron fissions. This is judged to be primarily due to the very large critical masses that would be associated with such low-density configurations. For large arrays such as vault storage operations, Woodcock speculated on a fission yield but it is not possible to analyze such an event and relatively easy to protect against the accident by appropriate packaging of individual items. For both of these accident types the Criticality Safety Evaluations (CSEs) have been able to document no credible accident sequences.

B.3.3 FISSION YIELDS OF AUTOCATALYTIC ACCIDENTS

This deals with a criticality accident where the reactivity initially increases as the fission reaction progresses, conceptually due to the effects of temperature and pressure causing material rearrangement within the fissioning medium. One early estimate of excursion yields in a specific facility postulated an unusual accident whose reactivity initially increased due to the initial energy release (Woodcock, 1966). This type of event has not been observed in accident history. However, if the accident being evaluated has the potential for self-propagation, this should be considered.

B.4 EVALUATION OF DIRECT RADIATION DOSES

The prompt dose depends only upon the number of fissions in the criticality accident, the distance from the accident site to the receptor, and the amount of intervening shielding material, such as self-attenuation within the fissioning medium or building walls, that can be credited as passive design features if protected by TSRs as discussed in Section B.2.1. The Nuclear Criticality Slide Rule gives curves of unshielded dose as a function of distance, number of fissions, and time after the criticality accident. There is also information on the shielding effect of typical construction materials. See discussion in Section 8.2.5, Prompt (Direct) Dose.

B.5 CRITICALITY ACCIDENT SOURCE TERMS

Chapter 5, Source Term Analysis, covers source term estimation in detail depending on the accident stress on the material. For criticality accidents, however, the source term is fundamentally defined by the number of fissions occurring. This specialized subject will therefore be covered as part of this Appendix.

There are two main contributors to the criticality accident source term: fission products generated by the excursion, and releases of neutrons and gamma rays from the fission process itself. From the fission products, the major components of concern have historically been the noble gases (i.e., isotopes of krypton and xenon) and isotopes of iodine, due to their propensity to become airborne and escape filtration. However, decay products also have to be accounted for in analyzing criticality accidents.

B.5.1 FISSION PRODUCT INVENTORIES

A criticality accident generates the same types of fission products generated in spent nuclear reactor fuel. These are the primary fission product isotopes along with the subsequent decay of the initial fission products into other radioactive isotopes that, in turn, continue the decay chain. The typical pattern for total fission product activity in a criticality accident is a decrease in activity by orders of magnitude in the first 30 seconds after the criticality accident terminates. This is due to the loss of high-energy, short half-life isotopes that decay almost immediately. The activity then continues to decrease at a slower rate, with the contributions from various elements and classes of elements changing due to the ongoing decay process.

In withdrawn Regulatory Guides 3.33, 3.34 and 3.35, the NRC provided an estimate of "the radioactivity of significant nuclides released" for fuel reprocessing solutions, uranium solutions, and plutonium solutions. The criticality accident assumed had a 1×10^{18} fissions initial burst followed by 47 bursts of 1.9×10^{17} fissions each over the next 8 hours for a cumulative total of 1×10^{19} fissions. This particular scenario has not often been justified in a technical document. The significant nuclides noted were isotopes of krypton, xenon, and iodine. Their activity levels were based on the cumulative yield for the fission energy spectrum, an assumption noted as "very conservative" since it did not consider decay schemes for these nuclides.

Historical practice for DOE DSAs has been to use the information in the withdrawn Regulatory Guides 3.33, 3.34, and 3.35 for all criticality accidents, simply scaling the results to reflect total fission yields less than 1 x 10^{19} fissions (and eliminating the 8-hr duration for single spike criticality accidents). With the availability of modern code systems and cross sections, it is entirely feasible to calculate the fission products from a postulated criticality accident.

B.5.2 PARTICULATE RELEASE AND HEALTH RELATED PARAMETERS

As presented in Chapter 5 of this Handbook and in Chapter 6 of Handbook 3010-94, the ARFs and RFs are major parameters in determining the amount of radioactive or other hazardous material released in an accident. These parameters are normally evaluated by comparing a given phenomenology to available experimental data such as boiling of solutions or oxidation of metal. Unfortunately, no direct criticality accident release experiments have ever been conducted. Furthermore, the fission yields assigned are intended to bound fission product formation of noble gases and radioiodines, as opposed to estimating the physical changes experienced by the fissionable/fissile material and how many particulates may become airborne.

Accordingly, criticality accident release fractions have been developed only in a general sense without attempting to extrapolate them back to detailed phenomenological modeling of different accident stresses. The majority of the effort expended in developing them has also focused on the fission product release of noble gases and radioiodines. However, as related to release of particulates due to melting of metal, boiling of a solution, heating of powders, or energetic dispersal of a powder, the recommended bounding ARFs and RFs are based on experimental data for those types of changes in the materials based on the accident stresses discussed in Chapter 5.

As presented in Chapter 8, Radiological Consequence Assessment, the dose a person might receive from the fission products released by a criticality accident depends on many factors such as half lives and dose conversion factors. The primary pathways of interest from a criticality accident to receptors outside the facility are inhalation, cloudshine, and groundshine; prompt (direct) radiation may be significant for the 100 m CW, but generally not for the offsite public (MOI) due to the longer site boundary distance. These pathways are discussed in Chapter 8. Dose conversion factors for these pathways are discussed in ICRP-68, *Dose Coefficients for Intakes of Radionuclides by Workers*, and in ICRP-72, *Age-Dependent Doses to Members of the Public from Intake of Radionuclides, Part 5*.

Release estimates for solution criticality accidents derive from the now withdrawn NRC Regulatory Guides 3.33, 3.34, and 3.35 (see Chapter 6 of Handbook 3010-94). In these guides, the NRC established three assumptions. First, all noble gases are assumed to be released from solution and subsequently leave the facility. Second, it assumed that 25 percent of radioiodine ultimately escapes from the facility, either because only that much escapes from solution or because only that much of this element does not react with physical surfaces within the facility. Third, it was generically assumed that the criticality accident terminates when 25 percent of the available solution evaporates. The bounding ARF for boiling liquid is 2×10^{-3} (see Chapter 5). Applying the 25 percent factor to this ARF yields an effective release fraction of 5×10^{-4} , which the NRC originally applied to the base matrix of fissile plutonium in solution in Regulatory Guide 3.35.

However, the numerous experiments associated with the data in Figures B-1 and B-2 and 20 of the 21 known solution criticality accidents produced negligible evaporation since the boiling temperature was not reached. For those that did not shut down quickly, but fissioned for many hours, such as Tokai-Mura, the fission energy deposition was easily removed by convection cooling from the exterior of the vessel at temperatures well below the boiling point, such that no measurable evaporation occurred. Therefore, the 2 x 10^{-3} ARF/RF assumption of particulate releases from vigorous boiling (which was based on 90% evaporation of the solution) and its 25% reduction factor (effective 5 x 10^{-4} ARF/RF) may be an overestimate, and a 3 x 10^{-5} ARF/RF for heating of solution in flowing air without surface rupture of bubbles (i.e., no visible surface disruption) from DOE-HDBK-3010-94 Section 3.2.1.1, Heating of Shallow Pools, may be an appropriate conservative estimate. This heating value bounds the experimental data from two experiments reported in DOE-HDBK-3010-94 Section 3.2.1.2, Heating of Pools, which exhibited simmering of the solution and a maximum ARF of 4.5 x 10^{-6} was measured.

The values cited above have been reiterated in NUREG/CR-6410, which also formally extended the 5 x 10^{-4} release fraction to the seven significant isotopes (Sr-91, Sr-92, Ru-106, Cs-137, Ba-139, Ba-140, and Ce-143). That document further noted that the 5 x 10^{-4} value is considered "applicable to all non-volatile compounds in the liquid." The portion of the actinides released is assumed to be proportional to the mass of actinides in the solution as the actinides are released through the spray caused by the bursting bubbles that reach the surface of the solution. The mass of the actinides depends upon their concentration in the solution. A more detailed discussion of this phenomenology and estimating particulate source terms is provided in DOE-HDBK-3010-94, Section 6.3.1, Solutions.

B.6 CRITICALITY ACCIDENT EXAMPLE

This example assumes that there is a fissile solution that inadvertently and very rapidly accumulates in a 150-liter vessel/volume and that the system just reaches the prompt critical state as the vessel becomes full. Thus, conservatively assuming that the prompt critical state is reached and that the system remains critical, and then applying the information from Figure B-2, the first spike, 10-minute, and 2- and 8-hour fissions can be calculated as:

First spike yield = 150 liters x 1 x 10^{15} fissions/liter = 1.5 x 10^{17} fissions. 10-minute yield = 150 liters x 1.5 x 10^{16} fissions/liter = 2.25 x 10^{18} fissions. 2-hour yield = 1.5 x 10^{17} x 20 = 3.0 x 10^{18} fissions 8-hour yield = 1.5 x 10^{17} x 30 = 4.5 x 10^{18} fissions.

Once the total fission yield is known, a fission product inventory is determined as discussed in Section B.5.1, and estimates of particulate releases are determined as discussed in Section B.5.2. With these criticality source terms, a DOE Toolbox dispersion and radiological dose assessment code can be used to calculate the doses to the CW at 100 m and the offsite public (MOI) at the site boundary. If important, the prompt (direct) dose can be calculated as discussed in Section B.4.