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	Software Integration for Environmental Radiological Release Assessments (SIERRA) Atmospheric Transport and Diffusion (ATD) Model			
	Technical Basis and Comparisons with Legacy Codes			
	March 2025			
	S Ghosh JE Flaherty GC Cornwell CD Mangini			
	Prepared for the U.S. Nuclear Regulatory Commission Office of Nuclear Regulatory Research Under Contract DE-AC05-76RL01830 Interagency Agreement: 31310024S0007			

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Pacific Northwest National Laboratory Richland, Washington 99354

Summary

The Software Integration for Environmental Radiological Release Assessments (SIERRA) application provides a consolidated framework for separate "functional engines" that can be used, individually or in certain combinations, for dose assessment to support the licensing of nuclear power plants (NPPs) and nonpower production or utilization facilities (NPUFs). The software consolidates and modernizes various existing codes within the U.S. Nuclear Regulatory Commission's (NRC's) Radiation Protection Computer Code Analysis and Maintenance Program (RAMP). RAMP develops, maintains, improves, distributes, and provides training on NRC-sponsored radiation protection and dose assessment computer codes. The SIERRA software is designed based upon existing RAMP codes and incorporates scientific methods for environmental (e.g., air or water) transport, diffusion, and dose assessment of radionuclides.

This document describes the mathematical basis of the Atmospheric Transport and Diffusion (ATD) model within the SIERRA software. The fundamental differences between the mathematical outputs from the ATD model and the corresponding RAMP legacy model outputs are provided. This is achieved through a description of the technical basis and statistical approaches used within the models, which highlights similarities and differences between the ATD model and RAMP legacy models.

The SIERRA ATD software has undergone testing to document whether it meets the functional requirements of the software and to document its performance in unit and integrated testing. Model comparisons were conducted with two meteorological datasets to demonstrate regulatory consistency between ATD and legacy models: a single synthetic dataset and an array of site-specific data from various NPPs. The synthetic data were created to control the meteorological factors that contribute to the model output, while the site-specific meteorological data are from 22 unique locations across the United States with varying content, including unique numbers of calm and missing data.

The synthetic data illustrated that the χ/Q values for single meteorological conditions were either identical or very similar between the ATD and legacy models. The primary differences were due to the joint frequency distribution (JFD) wind-speed bin selection for the PAVAN and XOQDOQ models, which could create differences between the true wind speed and the bin-averaged wind-speed values. The largest differences were observed in the model statistical calculations, which are necessarily different between the ATD model and legacy codes that use JFDs (PAVAN and XOQDOQ). These differences include the interpolation (or extrapolation) employed by the legacy codes to compute the exceedance values, which are computed more directly from the hourly data in the ATD model, as well as the influence of the JFD bin definition that was identified in the evaluation of single meteorological conditions.

Comparisons with site-specific data demonstrated a high level of agreement and consistency between the ATD model and legacy code outputs. The primary deviations result from the fundamental differences in PAVAN statistical methodologies and how they are applied to JFDs versus hourly data. However, users are cautioned to examine how calms are handled and distributed in PAVAN and XOQDOQ when drawing comparisons to the ATD model, as the analyses presented here assumed consistent handling of calms between the ATD and legacy models.

Acronyms and Abbreviations

ALARA	as low as is reasonably achievable
ARCON	computer code for Atmospheric Relative CONcentration in Building Wakes
ATD	atmospheric transport and diffusion
CDF	cumulative distribution function
CFR	Code of Federal Regulations
DBA	design basis accident
DOE	U.S. Department of Energy
EAB	exclusion area boundary
EPA	U.S. Environmental Protection Agency
F2	Factor of 2
F5	Factor of 5
Fortran	FORmula TRANslator
h	hour(s)
HDI	How Do I?
ISC	Industrial Source Complex Dispersion Model
JFD	joint frequency distribution
LPZ	outer boundary of the low population zone
m	meter(s)
m/s	meter(s) per second
MNMB	modified normalized mean bias
NMB	normalized mean bias
NPP	nuclear power plant
NPUF	nonpower production or utilization facility
NRC	U.S. Nuclear Regulatory Commission
P-G	Pasquill–Gifford (diffusion coefficients)
PAVAN	computer code for ground-level χ/Q for accidental release
PNNL	Pacific Northwest National Laboratory
RAMP	Radiation Protection Computer Code Analysis and Maintenance Program
RG	Regulatory Guide
s·m⁻³	second(s) per cubic meter
SIERRA	Software Integration for Environmental Radiological Release Assessments
SQA	software quality assurance
SRP	standard review plan
WD	wind direction
WS	wind speed

XOQDOQ computer code for evaluation of routine effluent releases at commercial nuclear power stations

Contents

Summ	ary			ii
Acrony	/ms and	Abbrevia	ations	iii
1.0	Introdu	ction		1
	1.1	Software	Quality Assurance	1
		1.1.1	Software Testing	2
2.0	ATD M	odel Reg	ulatory Bases	4
3.0	ATD M	odel Tec	hnical Basis Overview	7
	3.1	ARCON	Model Overview	7
	3.2	PAVAN	Model Overview	7
	3.3	XOQDO	Q Model Overview	8
	3.4	Meteoro	logical Data Processing	8
		3.4.1	Calm Wind Conditions	9
	3.5	Gaussia	n Plume Model	.10
		3.5.1	Statistical Calculations	.10
4.0	Overvie	ew of Co	mparisons with Legacy Code Output	.12
	4.1	ATD On: with AR(site Control Room Design Basis Accident Analysis Comparison CON	.13
	4.2	ATD Off	site Design Basis Accident Analysis Comparison with PAVAN	.15
	4.3	ATD Rou	utine Release Analysis Comparison with XOQDOQ	.21
5.0	Summa	ary		.24
6.0	Refere	nces		.25
Appen	dix A –	Model Te	chnical Basis	A.1
Appen	dix B –	Comparis	sons with Legacy Code OutputI	B.1
Appen	dix C –	Legacy C	Code Input File Examples	C.1

Figures

Figure 4.1.	Comparison of the 95th percentile χ/Q from ATD and ARCON at various averaging intervals using site data from 22 nuclear power plant locations for a ground-level release (10 m).	14
Figure 4.2.	Comparison of the 95th percentile χ/Q from ATD and ARCON at various averaging intervals using site data from 22 nuclear power plant locations for an elevated release (60 m).	15
Figure 4.3.	Comparison of the sector $0-2$ h χ/Q values from ATD and PAVAN using site data from 22 nuclear power plant locations for a ground-level release (10 m). The upper panel is for the EAB (800 m), and the lower panel is for the LPZ (3000 m).	17
Figure 4.4.	Comparison of the sector $0-2 h \chi/Q$ values from ATD and PAVAN using site data from 22 nuclear power plant locations for an elevated release (60 m). The upper panel is for the EAB (800 m), and the lower panel is for the LPZ (3000 m).	18
Figure 4.5.	Comparison of the annual average χ/Q values from ATD and PAVAN using site data from 22 nuclear power plant locations for a ground release (10 m). The upper panel is for the EAB (800 m), and the lower panel is for the LPZ (3000 m).	19
Figure 4.6.	Comparison of the annual average χ/Q values from ATD and PAVAN using site data from 22 nuclear power plant locations for an elevated release (60 m). The upper panel is for the EAB (800 m), and the lower panel is for the LPZ (3000 m)	20
Figure 4.7.	Comparison of the annual average χ/Q values from ATD and XOQDOQ using site data from 22 nuclear power plant locations for a ground-level release (10 m). The values of χ/Q are plotted for 1 and 10 miles in the upper and lower panels, respectively.	22
Figure 4.8.	Comparison of the annual average χ/Q values from ATD and XOQDOQ using site data from 22 nuclear power plant locations for an elevated release (60 m). The values of χ/Q are plotted for 1 and 10 miles in the upper and lower panels, respectively.	23
Figure A.1.	Open terrain correction factor	A.8
Figure A.2.	Plume depletion effect for ground-level releases (all atmospheric stability classes).	A.9
Figure A.3.	Plume depletion effect for 30 m releases and different atmospheric stability classes	A.9
Figure A.4.	Plume depletion effect for 60 m releases and different atmospheric stability classes	A.10
Figure A.5.	Relative deposition for ground-level releases (all atmospheric stability classes).	A.10
Figure A.6.	Relative deposition for 30 m releases and different atmospheric stability classes	A.11
Figure A.7.	Relative deposition for 60 m releases and different atmospheric stability classes.	A.11

Figure B.1.	Comparison of χ/Q values from ATD and the PAVAN CHIQ subroutine for a ground-level release without a building.	B.10
Figure B.2.	CHIQ output at 800 m from PAVAN for a ground-level release	B.11
Figure B.3.	CHIQ output at 3000 m from PAVAN for a ground-level release	B.11
Figure B.4.	Comparison of the downwind distances set within ATD and PAVAN for an EAB of 800 m	B.12
Figure B.5.	Comparison of χ/Q values from ATD and PAVAN's CHIQ subroutine for an elevated release	B.14
Figure B.6.	CHIQ output at 800 m from PAVAN for an elevated release.	B.14
Figure B.7.	CHIQ output at 3000 m from PAVAN for an elevated release	B.15
Figure B.8.	PAVAN output showing the statistical results for χ/Q values at 800 m computed using the ENVLOP and ONEOUT routines	B.16
Figure B.9.	Comparison of the annual average χ/Q values from ATD and XOQDOQ for a ground-level release. The XOQDOQ model used two variants of the same meteorological data that employed different wind-speed bins. Results without decay incorporated are presented in the left panel, while results with 8-day decay and depletion are presented in the right panel	B.17
Figure B.10.	Comparison of the annual average χ/Q values from ATD and XOQDOQ for an elevated release. The XOQDOQ model used two variants of the same meteorological data that employed different wind-speed bins. Results without decay incorporated are presented in the left panel, while results with 8-day decay and depletion are presented in the right panel	B.19
Figure C.1.	Example of an ARCON .rsf file used in the site-specific meteorological comparative analysis. This file is for the Levy site and represents the ground-level release scenario.	C.1
Figure C.2.	Example of a PAVAN .inp file used in the site-specific meteorological comparative analysis. This file is for the Levy site and represents the ground-level release scenario. The calms are evenly distributed in the 0.5 m/s wind-speed bin.	C.2
Figure C.3.	Example of a XOQDOQ .inp file used in the site-specific meteorological comparative analysis. This file is for the Levy site and represents the ground-level release scenario. The calms are evenly distributed in the 0.5 m/s wind-speed bin.	C.3

Tables

Table 2.1.	Regulations and NRC guidance documents related to assessment types	4
Table 3.1.	Summary of calm treatments for the ATD model and legacy codes	9
Table 4.1.	Sites used in the verification of the ATD model.	13
Table A.1.	Fortran format implemented in the meteorological reader routine	A.1
Table B.1.	Joint frequency distribution of the hourly meteorological data for the synthetic dataset.	B.2
Table B.2.	ATD and ARCON2 calculations of hourly χ/Q values for a ground-level release with synthetic meteorological data. The 1 m/s D stability case in bold font represents the results of the example "hand calculation."	B.5
Table B.3.	ATD and ARCON2 calculations of hourly χ/Q values for an elevated release with synthetic meteorological data. The 0.92 m/s D stability case in bold font represents the results of the example "hand calculation."	B.6
Table B.4.	ATD and PAVAN calculations of hourly χ/Q values for a ground-level release with synthetic meteorological data.	B.9
Table B.5.	Comparison of the key statistics relevant to regulatory applications from a ground-level release.	B.11
Table B.6.	ATD and PAVAN calculations of hourly χ/Q values for an elevated release with synthetic meteorological data.	B.13
Table B.7.	Comparison of key statistics used for regulatory purposes from an elevated release	B.15
Table B.8.	Routine release calculations at a receptor point located 0.44 miles (715 m) from a ground-level release (10 m).	B.18
Table B.9.	Routine release calculations at a receptor point located 0.44 miles (715 m) from an elevated release (60 m).	B.20

1.0 Introduction

The Software Integration for Environmental Radiological Release Assessments (SIERRA) application provides a consolidated framework for separate "functional engines" that can be used, individually or in certain combinations, for dose assessment to support the licensing of nuclear power plants (NPPs) and nonpower production or utilization facilities (NPUFs). The software consolidates and modernizes various existing codes within the U.S. Nuclear Regulatory Commission's (NRC's) Radiation Protection Computer Code Analysis and Maintenance Program (RAMP). RAMP develops, maintains, improves, distributes, and provides training on NRC-sponsored radiation protection and dose assessment computer codes. The SIERRA software is designed based upon existing RAMP codes and incorporate scientific methods for environmental (e.g., air or water) transport, diffusion, and dose assessment of radionuclides.

This document describes the mathematical basis of the Atmospheric Transport and Diffusion (ATD) model within the SIERRA software. The fundamental differences between the mathematical outputs from the ATD model and the corresponding RAMP legacy model outputs are provided. This is achieved through a description of the technical basis and statistical approaches used within the models, which highlights similarities and differences between the ATD model and RAMP legacy models. Model comparisons were conducted and are presented with two meteorological datasets to demonstrate regulatory consistency between ATD and legacy models: a single synthetic dataset and an array of site-specific data from various NPPs.

The remainder of this section will provide a brief overview of the software quality assurance approach for the SIERRA ATD software. Section 2.0 describes the regulatory basis of these codes; Section 3.0 provides an overview of the ATD model technical basis, along with the primary technical differences with the legacy codes; and Section 4.0 provides a comparison of the mathematical outputs of the ATD and legacy models for an array of site-specific meteorological monitoring data from various NPPs. Appendix A contains a detailed technical basis of the ATD model, Appendix B provides a detailed discussion of the synthetic dataset analysis, and Appendix C provides examples of the legacy model input files.

1.1 Software Quality Assurance

The NRC and subscribers to RAMP (e.g., licensees and applicants) intend to use the SIERRA ATD software solely as a confirmatory tool for independent safety and environmental projections related to atmospheric dispersion, dose, and consequences for NPP licensing, emergency responses, and site decommissioning. The Pacific Northwest National Laboratory (PNNL) project team, its software quality practitioner, and the NRC have determined the intended use of the SIERRA ATD software shall be qualified per NUREG/BR-0167 as Level 1 software: Technical application used in a safety decision by the NRC.

The SIERRA ATD software is maintained by PNNL using a graded software quality assurance (SQA) approach compliant with the requirements specified in NUREG/BR-0167. The applicable SQA process for the project team is the PNNL "How Do I?" (HDI) "Develop Software for Delivery" workflow. The level of rigor applied to the software life cycle phases is based on the following identified risks, given the intended use:

• Software results could significantly impact PNNL's customer (i.e., NRC) decisions; therefore, data quality is a key parameter.

• Software failure or performance other than as intended could result in a violation of NRC's regulatory limits.

Any software use beyond this intended purpose requires additional SQA evaluation.

1.1.1 Software Testing

Software testing to meet the Software Quality Assurance Plan for the SIERRA software has been conducted. The project software verification and validation methodology was used to perform tests to demonstrate that the software correctly performs all intended functions. For this software, the mathematical models and the user interfaces were tested. A brief description of software testing is described in the sections below.

1.1.1.1 Mathematical Model Testing

Tests are implemented to determine whether the codes executing the mathematical models are performing as expected. This testing falls into two general categories: unit testing and integrated testing (or functional testing). Unit testing is performed on the methods and functions in the software codes that either generate or modify data values. This testing is done against the individual function code separate from the testing performed against the software. Unit testing on a function is done by running function code using a set of predefined input values and comparing the results against the expected result values. Unit testing is focused on the smallest separable functions of the underlying code.

Following unit testing, integrated testing is implemented on the executable to test that the mathematical models are performing as executed together (i.e., at a level above unit testing). Integrated testing of the mathematical model involves numerous cases with varying input parameters performed with sets of meteorological data. These cases were replicated, to the extent possible, with the corresponding legacy software.

1.1.1.2 User Interface Testing

User interface testing is performed to determine that the user experience is performing as expected as a user interacts with the interface (i.e., buttons function, screens progress, etc.). This testing must identify that the user interface performs as expected and that it will also provide the correct error message or restrict the user if an input falls outside an acceptable range. Unit tests of the user interface have been performed to assess the performance of the navigation between screens and data input. Functional testing of SIERRA and the ATD model user interfaces was performed using several different types of tests:

- invalid input (e.g., a string instead of a number)
- out-of-range input (e.g., 1001 in the field that has an upper limit of 1000)
- valid input and running the analysis (including ensuring inputs are transferred appropriately to the model and to the output files)
- control testing (the functionality of buttons, checkboxes, drop-down lists, etc.)
- input values with many decimal places (e.g., 0.111111111)
- form navigation ("Next" buttons and left navigation menu)
- saving and loading input files

• application logic (e.g., does clicking on "Run Analysis" run the model?).

2.0 ATD Model Regulatory Bases

The ATD model within SIERRA is a unified code in FORmula TRANslator (Fortran) 90 that allows the computation of χ/Q for three assessment types: (1) onsite control room habitability design basis accidents (DBAs), (2) offsite DBAs, and (3) routine releases. NRC staff and RAMP users have employed ARCON2 (and earlier ARCON96) for short-term consequence assessment of the onsite control room DBA, PAVAN for analyzing offsite DBAs, and XOQDOQ for consequence assessment of routine releases from NPPs. A summary of these assessments, along with their respective regulatory bases, is provided in Table 2.1.

SIERRA ATD		NRC Guidance		
Analysis Type	Legacy Model	Document	Regulations	Applicability
Onsite control room habitability design basis accident assessment	ARCON96	RG 1.194 and SRP 2.3.4	10 CFR Part 50, Appendix A, General Design Criterion 19 10 CFR 50.34(a)(1)	Input to evaluating personnel exposures in the onsite control room during accidents
Onsite control room habitability design basis accident assessment	ARCON96	SRP 15.0.3 and SRP 13.3	10 CFR Part 50, Paragraph IV.E.8 of Appendix E	Protection against radiation inside the onsite technical support center
Offsite design basis accident dispersion analyses	PAVAN	RG 1.145 and SRP 2.3.4	10 CFR 50.34(a)(1)(ii)(D) 10 CFR 52.47(a)(2)(iv) and 10 CFR 52.137(a)(2)(iv)	Offsite consequence at EAB and LPZ for plant design (Design Certifications and Standard Design Approvals, respectively)
Offsite design basis accident dispersion analyses	PAVAN	RG 1.145 and SRP 2.3.4	10 CFR 52.17(a)(1)(ix)	Offsite consequence at EAB and LPZ for safety assessment (Early Site Permits)
Offsite design basis accident dispersion analyses	PAVAN	RG 1.145 and SRP 2.3.4	10 CFR 52.79(a)(1)(vi)	Offsite consequence at EAB and LPZ for safety assessment (Combined Licenses)
Offsite design basis accident dispersion analyses	PAVAN	RG 1.145 and SRP 2.3.4	10 CFR 52.157(d)	Offsite consequence at EAB and LPZ for safety assessment (Manufacturing Licenses)
Offsite design basis accident dispersion analyses	PAVAN	RG 1.145 and SRP 2.3.4	10 CFR 100.21(a)	Determine acceptable EAB and LPZ for siting

Table 2.1. Regulations and NRC guidance documents related to assessment types.

SIERRA ATD		NRC Guidance				
Analysis Type	Legacy Model	Document	Regulations	Applicability		
Offsite design basis accident dispersion analyses	PAVAN	RG 1.145 and SRP 2.3.4	10 CFR 100.21(c)(2)	Offsite consequence at EAB and LPZ for postulated accidents		
Routine release analyses	XOQDOQ	RG 1.111 and SRP 2.3.5	10 CFR Part 20 Subpart D	Annual dose assessment to meet as low as is reasonably achievable (ALARA) criterion during preliminary plant design and limiting conditions for operations		
Routine release analyses	XOQDOQ	RG 1.111 and SRP 2.3.5	10 CFR Part 50, Appendix I	Annual dose assessment to meet ALARA criterion during preliminary plant design		
ALARA = as low as is reasonably achievable; ARCON = computer code for Atmospheric Relative CONcentrations						

in Building Wakes; CFR = Code of Federal Regulations; EAB = exclusion area boundary; LPZ = outer boundary of the low population zone; PAVAN = atmospheric dispersion program for evaluating design basis accident releases; RG = Regulatory Guide; SRP = standard review plans; XOQDOQ = atmospheric dispersion program for the meteorological evaluation of routine releases.

Sources: NRC 1977, 1982, 2003, 2007a, 2007b, 2007c, 2007e.

A summary of the guidance document content related to onsite control room habitability DBA assessments is provided below:

- General Design Criterion 19 of Title 10 of Code of Federal Regulations, Part 50 (10 CFR) Part 50), Appendix A states that "Adequate radiation protection shall be provided to permit access and occupancy of the control room under accident conditions without personnel receiving radiation exposures >5 rem whole body, or its equivalent to any part of the body, for the duration of the accident."
- Regulatory Guide (RG) 1.194 (NRC 2003), "Atmospheric Relative Concentrations for Control Room Radiological Habitability Assessments at Nuclear Power Plants," presents criteria for characterizing atmospheric transport and diffusion conditions for evaluating the consequences of radiological releases to the control room.
- RG 1.194 (NRC 2003) requires determination of the 95th percentile x/Q (exceeded no more than 5 percent of the assessment period) for each of the source-to-receptor combinations.
- Currently, RG 1.194 (NRC 2003) prescribes Atmospheric Relative CONcentration in Building Wakes (ARCON) as an acceptable methodology for assessing control room χ/Q values.
- ARCON is designed to estimate concentrations for sources and receptors in the vicinity of buildings. The model includes an explicit treatment of low-wind-speed dispersion and building wakes. The stability-based Pasquill–Gifford (P-G) diffusion coefficients were modified based on field experimental data as described in Ramsdell and Fosmire (1998). These dispersion coefficients are valid only for distances within a few hundred meters from the source.
- ARCON currently considers ground-level releases, vent releases, or elevated releases. However, RG 1.194 states that the vent release mode within ARCON should not be used for offsite DBAs.

A summary of the regulatory and guidance document content related to offsite DBA analyses is provided below:

- 10 CFR 100.11 requires that an applicant determine the following for siting considerations:
 - An individual at an exclusion area boundary (EAB) does not receive a total whole body radiation dose over 25 rem over the first two hours of exposure.
 - An individual in a low population zone (LPZ) does not receive a total radiation dose over 25 rem over the entire period of the plume passage.
- RG 1.145 (NRC 1982) provides guidance on ATD models for potential accident consequence assessment at NPPs.
 - This guide provides specific χ/Q calculation methods for ground-level release and elevated releases that were implemented in PAVAN. The sector-averaged Gaussian plume equation is modified with corrections for the building wake and meander for ground-level release.
- RG 1.145 (NRC 1982) requires the calculation of the 2-hour χ/Q at the EAB that is exceeded 0.5 percent of the time for each of 16 directions (22.5° each).
- RG 1.145 (NRC 1982) requires the calculation of the ≥8-hour χ/Q in the LPZ that is
 exceeded 0.5 percent of the time for each of 16 directions and 5 percent for the overall site
 (all directions).

A summary of the regulatory and guidance document content related to offsite routine release analyses is provided below:

- 10 CFR Part 50, Appendix I requires that a nuclear facility be operated to meet the criterion "as low as is reasonably achievable" (ALARA).
- 10 CFR 20.1301 sets the radiation dose limits to the public from the routine release of airborne radioactive effluents from a nuclear facility and thus regulates the amount of annual releases.
- RG 1.111 (NRC 1977) provides acceptable methods for the estimation of atmospheric transport and dispersion of gaseous effluents in routine releases.
- XOQDOQ implements the long-term dispersion and deposition calculation for routine operational releases based on Sagendorf (1994).
- Unlike the legacy models for onsite control room DBA analysis and offsite DBA analysis, XOQDOQ accounts for removal processes due to dry deposition and radioactive decay.
- This analysis considers ground-level releases, vent releases, or elevated releases.
- Detailed user guidance for the XOQDOQ dispersion model is provided in NUREG/CR-2919 (Sagendorf et al. 1982).

3.0 ATD Model Technical Basis Overview

Although the objectives of the three assessment types are different, the underlying technical basis is a simple near-field straight-line Gaussian plume model that takes as common input the meteorological fields of wind speed, wind direction, and atmospheric stability for a site. The three separate legacy model codes were reengineered and consolidated with a common input of hourly meteorological data based on the RG 1.23 (NRC 2007d) format. Appendix A describes the meteorological data processing and Gaussian plume model equations used in the ATD engine. In this section, a basic overview of the ATD model and legacy models' technical basis is presented, along with the salient differences between the ATD model and legacy codes.

3.1 ARCON Model Overview

Experimental studies have demonstrated that the straight-line Gaussian plume model typically overestimates concentrations in the vicinity of buildings (Ramsdell 1990). ARCON95/96 was developed to address this concern by using a statistical model to make more reliable predictions in building wakes. RG 1.194, which is largely based on the ARCON code, prescribes methods and procedures to determine atmospheric relative concentrations (χ/Q) for assessing the potential control room radiological consequences for a range of postulated accidental releases of radioactive materials to the atmosphere. RG 1.194 states the requirement for the determination of the 95th percentile χ/Q value for a specific source–receptor direction. ARCON96 was later slightly revised to ARCON2 (Rishel 2021).

ARCON is a code for potential use by NRC staff in the review of license submittals related to onsite control room habitability. ARCON takes as input hourly meteorological data with wind speed and direction at the lower and upper measurement heights and a stability class. SIERRA ATD also takes as input hourly meteorological data with the format provided in RG 1.23 (NRC 2007d). Stability is calculated based on the vertical temperature difference (d*T*/d*z*). Both ground-level and elevated releases can be modeled. Mixed-mode releases for vents were excluded from SIERRA ATD onsite control room DBA analyses.

3.2 PAVAN Model Overview

RG 1.145 provides the regulatory basis for potential accident consequence assessments and an acceptable methodology to determine site-specific χ/Q at the EAB and LPZ. RG 1.145 requires meteorological data as input for consequence assessment that represent hourly averages, as defined in RG 1.23 (NRC 2007d). The U.S. NRC developed PAVAN (Bander 1982) to implement the guidance and regulatory positions in RG 1.145. PAVAN was developed in Fortran 77 and uses a joint frequency distribution (JFD) of the wind speed and stability along 16 directions as the meteorological input. The SIERRA ATD engine reengineered the implementation of RG 1.145 to use hourly meteorological data. Both SIERRA ATD and NRC PAVAN have the same governing equations and diffusion parameters and implement the regulatory basis that users would need for dose calculations for 10 CFR Part 100 and 10 CFR Part 50. The statistical routines within SIERRA ATD are updated to process hourly data directly, rather than a conversion from the JFD. The SIERRA ATD model meets the objectives of the offsite design basis consequence analyses as outlined in RG 1.145:

- 1. compute χ/Q on a directional basis
- 2. compute χ/Q on an overall site basis
- 3. choose χ/Q values to be used in evaluations to meet RG 1.3 and RG 1.4.

RG 1.145 requires the calculation of peak χ/Q values for a 2-hour period at the EAB and longer time periods for the LPZ including 8, 16, 72, and 624 hours. The maximum values for these time periods are selected from the maximum sector χ/Q or the 5 percent overall site χ/Q , whichever is higher. RG 1.145 also requires the determination of 2-hour and annual average χ/Q values at the LPZ.

3.3 XOQDOQ Model Overview

As stated in 10 CFR Part 50, NPPs are required to limit radioactive releases to the atmosphere ALARA, and Appendix I of 10 CFR Part 50 provides numerical guidance to meet these design objectives. RG 1.111 provides procedures and models to implement the numerical guidance in Appendix I. This RG describes the basic features of the model calculations and assumptions to facilitate estimates of the atmospheric transport and dispersion of gaseous effluents in routine releases. RG 1.111 highlights that the recommended procedures and models will be subject to continuing review by the NRC staff, providing flexibility to the applicant in meeting the requirements of Appendix I. The XOQDOQ code (Sagendorf et al. 1982) implements RG 1.111 and is used by NRC staff in their independent evaluation of routine or intermittent releases from nuclear power reactors. It is not intended to evaluate the consequences of accidental releases.

The XOQDOQ code computes the relative atmospheric dispersion (χ/Q) and deposition factors (D/Q) for 22 specific distances to 50 miles from the site for each directional sector. XOQDOQ implements a straight-line Gaussian plume model with plume depletion due to dry deposition and radioactive decay and also accounts for plume recirculation. Meteorological data are input into the program as a JFD that includes the stability class, wind direction, and wind-speed class. The "Routine Release" algorithm within ATD implements RG 1.111 in a method like XOQDOQ, with the primary difference of incorporating hourly meteorological data rather than a JFD.

3.4 Meteorological Data Processing

Meteorological data in a Fortran format provided in Appendix A of the RG 1.23 guidance document are used as model input for all three models. The PAVAN and XOQDOQ legacy codes used JFDs instead. As a result, there are intrinsic differences in the approach to processing the model output, which will be described in Section 3.5.1.

Another difference between the ATD model and legacy codes is that the atmospheric stability for each hour is determined from hourly records of the temperature difference (dT/dz) using the classification (A through G) in Table 1 of RG 1.23. While the ARCON meteorological input is hourly as well, the stability class, entered as a number from 1 through 7, is included directly in the hourly record. In a similar vein, the JFDs for the PAVAN and XOQDOQ meteorological data are sorted according to stability class.

The wind speed at the measurement height is corrected for the stack (release) height using Monin–Obukhov length similarity theory for a control room assessment (Ramsdell and Simonen 1997). A simple power law relationship (Bander 1982) is used to adjust the wind speed for the other two assessments.

The ATD model and legacy codes may also take a different approach to calm winds. With the RG 1.23 formatted meteorological file, records are identified as calm by entering 77777 within the wind direction field. In the case of the onsite control room DBA analysis, the ATD model matches the behavior of the ARCON code and applies all calm winds to the direction to the downwind receptor. This is considered conservative because it substitutes nonzero values of

 χ/Q for values that would normally be zero if the wind direction were considered (Ramsdell and Simonen 1997).

3.4.1 Calm Wind Conditions

For the routine release and offsite DBA analyses, the ATD model assumes that the calm winds represent a light and variable wind that does not have a distinct wind direction and applies the calm periods evenly across all of the 16 wind direction sectors for a given stability class. This treatment is supported by the RG 1.23 format, which defines calms as an unknown wind direction (assigns 77777 in the wind direction field). In the PAVAN legacy code, the calm winds may be distributed into separate wind direction bins by the user creating the JFD. However, if they have not been previously assigned a wind direction, the PAVAN code distributes occurrences of calm wind by assigning them in proportion to the directional distribution of noncalm winds with speeds less than 1.5 meters per second (Bander 1982). Finally, the XOQDOQ JFD may also be similarly distributed by the user into wind direction bins, or the calms will be distributed according to the directional distribution of the first noncalm wind-speed class (Sagendorf et al. 1982). The handling of calms in both legacy codes provide the user with the flexibility to distribute calms in a few ways. For example, the calms can be distributed evenly-as they are in ATD-by creating a wind-speed bin for calms and evenly dividing the calm hours across all 16 sectors for a given stability class. In doing so, a more direct testing comparison to ATD can be made. As such, calms in the legacy codes are evenly distributed for the analyses discussed in the next section. Table 3.1 summarizes the calm treatments for the various codes.

ATD	ARCON	PAVAN	XOQDOQ
For Onsite Control Room DBA: All calms are assigned to the direction to the receptor.	All calms are assigned to the direction to the receptor.	If a WD is provided, use the given WD. If no WD is provided, distribute the calm occurrences by assigning them in	If a WD is provided, use the given WD. If no WD is provided, distribute the calm occurrences by assigning them in
For Offsite Design Basis Accident and Routine Release Analyses: All calms are distributed equally across all wind directions.		proportion to the directional distribution of noncalm winds with speeds less than 1.5 m/s. If no WD is provided and there are no winds below 1.5 m/s, distribute the calms equally across all wind directions.	proportion to the directional distribution of the first noncalm wind- speed class.

Table 3.1. Summary of calm treatments for the ATD model and legacy codes.

ARCON = computer code for Atmospheric Relative CONcentration in Building Wakes; ATD = atmospheric transport and diffusion; m/s = meter(s) per second; PAVAN = computer code for ground-level χ/Q for accidental release; WD = wind direction; XOQDOQ = computer code for evaluation of routine effluent releases at commercial nuclear power stations.

3.5 Gaussian Plume Model

The atmospheric engine implements a straight-line Gaussian plume model. The concentrations (and deposition) at receptor distances are computed for each hour by the ATD model using the same equations that are used by the legacy codes. There is only a slight difference in the equations for the sector-averaged Gaussian plume models for the PAVAN and XOQDOQ codes, necessitated by the use of JFDs in the legacy codes (the frequency of occurrence is included in the equations for the legacy code, which are not necessary for the ATD model, because of the hourly meteorological input).

3.5.1 Statistical Calculations

Although the consolidated ATD model calculates the hourly normalized concentration and deposition values, regulatory guides require different statistical outputs for different model assessments. Post-processing generates statistics and output as required by the regulatory guides—RG 1.194 for onsite control room DBA analyses, RG 1.145 for offsite DBAs, and RG 1.111 for routine release analyses.

The primary contributor to the differences between the final results from the ATD, PAVAN, and XOQDOQ codes stems from the different approaches for computing the percentiles and averages based on whether the data are hourly or from a JFD. The PAVAN code produces several different statistical results, including 0.5% per sector, 5% (overall site), and different averaging times (e.g., 0–2 h). The XOQDOQ code, on the other hand, computes annual averages.

The PAVAN ENVLOP routine interpolates (or extrapolates) the 0.5% and 5% results based on the occurrences of the χ/Q values on a lognormal plot. It computes a slope from the highest χ/Q to 10 lower values on the cumulative frequency distribution plot and uses the lowest slope (closest to horizontal) to interpolate the 0.5% (sector) or 5% (overall site) χ/Q value. If the frequency has a starting value greater than 0.5% (or 5%), ENVLOP extrapolates the first slope.

Since the ATD model uses hourly data, it has significantly more χ/Q records than the PAVAN code. The algorithm in the ATD model generates a cumulative distribution of hourly χ/Q values. It utilizes the slope between the frequencies where the 0.5% (or 5%) falls. If the cumulative frequency distribution has a starting value greater than 0.5% (or 5%), then the ATD model assigns the upper limit as the 0.5% (or 5%) χ/Q value. Unlike PAVAN, the ATD model currently does not extrapolate the first slope. Since the distributions are inherently different between the PAVAN and ATD models, the interpolations could be significantly different. Section 4.11 of the PAVAN documentation (Bander 1982) notes the following:

The values calculated in ONEOUT must be considered as approximations only. The enveloped frequency distributions generated in Subroutine ENVLOP may not always be reasonable. These should <u>always</u> be checked, and the values listed by ONEOUT adjusted accordingly.

The PAVAN ONEOUT subroutine computes χ/Q for intermediate time periods by interpolating the 0–2 h values and annual average values for each sector and overall site. In contrast, ATD uses moving averages of hourly data to compute χ/Q for each of the intermediate time periods and then computes the 0.5% and 5% values in a manner similar to the calculation of the short-term χ/Q values. RG 1.145, Section 2.2.1, states the following:

For a given sector, the average χ/Q values for the various time periods may be approximated by a logarithmic interpolation between the 2-hour sector χ/Q and the annual average (8760-hour) χ/Q Alternate methods should also be consistent with these studies and should produce results that provide a monotonic decrease in average χ/Q in time.

Since SIERRA ATD takes as input hourly data, the averages for various time periods are directly computed using moving (rolling) averages of the hourly data, and no logarithmic interpolation implemented. The moving averages generate a monotonic decrease in χ/Q values for longer time periods.

4.0 Overview of Comparisons with Legacy Code Output

The SIERRA ATD model results were compared with the legacy code outputs using two meteorological datasets:

- 1. a single synthetic meteorological dataset
- 2. an array of site-specific meteorological monitoring data from various NPPs.

Appendix B contains a detailed comparative analyses with synthetic data for the purpose of highlighting the fundamental differences between the legacy models and the ATD model. Comparisons with site-specific data are presented in this section in order to demonstrate ATD model agreement and consistency with prior regulatory code outputs.

The site-specific meteorological data are from 22 unique locations across the United States. Each file contains 1–5 years of data, and each file contains a unique number of calm and missing data. Table 4.1 presents a summary of the abbreviated site names (which include the years of data contained in the file) along with the hours of calm and missing data at the two heights. The mean wind speed at each height is also included in Table 4.1, along with the lower and upper measurement height values.

The primary comparison statistic used for comparing the ATD model to the legacy models is the modified normalized mean bias (MNMB). The MNMB describes the difference between the ATD model and legacy codes as a percentage of the average between the two outputs and is expressed as follows:

$$MNMB = \frac{100}{n} \sum_{i} \frac{M_i - O_i}{\frac{1}{2}(M_i + O_i)}$$
(1)

where M_i is the model result (χ/Q or D/Q) predicted using the ATD model and O_i is the corresponding model result (χ/Q or D/Q) predicted using the legacy code. MNMB values closer to zero show greater agreement between the models.

Additional statistics used in the comparison are the Factor of 2 (F2) and Factor of 5 (F5), which describe the percentage of ATD results that are within a factor of 2 ($0.5 \le ATD/Legacy \le 2.0$) of the legacy model result or within a factor of 5 ($0.2 \le ATD/Legacy \le 5.0$) of the legacy model result, respectively. The comparison results for the site-specific meteorology are presented as scatterplots for each legacy model. Perfect agreement between the two models would present as data aligned on the 1:1 line. Given that the models are fundamentally different, some spread is expected, and the 1:10 and 10:1 lines are included in each figure to give readers a sense of the spread of the data for different plots, which have different scales.

Number	Site Abbreviation	Total Hours	Missing + Calm Hours, Lower	Missing + Calm Hours, Upper	Average Lower WS (m/s)	Average Upper WS (m/s)	Lower Height (m)	Upper Height (m)
1	Belle 0607	8,760	1,440	523	2.04	2.89	10	60
2	BF 8791	43,824	4,401	3,110	4.56	8.39	10	55
3	BV 8690	43,824	15,338	2,275	1.88	4.16	10	46
4	CC 9193	26,304	976	597	3.07	4.91	10.1	49.4
5	Clint 0002	26,304	2,521	2,440	3.54	5.63	10	60
6	Hatch 9498	43,832	4,188	1,959	1.66	5.13	15	122
7	HMS 8387	43,824	1,354	1,233	3.41	4.84	12	61
8	Lee 0506	8,760	232	88	2.28	3.48	10	100
9	Levy0709	17,547	3,929	576	2.43	4.31	10	60
10	Mont 9192	8,760	790	444	2.93	6.06	10	60
11	NA 9698	26,304	730	261	2.47	3.74	10	60
12	Ocon 9498	43,824	3,021	2,777	2.08	3.30	10	48
13	Perry 9397	43,824	3,280	1,710	3.41	5.31	10	60
14	PSEG0609	26,304	542	884	3.79	6.33	10	60
15	SH 9499	43,824	5,423	895	1.95	3.71	10	91
16	STP9900	17,544	589	1,564	4.06	5.97	10	60
17	Surry 9296	43,848	4,788	874	2.17	4.19	9.6	44.9
18	TP0206	26,280	1,021	2,347	3.77	5.57	10	60
19	Vogtle 9802	43,824	2,311	2,750	2.21	3.84	10	90
20	VY 9599	43,824	2,822	3,338	2.44	4.48	10	60
21	WB 8993	43,824	12,305	4,779	2.04	3.30	9.5	91.2
22	Zion 8992	35,064	589	452	3.43	5.22	10	60

Table 4.1. Sites used in the verification of the ATD model.

m = meter(s); m/s = meter(s) per second; WS = wind speed.

4.1 ATD Onsite Control Room Design Basis Accident Analysis Comparison with ARCON

An onsite control room DBA analysis was performed using 21 sites from the site-specific data described in Table 4.1 (CC 9193 was absent from this analysis because of a missing input file for ARCON96). A single ground-level release case and a single elevated release case were prescribed for this evaluation. The ground-level release case had a release height of 10 m, a receptor distance of 45 m, and an intake height of 15 m, at 326°. The elevated release case had a release height of 60 m, a receptor distance of 210 m, and an intake height of 25 m, at 284°. An example of the ARCON input files used in this analysis is provided in Appendix C.

A comparison of the 95th percentile χ/Q values at each site for various averaging periods are plotted in Figure 4.1 for the ground-level release and in Figure 4.2 for the elevated release. The ground-level release results were very similar between the two models, with an MNMB of -0.26%, and 100% of values within a factor of 2. The elevated release results were also nearly identical between the two models. The normalized mean bias was 0.04%, and the F2 value was 100%. This level of agreement demonstrates a very high level of confidence in using the ATD model in place of the ARCON legacy code.



Figure 4.1. Comparison of the 95th percentile χ/Q from ATD and ARCON at various averaging intervals using site data from 22 nuclear power plant locations for a ground-level release (10 m).



Figure 4.2. Comparison of the 95th percentile χ/Q from ATD and ARCON at various averaging intervals using site data from 22 nuclear power plant locations for an elevated release (60 m).

4.2 ATD Offsite Design Basis Accident Analysis Comparison with PAVAN

An offsite DBA analysis was performed using the site-specific data described in Table 4.1. The hourly data in the RG 1.23 format were converted to a JFD and incorporated within PAVAN input files for this comparison. The calms in each meteorological file were assigned a direction and distributed uniformly within the first wind-speed class in the PAVAN input file. This allowed for a direct model comparison with ATD. A single ground-level release case and a single elevated release case were prescribed for this evaluation. The ground-level release case had a release height of 10 m and a building area of 0 m². The elevated release case had a release height of 60 m and a stack flow of 0 m/s. An example of the PAVAN input files used in this analysis is provided in Appendix C.

Comparisons of the 16 sector 0-2 h χ/Q values for the ground-level and elevated releases are presented in Figure 4.3 and Figure 4.4. The MNMBs for the ground-level release case were 0.7% at the EAB and 2.4% at the LPZ. At both distances, 96.6% of the values were within a factor of 2, and 100% of the values were within a factor of 5. For the elevated case, the MNMBs were 15.9% at the EAB and 7.5% at the LPZ. As was seen for the ground case, 99.7% or more of the values were within a factor of 2, and 100% of the values were within a factor of 5.

As noted in Section 3.5.1, the differences between these results primarily stem from the statistical interpolation (or extrapolation) of the short-term χ/Q values, which are variably distributed between the ATD and PAVAN simulations. Additional detail on the PAVAN statistical comparisons can be found in Appendix B with the synthetic data analysis.

Comparisons of the annual average χ/Q values for the ground-level and elevated releases are presented in Figure 4.5 and Figure 4.6. All values are within a factor of 2, with MNMBs for the ground-level release case of 5.0% and 5.6% at the EAB and LPZ, respectively. MNMBs for the elevated release case were -0.5% at the EAB and 1.3% at the LPZ. As with the ARCON analysis, the ATD model is shown to be consistent and agrees very well when compared to the legacy PAVAN code.



Figure 4.3. Comparison of the sector $0-2 h \chi/Q$ values from ATD and PAVAN using site data from 22 nuclear power plant locations for a ground-level release (10 m). The upper panel is for the EAB (800 m), and the lower panel is for the LPZ (3000 m).



Figure 4.4. Comparison of the sector $0-2 h \chi/Q$ values from ATD and PAVAN using site data from 22 nuclear power plant locations for an elevated release (60 m). The upper panel is for the EAB (800 m), and the lower panel is for the LPZ (3000 m).



Figure 4.5. Comparison of the annual average χ/Q values from ATD and PAVAN using site data from 22 nuclear power plant locations for a ground release (10 m). The upper panel is for the EAB (800 m), and the lower panel is for the LPZ (3000 m).



Figure 4.6. Comparison of the annual average χ/Q values from ATD and PAVAN using site data from 22 nuclear power plant locations for an elevated release (60 m). The upper panel is for the EAB (800 m), and the lower panel is for the LPZ (3000 m).

4.3 ATD Routine Release Analysis Comparison with XOQDOQ

A routine release analysis was performed using the site-specific data described in Table 4.1. The hourly data in the RG 1.23 format were converted to a JFD and incorporated within XOQDOQ input files for this comparison. The calms in each meteorological file were assigned a direction and distributed uniformly within the first wind-speed class in the XOQDOQ input file. This allowed for a direct model comparison with ATD. A single ground-level release case and a single elevated release case were prescribed for this evaluation. The ground-level release case had a release height of 10 m, while the elevated release case had a release height of 60 m. In each case, receptors at each of the 16 directional sectors at distances of 1 and 10 miles were evaluated. An example of the XOQDOQ input files used in this analysis is provided in Appendix C.

A comparison of the χ/Q values for the ground-level release case is presented in Figure 4.7 for receptors at 1 and 10 miles. The MNMBs were 6.3% and 1.9% and at 1 and 10 miles, respectively, with 100% of the results within a factor of 2. The elevated release case is presented in Figure 4.8 for receptors at 1 and 10 miles. As with the ground-level release, all results are within a factor of 2, with MNMBs of -8.2% and -4.8% for the 1-mile and 10-mile distances, respectively.

The level of agreement demonstrated with this analysis shows that ATD model, while using hourly meteorological data, is consistent with the XOQDOQ legacy code, which uses JFD inputs. However, as with PAVAN, users are cautioned to examine how calms are handled and distributed in XOQDOQ when drawing comparisons to the ATD model. If the user does not assign a uniform wind direction to the calms and allows XOQDOQ to distribute the calms in the default manner, the comparisons will be quite different because of the fundamental differences in calm wind assumptions. This will be of particular importance for sites with high percentages of calms.



Figure 4.7. Comparison of the annual average χ/Q values from ATD and XOQDOQ using site data from 22 nuclear power plant locations for a ground-level release (10 m). The values of χ/Q are plotted for 1 and 10 miles in the upper and lower panels, respectively.



Figure 4.8. Comparison of the annual average χ/Q values from ATD and XOQDOQ using site data from 22 nuclear power plant locations for an elevated release (60 m). The values of χ/Q are plotted for 1 and 10 miles in the upper and lower panels, respectively.

5.0 Summary

The ATD model within SIERRA was designed to consolidate and modernize the computation of χ/Q for three assessment types: (1) onsite control room habitability DBAs, (2) offsite DBAs, and (3) routine releases. NRC staff and RAMP users have employed ARCON2 (and earlier ARCON96) for short-term consequence assessment of the control room, PAVAN for analyzing offsite DBAs, and XOQDOQ for consequence assessment of routine releases from NPPs. The SIERRA ATD engine reengineered the implementation of RG 1.145 and RG 1.111 to use hourly meteorological data for PAVAN and XOQDOQ analyses, respectively, and allows for ARCON-equivalent onsite control room DBA calculations pursuant to RG 1.194 all within the same code. Given the regulatory basis and governance of the legacy codes, it is of utmost importance to demonstrate agreement and consistency between the ATD model and the legacy codes.

Comparisons with site-specific data demonstrated this high level of agreement and consistency between ATD model and legacy code outputs. For ARCON, the ground-level and elevated release comparison produced MNMB values within ±1%. The XOQDOQ comparisons had similar alignment, with MNMB values within ±4%. For PAVAN, the primary deviations resulted from fundamental differences in PAVAN statistical methodologies and how they are applied to JFDs versus hourly data. Despite this, MNMB values were within ±8% for statistical-based results.

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Appendix A – Model Technical Basis

A.1 Meteorological Data Processing

Meteorological data in a Fortran format provided in the Regulatory Guide (RG) 1.23 guidance document are used as the model input. The meteorological reader routine within the Atmospheric Transport and Diffusion (ATD) engine reads the wind speed, wind directions collected at lower and upper tower measurement heights, and the temperature difference between these two heights (i.e., upper minus lower). There are other variables (e.g., sigma theta) that can be provided by the user, as described in RG 1.23. However, the reading routine ignores these values and treats them as blank space. The Fortran format used in this routine is described in Table A.1.

Fortran Read	
Specification	Variable Description
A4	Identifier
I4	Year
13	Julian day
14	Hour (01 to 24)
F5.1	Upper measurement height (m)
F5.1	Wind direction (degrees) at upper measurement height
F5.1	Wind speed (m/s) at upper measurement height
55X	Not used as a variable
F5.1	Lower measurement height (m)
F5.1	Wind direction (degrees) at lower measurement height
F5.1	Wind speed (m/s) at lower measurement height
20X	Not used as a variable
F5.1	Temperature Difference (Upper – Lower) (°C/100 m)
°C = degrees Celsius; m = m	neter(s); m/s = meter(s) per second.

Table A.1. Fortran format implemented in the meteorological reader routine.

Thereafter, the meteorological processor routine selects the measurement height that will be used for dispersion calculations. If the stack height is greater than the average of the lower and upper air measurement heights, then the upper air measurements are used for dispersion modeling; otherwise, the lower measurements are used.

Once a measurement height is selected, the routine determines the "calm" wind from the hourly data for the selected height using the following criteria:

- wind direction with values "77777" as prescribed in RG 1.23 to indicate calm
- less than or equal to the minimum calm threshold provided by the user in the input.

The missing data are determined within the engine based on following criteria:

• wind direction or temperature difference with values "99999" as prescribed in RG 1.23 for a lost or invalid hourly record or parameter value

A "calm" hour missing data criterion being met is treated as missing data and not included in calculations. χ/Q and/or D/Q is not computed for hours with missing data and also excluded from statistical averages during post-processing.

The atmospheric stability for each hour is then determined from the temperature difference (dT/dz) using the classification (A through G) in Table 1 of RG 1.23. The wind speed at the measurement height is corrected for the stack (release) height using Monin–Obukhov length similarity theory for an onsite control room design basis accident (DBA) assessment (Ramsdell and Simonen 1997). A simple power law relationship (Bander 1982) is used to adjust the wind speed for the other two assessments.

A.2 Effective Stack (Release) Height

An effective stack height is computed for elevated and vent releases (routine release analyses only). The effective stack height is determined from a combination of the stack (release) height, plume rise, downwash, and terrain. The effective height is also adjusted for the surrounding terrain heights and receptor height to adjust for the difference between the plume centerline and receptor heights:

$$H = H_{\text{stack}} + \Delta H_{\text{rise}} + \Delta H_{\text{d}} + (T_{\text{stack}} - T_{\text{rec}}) - H_{\text{intake}}$$
(A.1)

where

Н	=	effective stack height used in the computation of relative concentrations
H_{stack}	=	physical height of the stack
ΔH_{rise}	=	increase in plume height due to the plume rise
$\Delta H_{\rm d}$	=	stack downwash (onsite control room DBA analysis only)
$T_{\rm stack}$	=	terrain height at the stack location
$T_{\rm rec}$	=	terrain height at the receptor location
<i>H</i> intake	=	height of intake (onsite control room DBA analysis only).

ATD only allows the user to provide the receptor height for the onsite control room DBA analyses. The receptor height is assumed to be zero at ground level for offsite DBA and routine release analyses. The terrain height (T_{rec}) for a single receptor is directly retrieved from the input for onsite control room DBA analyses. This value is interpolated from a range of user inputs within the input file for the other two assessments, which may have terrain information at different distances for each directional sector. The ATD engine currently allows the user to enter terrain data as a function of two or more distances and 16 directions. The ATD engine interpolates the terrain data at a particular hour for a receptor of a certain distance and a directional sector where the concentration is being computed.

The plume rise (ΔH_{rise}) is also calculated for elevated releases caused by either momentum or buoyancy based on the formulations outlined in (Sagendorf et al. 1982). It is calculated separately for stable conditions and neutral/unstable conditions.

The plume rise due to buoyancy is calculated if the heat emission rate is greater than zero. Otherwise, the plume rise due to momentum is calculated using the input of the volumetric flow rate from the stack or vent. If both values are zero or the stack diameter is zero, then plume rise is assumed to not be included. If the exit velocity is less than 1.5 times the wind speed at the release height, a correction for the downwash is made for momentum-based plume rise. The ATD engine calculates the exit velocity using the user inputs of the stack flow rate and stack inside diameter:

$$w_0 = \frac{Q}{\pi \left(\frac{D}{2}\right)^2} \tag{A.2}$$

where

 w_0 = exit velocity

 $Q = \text{stack flow rate } (m^3/s)$

D =stack inside diameter (m).

Plume rise calculations are a user option for offsite DBA analyses. An applicant or licensee may propose adjustments to the release height for the plume rise that are due to buoyancy or momentum effects on a case-by-case basis. However, in order to credit any such adjustments, an applicant or licensee must be able to demonstrate that the assumed buoyancy or vertical velocity of the effluent plumes will be maintained throughout the time intervals that the plume rise is to be credited. If the plume rise effects are determined to not last throughout every averaging period, SIERRA could be run twice (both with and without the plume rise included), and the appropriate values reported for the applicable time periods. Planned future updates will allow the user to select the averaging periods for which the plume rise effects apply in a single run.

Currently, the plume rise is not calculated for the onsite control room DBA assessment. A stack tip downwash is computed for an onsite control room DBA assessment using the following equation:

$$\Delta H_{\rm d} = 4 \frac{D}{2} \Big[\frac{w_0}{U} - 1.5 \Big] \tag{A.3}$$

where U is the wind speed in meters/second.

A.3 The Gaussian Plume Model

The concentrations (and deposition) at receptor distances are computed for each hour including inputs of wind speed (adjusted as needed based on the effective release height), wind direction, and atmospheric stability. The atmospheric engine implements a straight-line Gaussian plume model. The complete straight-line Gaussian plume model (including ground reflection) is expressed as follows:

$$\frac{\chi}{Q} = \frac{1}{2\pi U \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \left[\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right)\right]$$
(A.4)

where

 χ = concentration (Ci/m³) at downwind distance *x*, crosswind distance *y*, and height *z* in a plume with an axis at the effective stack height *H*

- Q = release rate (Ci/s)
- χ/Q = relative concentration (s/m³)
 - U = mean wind speed (m/s)
 - x = downwind distance (m)
 - y = crosswind distance (m)
 - z = height in the plume (m)
 - H = effective stack height (m)

σ_y, σ_z = diffusion coefficients in the horizontal and vertical directions, respectively (m).

A.3.1 Centerline Plume Model

The Gaussian plume model in Equation (A.4) can be simplified for ground-level (z = 0) centerline (y = 0) concentrations as follows:

$$\frac{\chi}{Q} = \frac{1}{\pi U \sigma_y \sigma_z} \exp\left(-\frac{H^2}{2\sigma_z^2}\right) \tag{A.5}$$

This equation provides the centerline relative concentrations for an elevated release with the effective stack height H (m). For ground-level sources, H is equal to zero, and the equation is further simplified to

$$\frac{\chi}{Q} = \frac{1}{\pi U \sigma_{\rm y} \sigma_z} \tag{A.6}$$

A.3.2 Sector-Averaged Plume Model

The centerline relative concentrations in Equations (A.5) and (A.6) are appropriate for short averaging periods. It is unlikely that the plume position will remain constant in the same direction for long periods. Therefore, a sector-averaged model is used to estimate the relative concentrations for averaging periods longer than 8 h. The sector-averaged plume model is derived by integrating the concentration across the normal plume model and dividing the result by the sector width, W (m). The sector-averaged relative concentration for elevated sources is given by

$$\frac{\chi}{Q} = \frac{2}{\sqrt{2\pi}U\sigma_z W} \exp\left(-\frac{H^2}{2\sigma_z^2}\right)$$
(A.7)

Further, for ground-level sources, the sector-averaged plume model is

$$\frac{\chi}{Q} = \frac{2}{\sqrt{2\pi}U\sigma_z W} \tag{A.8}$$

where *W* is the width of a 22.5° wind direction sector, which is a function of the downwind distance (m). It can be calculated from the circumference of a circle with a radius equal to the downwind distance *x* divided by number of wind direction sectors (conventionally 16 directions, which are each 22.5° wide).

$$W = \frac{2\pi x}{16} \tag{A.9}$$

Using this value of W, the sector-averaged relative (or normalized) concentration for elevated and ground-level sources can be expressed, respectively, as follows:

$$\frac{\chi}{Q} = \frac{2.0318}{U\sigma_z x} \exp\left(-\frac{H^2}{2\sigma_z^2}\right) \tag{A.10}$$

$$\frac{\chi}{Q} = \frac{2.0318}{U\sigma_z x} \tag{A.11}$$

These two equations are used for calculations within the SIERRA atmospheric engine for determining relative concentrations, based on the distance-based sector width, that mimic the functionality of PAVAN and XOQDOQ. It should be noted that NRC codes PAVAN (Bander 1982) and XOQDOQ (Sagendorf et al. 1982) also utilize a factor for the joint frequency distribution (JFD) of meteorological data in the sector-averaged model. The SIERRA atmospheric engine is based on hourly simulations; therefore, the equations implemented here do not incorporate the frequency factor. All hourly χ/Q values are collected in an array, and long-term averages (including annual averages) are computed during post-processing.

A.3.3 Calculations for Onsite Control Room Design Basis Accident Analyses

For onsite control room DBA analyses, the sector width W is calculated assuming that 95 percent of the Gaussian plume is generally within $\pm 2\sigma_y$ of the plume centerline (Ramsdell and Simonen 1997).

$$W = 4.3\sigma_{\rm v} \tag{A.12}$$

The slant path is generally used as the distance to the receptor in lieu of the straight-line (ground-level) distance between the receptor (typically the control room) and the source of release. The slant path is computed using the Pythagorean theorem from the effective release height (i.e., the difference between the source and receptor heights) and distance to the receptor:

$$X_{\text{slant}} = \sqrt{(X)^2 + (H)^2}$$
 (A.13)

The relative concentration is corrected for the stack flow rate as prescribed in Section 3.4 of Ramsdell and Simonen (1997):

$$\left(\frac{\chi}{Q}\right)^* = \frac{1}{\frac{1}{\chi/Q} + F} \tag{A.14}$$

where *F* is the stack flow rate (m^3/s) .

A.3.4 Calculations for Offsite Design Basis Accident Analyses

The relative concentrations for elevated releases under nonfumigation conditions are calculated at various predetermined distances up to a maximum of 90,000 m. The χ/Q values at given boundary distances (exclusion area boundary [EAB] and low population zone [LPZ]) are compared to concentrations at various distances beyond the boundary to assure that the maximum χ/Q does not occur outside the boundary. For EAB values, maximum values are not searched beyond the LPZ boundary. For LPZ values, comparisons are made with iterations out to 12.8 km beyond the LPZ boundary. Thus, the maximum χ/Q values at or beyond the boundary are used like that for PAVAN (Bander 1982).

Fumigation conditions are determined at each hour based on the stable atmospheric conditions (E, F, or G categories) at that hour and unstable conditions (A, B, or C categories) at the next

hour. For hours with fumigation conditions, the following equation is used to determine the centerline relative concentrations consistent with Regulatory Position 1.3.2(b) of RG 1.145:

$$\frac{\chi}{Q} = \frac{1}{\sqrt{2\pi}U\sigma_{\nu}H} \tag{A.15}$$

The wind speed used in this equation is representative of the fumigation layer. A value of 2 m/s is used as a reasonably conservative assumption for an effective stack height of about 100 m (RG 1.145). The lateral plume spreads at given distances are based on a moderately stable atmosphere (Pasquill stability category F).

The "fumigation χ/Q " from equation (A.15) can approach unrealistically large values, as the effective stack height becomes small. To limit the "fumigation χ/Q " value, the ATD routine also calculates χ/Q from equation (A.5) assuming a stability category of F, a wind speed of 2 m/s, and an effective height of 0 m. The χ/Q values calculated using both equations are compared, and the lower value is selected as the "fumigation χ/Q " consistent with Regulatory Position 1.3.2(b) of RG 1.145. At coastal sites (i.e., less than 3.2 km from a large body of water), the 0–2 h average χ/Q at the EAB for each sector is selected from the maximum of either the "fumigation χ/Q " or nonfumigation χ/Q " and nonfumigation χ/Q is used for inland sites. Methods for the determination and use of fumigation and nonfumigation χ/Q values for elevated releases are described more fully in Regulatory Positions 1.3.2, 2.1.2, and 2.2.2 of RG 1.145.

A.3.5 Calculations for Routine Release Analyses

The annual average is processed from hourly normalized relative concentrations (χ/Q) (sectoraveraged only) and relative deposition (D/Q) values in the post-processing routine. Hourly χ/Q values are calculated using modified forms of the elevated and ground-level release equations. RG 1.111 calls for calculations of radionuclide transport and diffusion for long durations (typically annual averages) and distances (typically out to 50 miles). Therefore, the open terrain recirculation and removal mechanisms due to radioactive decay (or depletion) and dry deposition are accounted for in the routine release analysis. Standard multiplicative factors as a function of atmospheric (Pasquill) stability class and distance are provided for the radioactive decay (depletion) and dry deposition processes in the January 1977 Errata to RG 1.111. The sector-averaged χ/Q and D/Q values are multiplied by these factors, as in (Sagendorf et al. 1982):

$$\frac{\chi}{Q} = \frac{2.0318}{U\sigma_z x} \exp\left(-\frac{H^2}{2\sigma_z^2}\right) \times RF(x) \times DEC(x, U) \times DEPL(x, stab, H)$$
(A.16)

$$\frac{\chi}{Q} = \frac{2.0318}{U\sigma_z x} \times RF(x) \times DEC(x, U) \times DEPL(x, stab)$$
(A.17)

where

stab = stability condition

RF = open terrain recirculation factor at distance x
 DEC = reduction factor due to radioactive decay at distance x and wind speed U
 DEPL = reduction factor due to plume depletion at distance x, stability stab, and height H (for elevated sources).

The correction factor for open terrain recirculation is calculated using polynomial equations (a function of the downwind distance, x) based on Figure 3.2 in the XOQDOQ user manual

(Sagendorf et al. 1982). If the user does not select the option of recirculation factor, then *RF* is equal to 1. The factor *DEC* is computed using simple first-order radioactive decay based on a predefined half-life:

$$DEC(x) = \exp\left(\frac{-0.693 \times t}{24 \times T_{1/2}}\right)$$
 (A.18)

$$t = \frac{x}{3600 \times U} \tag{A.19}$$

where

t = travel time in hours calculated from the hourly wind speed U (m/s) $T_{1/2}$ = half-life of the radioactive material (days).

Three different values for relative concentrations are calculated based on three half-life values that have been predefined in RG 1.111 and implemented in XOQDOQ (Sagendorf et al. 1982):

- no decay, undepleted
- an overall half-life of 2.26 days for short-lived noble gases (undepleted)
- a half-life of 8 days for all iodines (depleted)

The plume depletion factor is also calculated using polynomial equations based on Figures 3 through 6, as numbered, in the January 1977 Errata of the March 1976 issue of RG 1.111. The plume depletion is a function of the release height (*H*) and downwind distance (*x*). For releases >15 m, the depletion factor also varies for the stability condition (*stab*).

The relative deposition (dry) is calculated as follows:

$$\frac{D}{Q} = \frac{F(x, stab, H)}{(2\pi/16)x} \times RF$$
(A.20)

where

D/Q = relative deposition

F = polynomial equation from XOQDOQ.

The function *F* is a polynomial equation from XOQDOQ based on the distance, stability condition, and release height. These polynomials were derived from Figures 7 through 10, as numbered, in the January 1977 Errata of the March 1976 issues of RG 1.111. For release heights \leq 15 m, the deposition is only function of the downwind distance, like the depletion factors. The function plots for the recirculation factor, plume depletion, and relative deposition are shown in Figure A.1 through Figure A.7.

In addition to ground-level and elevated sources, relative concentration and deposition values are also calculated for vent releases. An entrainment coefficient is calculated based on the ratio of the plume exit velocity (w_0) to the hourly wind speed at the release height. If the ratio is <1 (i.e., the exit velocity less than the wind speed), then it is treated as a ground-level source. If the ratio is >5, then the plume is treated as an elevated source. For cases where the ratio of the exit velocity to the wind speed is between one and five, a mixed release model is assumed, in which the plume is considered as an elevated release during part of the time and as a ground-level release during remainder of the time. The entrainment coefficient (E_t) is determined for these cases as follows:

$$E_t = 1 \text{ for } \frac{w_0}{u} \le 1 \tag{A.21}$$

$$E_t = 2.58 - 1.58 \left(\frac{w_0}{u}\right)$$
 for $1 < \frac{w_0}{u} \le 1.5$ (A.22)

$$E_t = 0.3 - 0.06 \left(\frac{w_0}{U}\right)$$
 for $1.5 < \frac{w_0}{U} \le 5$ (A.23)

$$E_t = 0 \text{ for } \frac{w_0}{u} > 5 \tag{A.24}$$

The release is considered to occur as an elevated release during a $(1 - E_t)$ time fraction and as a ground release during an E_t time fraction, as shown below. For mixed-mode vent releases, relative concentrations and deposition rates are calculated using the respective Gaussian equations for elevated and ground-level releases and as adjusted by either Equation (A.25) or (A.26).

$$\left(\frac{\chi}{Q}\right)_{\text{vent}} = (1 - E_t) \left(\frac{\chi}{Q}\right)_{\text{ground}} + E_t \left(\frac{\chi}{Q}\right)_{\text{elevated}}$$
(A.25)

$$\left(\frac{D}{Q}\right)_{\text{vent}} = (1 - E_t) \left(\frac{D}{Q}\right)_{\text{ground}} + E_t \left(\frac{D}{Q}\right)_{\text{elevated}}$$
(A.26)



Figure A.1. Open terrain correction factor.



Figure A.2. Plume depletion effect for ground-level releases (all atmospheric stability classes).



Figure A.3. Plume depletion effect for 30 m releases and different atmospheric stability classes.



Figure A.4. Plume depletion effect for 60 m releases and different atmospheric stability classes.



Figure A.5. Relative deposition for ground-level releases (all atmospheric stability classes).



Figure A.6. Relative deposition for 30 m releases and different atmospheric stability classes.





A.3.6 Diffusion Coefficients

The spread of a plume in the horizontal (σ_y) and vertical (σ_z) directions at a prescribed downwind distance is described by diffusion coefficients. These coefficients are standard

deviations of the Gaussian plume distribution and are related to the atmospheric stability and downwind distance. There are many schemes for estimating these coefficients based on empirical data. The diffusion coefficients have the general form (Ramsdell and Simonen 1997)

$$\sigma = ax^b + c \tag{A.27}$$

where

 σ = diffusion coefficients (m) x = downwind distance (m)

a, b, c = parameters as functions of the atmospheric stability.

The most widely used stability classification approach for atmospheric dispersion modeling purposes is based on the Pasquill–Gifford (P-G) diffusion coefficients. It is noted that the P-G diffusion coefficients have been established by the U.S. Nuclear Regulatory Commission (NRC) for seven stability categories (A–G), while the U.S. Environmental Protection Agency (EPA) defines them for six stability categories only (A–F). The atmospheric stability at each hour is calculated using the vertical temperature gradient (dT/dz) (i.e., as measured between the upper and lower levels) from meteorological data in the RG 1.23 format based on guidance provided in Table 1 of RG 1.23 (NRC 2007d).

The atmospheric engine allows five empirical methods for calculating diffusion coefficients:

- P-G relationships implemented in NRC models (NRC regulatory default method)
- P-G relationships implemented in the EPA ISC3 model (non-NRC alternate regulatory approach)
- Briggs open country conditions (non-NRC alternate regulatory approach)
- Briggs urban conditions (non-NRC alternate regulatory approach)
- desert diffusion curves by Markee implemented in XOQDOQ (Sagendorf et al. 1982) (NRC regulatory default method when appropriate).

These empirical relationships are elaborated in a report by Napier et al. (2011). NRC P-G coefficients and Markee's desert diffusion curves are discussed in Section 4.16 of the PAVAN model users guide (Bander 1982) for offsite DBA analyses. Horizontal (lateral) and vertical diffusion curves (i.e., σ_y and σ_z , respectively) as a function of distance are illustrated in Figures 1 and 2 of RG 1.145 but do not include plume meander and building wake effects, which can be accounted for by other model options. Further, note that only six P-G stability classes (i.e., A through F) are shown; footnotes to those curves indicate approximations for stability class G. NRC P-G coefficients and Markee's desert diffusion curves are discussed (the latter when applicable) in Sections 3.2 and 4.21 of the XOQDOQ model user's guide (Sagendorf et al. 1982) for routine release analyses. Only the vertical diffusion curve (σ_z) is illustrated by Figure 1 of RG 1.111 because the plume is typically assumed to cover the width of the entire direction sector on a long-term basis. Building wake effects can be accounted for as an option; consideration of plume meander effects is reflected in the desert diffusion curves under limited conditions.

The airflows over and around buildings create a complex dispersion pattern for plumes. The recirculation airflow near the edge of the building creates enhanced turbulence and accelerated diffusion of the plume. Such "building wake" effects near buildings are accounted for through simple statistical modification of the diffusion coefficients in the Gaussian plume model.

A.3.6.1 Diffusion Coefficient Adjustments for Onsite Control Room Design Basis Accident Analyses

A building wake model based on work by Ramsdell and Fosmire (1998) is used for near-field calculations similar to ARCON2 and ARCON96. The modified diffusion coefficients are calculated as follows:

$$\Sigma_{y} = \left(\sigma_{y}^{2} + \Delta \sigma_{y1}^{2} + \Delta \sigma_{y2}^{2}\right)^{1/2}$$
(A.28)

$$\Sigma_z = (\sigma_z^2 + \Delta \sigma_{z1}^2 + \Delta \sigma_{z2}^2)^{1/2}$$
(A.29)

where $\Sigma_{y}, \Sigma_{z} = \text{modified diffusion coefficients}$ $\sigma_{y}, \sigma_{z} = \text{diffusion coefficients in a specified direction (m)}$ $\Delta \sigma_{y1}, \Delta \sigma_{z1} = \text{low-wind-speed corrections}$ $\Delta \sigma_{y2}, \Delta \sigma_{z2} = \text{building wake corrections.}$

These corrections are described in the ARCON96 user manual (Ramsdell and Simonen 1997).

A.3.6.2 Diffusion Coefficient Adjustments for Offsite Design Basis Accident and Routine Release Analyses

The building wake model implementations for mid- and far-field analyses are based on the equations provided in RG 1.145 and the PAVAN and XOQDOQ user manuals. RG 1.145 recommends two classifications based on meteorological conditions: (i) neutral (category D) or stable (categories E, F, or G) or (ii) unstable (categories A, B, or C). The three equations below are simultaneously calculated for centerline relative concentrations for ground-level releases. For offsite DBA analyses, these equations apply to sources effectively lower than 2.5 times the height of adjacent solid structures.

$$\frac{\chi}{Q} = \frac{1}{U(\pi\sigma_y\sigma_z + C\cdot A)} \tag{A.30}$$

$$\frac{\chi}{Q} = \frac{1}{U(3\pi\sigma_y\sigma_z)} \tag{A.31}$$

$$\frac{\chi}{Q} = \frac{1}{U(\pi \Sigma_{My} \sigma_y \sigma_z)} \tag{A.32}$$

where

A = smallest vertical-plane cross-sectional area of the reactor building or other appropriate structure

- C = mixing volume coefficient in the building wake term (internally set to 0.5)
- Σ_{My} = meander factor for the lateral plume spread as a function of the stability and wind speed.

The product of the meander factor (Σ_{My}) and horizontal diffusion coefficient (σ_y) for downwind distances greater than 800 m is adjusted as shown below:

$$\Sigma_{My}\sigma_y = \sigma_y + [\Sigma_{My} - 1]\sigma_{y,800m}$$
(A.33)

where $\sigma_{y,800m}$ is the horizontal diffusion coefficient at an 800 m distance for the particular stability class.

For the determination of Σ_{My} and a complete discussion on plume meander, refer to Regulatory Position 1.3.2, Figure 3, and Appendix A of RG 1.145. For unstable conditions, the higher concentration between the results of Equations (A.30) and (A.31) is used, and Equation (A.32) is not used. For neutral and stable conditions, the higher relative concentration between the results of Equations (A.30) and (A.31) is compared with the result from Equation (A.32), and the minimum is selected.

Simpkins (2007) compared the building wake calculations using equations and parameters from ARCON and RG 1.145. This investigative study showed that the ARCON wake corrections generated much lower values compared to a Gaussian plume model simulation without any building (about 100 times lower) for the F stability category. The RG 1.145 method was slightly lower than the no-building simulations for the F stability category (less than a factor of 10).

The building wake corrections for sector-averaged concentrations are based on RG 1.111 and applicable for long-term averages (>8 h) in offsite DBA and routine release analyses.

The vertical diffusion coefficient (σ_z) in Equations (A.10) and (A.11) is modified using the following equation:

$$\Sigma_z = \min\left[(\sigma_z^2 + C \cdot D^2/\pi)^{1/2}, \sqrt{3}\sigma_z\right]$$
(A.34)

where

- Σ_z = modified diffusion coefficient
- \overline{D} = the minimum adjacent building height either up- or downwind from the release point.

A.3.7 Statistical Calculations

Although the consolidated ATD model calculates the hourly normalized concentration and deposition values, regulatory guides require different statistical outputs for different model assessments. Post-processing generates statistics and output as required by the regulatory guides—RG 1.194 for onsite control room DBA analyses, RG 1.145 for offsite DBAs, and RG 1.111 for routine release analyses.

A.3.7.1 Statistical Calculations for Onsite Control Room Design Basis Accident Analyses

For onsite control room DBA analyses, χ/Q is computed for all calm hours and any populated hour when the wind is within the wind direction window, i.e., the direction to the source is within ±45°. For other hours when the wind direction is outside this window, or not calm, the χ/Q value for that hour is assigned as zero. The intention is to assess the frequency of χ/Q at the receptor site (typically at the control room but may also be an onsite technical support center) during the entire period of meteorological data.

Time-averaged values of relative concentrations are computed as running mean values of the hourly concentrations. Time averages are calculated for 1, 2, 4, 8, 12, 24, 96, 168, 360, and 720 h. For averaging time periods \leq 8 h in duration, the running average is calculated using the centerline concentrations consistent with Section 2.4.3 and 3.6 of Ramsdell and Simonen (1977):

$$\frac{\overline{\chi}}{Q} = \frac{1}{N} \sum_{i=1}^{N} \left(\frac{\chi}{Q} \right)_{i} \Big|_{\text{centerline}}$$

where N is 1, 2, 4, or 8 h for the averaging period. ATD is not limited to 10,000 hours, as described in Section 2.4.3 of Ramsdell and Simonen (1977).

For periods longer than 8 h, the time averages include both the centerline and sector-averaged concentrations consistent with Section 2.4.3 and 3.6 of Ramsdell and Simonen (1977):

$$\frac{\overline{\chi}}{Q} = \frac{1}{N} \left[\sum_{i=1}^{8} \left(\frac{\chi}{Q} \right)_{i} \right|_{\text{centerline}} + \sum_{i=9}^{N} \left(\frac{\chi}{Q} \right)_{i} \right|_{\text{sector average}}$$
(A.36)

where N is 12, 24, 96, 168, 360, or 720 h.

Cumulative frequency distributions are then computed for each averaging interval. The 95th percentile values, which support onsite control room DBA analysis and any other user-provided customized percentile values (e.g., 99.5th), which may or may not support other regulatory analyses, are then calculated from these frequency distributions. In addition to calculating percentile values for each averaging period, the algorithm determines the 95th percentile values for standard averaging intervals: 0–2 h, 2–8 h, 8–24 h, 1–4 days, and 4–30 days. The average 95th percentile relative concentrations for the 2–8 h period are calculated as follows:

$$\frac{\left(\frac{\chi}{Q}\right)_{95}}{8-2} = \frac{8 \times \left(\frac{\chi}{Q}\right)_{95}}{8-2} = \frac{$$

The relative concentrations for the other standard time intervals are calculated in a similar manner.

If at least one of the meteorological variables (i.e., wind speed, wind direction, dT/dz) required for a χ/Q calculation is not defined, the record is considered missing. Missing data are accounted for by deleting hours with missing data from the calculation of the running average relative concentrations. A missing data tolerance criterion is used to determine when the number of hours with missing data make a specific average unacceptable. This tolerance criterion is a user input, which by default is 10 percent, consistent with the default for this parameter as given in Table A-2 of RG 1.194. No missing hours are allowed for averaging periods of 8 hours or less. Time averages longer than 8 hours are not calculated for periods in which the number of hours with missing data exceed the missing data tolerance criteria.

A.3.7.2 Statistical Calculations for Offsite Design Basis Accident Analyses

This algorithm calculates the relative concentrations at two sets of distances, labeled EAB and LPZ per typical regulatory applications. For both sets of boundaries, two different procedures are utilized based on RG 1.145 and NUREG/CR-2260 (Snell and Jubach 1981) for statistical calculations:

• The direction-dependent approach described in Regulatory Position 2 of RG 1.145. Timeaveraged values and consequent exceedance values are calculated for each direction sector. For example, the relative concentration in each sector that is exceeded by χ/Q

(A.35)

values in that sector 0.5 percent of the total time relative to all sectors (i.e., sectordependent χ/Q), which is similar to the 99.5th percentile.

• The overall site approach described in Regulatory Position 3 of RG 1.145. In this procedure, a χ/Q from among all sectors that is exceeded 5 percent of the total time is determined (i.e., the overall site χ/Q).

The following averaging time periods (computed as a moving average) are considered: 0–2 h (maximum of 1 h and 2 h), 0–8 h, 8–24 h (16 h), 1–4 days (72 h), 4–30 days (624 h), and annual average. Relative concentrations for short periods (≤8 h) are calculated using centerline values, and those for longer periods (>8 h) are calculated using both centerline and sector-averaged values. Exceedance values of 0.5% and 5% are calculated for both direction-dependent and overall site relative concentrations. The exceedances are computed by generating cumulative distributions of χ/Q values. The ATD model utilizes the slope between the frequencies where the 0.5% (or 5%) falls. If the starting value of the frequency distribution is greater than 0.5% (or 5%), then the ATD model uses the upper limit χ/Q as 0.5% (or 5%). The 50% exceedances are calculated for the overall site. The calm hours are equally distributed in all directions.

Direction-dependent annual averages are calculated from the sum of all values in each wind direction sector and dividing by the total valid simulation hours (i.e., the total number of hours in the meteorological data – the number of hours with missing data). The χ/Q value that is exceeded 0.5% of the total time in each sector is calculated.

For the overall site approach, the χ/Q value that is exceeded 5% of the total time for all sectors is used as the annual average and for the site limit

A.3.7.3 Statistical Calculations for Routine Release Analyses

For routine release analyses, the algorithms calculate the annual average relative concentrations (χ/Q) and deposition values (D/Q) at user-specified discrete locations at 22 standard radial distances and 10 distance segments for 16 downwind sectors. Annual averages are computed from the hourly values. The program internally sets the 22 fixed distances between 0.25 and 50 mi, and the 10 distance segments over 0.5 and 50 mi, consistent with the XOQDOQ model users guidance in NUREG/CR-2919 (Sagendorf et al. 1982).

Additionally, the average values bounded by the segment boundaries are computed from the values at these fixed distances. The following method is used to compute the average χ/Q values for distance segments (the term D/Q is substituted when determining relative deposition values for a given distance segment):

$$\overline{\chi/Q}_{seg}(K) = \frac{R_1 \times \overline{\chi/Q}(R_1, K) + r_1 \times \overline{\chi/Q}(r_1, K) + \dots + r_n \times \overline{\chi/Q}(r_n, K) + R_2 \times \overline{\chi/Q}(R_2, K)}{R_1 + r_1 \dots + r_n + R_2}$$
(A.38)

where $\overline{\chi/Q}_{seg}(K)$ = average value for the segment for the directional sector K $\overline{\chi/Q}(R_1,K)$ = value at the downwind distance R_1 for the directional sector K $\overline{\chi/Q}(r_1,K)$ = value at intermediate downwind distance r_1 for the directional sector K R_1, R_2 = downwind distances of the segment boundaries $r_1, ..., r_n$ = selected radii between R_1 and R_2 . For example, an average χ/Q value for the segment 10–20 mi in the North sector represents an average value for any point between 10 and 20 mi north of the site.

The algorithm additionally calculates relative concentrations and deposition factors for userprovided discrete receptor locations (e.g., cow, garden, site boundary). As mentioned earlier in the document, the routine release analysis algorithm performs χ/Q calculations for three decay and depletion scenarios: (1) no decay (101-day half-life) with no depletion, (2) 2.26-day half-life with no depletion, and (3) 8-day half-life with depletion. The algorithm computes χ/Q values for each of the decay and depletion scenarios and D/Q values at 22 radial distances and 10 distance segments and for any user-defined discrete receptor locations.

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Appendix B – Comparisons with Legacy Code Output

The Software Integration for Environmental Radiological Release Assessments (SIERRA) Atmospheric Transport and Diffusion (ATD) model results were compared with the legacy code outputs using two meteorological datasets:

- 1. a single synthetic meteorological dataset
- 2. an array of site-specific meteorological monitoring data from various nuclear power plants (NPPs).

The site-specific meteorological data comparisons were discussed previously. This appendix discusses the synthetic meteorological dataset and associated results.

The synthetic meteorological data were created for this comparison to control the meteorological factors that contribute to the model output. The synthetic data used in this analysis included 3 unique wind-speed values and 3 unique stability classes with wind directions in each of the 16 wind direction sectors. These data were generated for both the Regulatory Guide (RG) 1.23 formatted hourly data and joint frequency distribution (JFD) data for use with the legacy codes. Winds are distributed among 1 m/s (3.333% occurrence), 2 m/s (10% occurrence), and 3 m/s (20% occurrence) for each of the three stability classes along each directional sector. Table B.1 presents the JFD for these synthetic data. No calm or missing data are included in the synthetic data.

 Table B.1.
 Joint frequency distribution of the hourly meteorological data for the synthetic dataset.

Stability Class	WS (m/s)	N	NNE	NE	ENE	E	ESE	SE	SSE	S	SSW	SW	WSW	W	WNW	NW	NNW
А	1	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208
А	2	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625
А	3	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250
D	1	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208
D	2	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625
D	3	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250
G	1	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208	0.208
G	2	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625	0.625
G	3	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250	1.250
WS = win	id spee	ed.															

In the comparisons presented in the subsections below, the use of synthetic meteorological data illustrated that the χ/Q values for single meteorological conditions were either identical or very similar between the ATD model and legacy codes. For the calculations performed before the statistical calculations, the primary differences between the ATD model and legacy codes are attributable to the influence of the JFD wind-speed bin selection. In the examples presented for the XOQDOQ case, the χ/Q values for the case with three wind-speed bins were approximately 60% larger than the χ/Q values for the case with two wind-speed bins. In this example, the larger number of bins resulted in χ/Q values that had larger differences from the ATD values because the bin definitions resulted in the use of lower wind speeds in the calculations.

Simulations with synthetic meteorological data were also used to compare the results after statistical calculations of values such as the annual average or values exceeded 0.5% and 5% of the time. The ATD model processes the hourly data, while the PAVAN and XOQDOQ models employ an interpolation (or extrapolation) approach to obtain the exceedance values. The influence of the JFD bin definition also contributes to the differences in the statistical results from the PAVAN and XOQDOQ models.

B.1 SIERRA ATD Onsite Control Room Design Basis Accident Analysis Comparison with ARCON

Experimental studies have demonstrated that the straight-line Gaussian plume model typically overestimates concentrations in the vicinity of buildings (Ramsdell 1990). ARCON95/96 was developed to address this concern by using a statistical model to make more reliable predictions in building wakes. RG 1.194, which is largely based on the Atmospheric Relative CONcentration in Building Wakes (ARCON) code, prescribes methods and procedures to determine atmospheric relative concentrations (χ/Q) for assessing the potential onsite control room radiological consequences for a range of postulated accidental releases of radioactive materials to the atmosphere. RG 1.194 states the requirement for the determination of the 95th percentile χ/Q value for a specific source–receptor direction. ARCON96 was later slightly revised to ARCON2 (Rishel 2021).

ARCON is a code for potential use by NRC staff in the review of license submittals related to onsite control room habitability. ARCON takes as input hourly meteorological data with wind speed and direction at the lower and upper measurement heights and a stability class. SIERRA ATD also takes as input hourly meteorological data with the format provided in RG 1.23 (NRC 2007). Stability is calculated based on the vertical temperature difference (dT/dz). Both ground-level and elevated releases can be modeled. Mixed-mode releases for vents were excluded from SIERRA ATD onsite control room DBA analyses.

B.1.1 Assessments with Synthetic Meteorological Data

An onsite control room DBA analysis was performed using the synthetic data described in Table B.1. For this analysis, only the wind direction associated with the direction toward the receptor is considered, and winds in other directions are not incorporated. The direction to the source from the receptor was defined as 22.5° with a 5° window. As a result, 6.25% of winds are in the direction of the receptor. Simulations with a ground-level release and an elevated release are described in the subsections to this section.

B.1.1.1 Ground-Level Release with an Adjacent Building

The ground-level release case had a release height set to 10 m with a building area of 1900 m². The intake room receptor was prescribed at a 45 m distance with a 10 m height. Table B.2 presents the centerline and sector-averaged χ/Q values calculated from ATD and ARCON2 for the synthetic data conditions. Diffusion coefficients are available from the ATD model, while they are not reported by ARCON2. The χ/Q values presented in Table B.2 are identical between the two codes.

A set of "hand calculations" were performed for a case with a wind speed of 1 m/s and stability category D. The Pasquill–Gifford (P-G) diffusion coefficients were approximated from Figures 4 and 5 in RG 1.194.

First, the low-wind-speed corrections to the lateral (σ_y) and vertical (σ_z) diffusion coefficients, which are presented in Equation 6 of the ARCON96 documentation (Ramsdell and Simonen 1997), are computed.

Equation 6 Calcs:
$$\sigma_{y1}^2 = 9.13 \times 10^5 \left[1 - \left(1 + \frac{45}{1000 \times 1} \right) \exp \left(\frac{-45}{1000 \times 1} \right) \right] = 897.1$$

 $\sigma_{z1}^2 = 6.67 \times 10^2 \left[1 - \left(1 + \frac{45}{100 \times 1} \right) \exp \left(\frac{-45}{100 \times 1} \right) \right] = 50.3$

Next, the building wake corrections to the diffusion coefficients, which are presented in Equation 7 of the ARCON96 documentation (Ramsdell and Simonen 1997), are computed.

Equation 7 Calcs:
$$\sigma_{y2}^2 = 5.24 \times 10^{-2} \times 1^2 \times 1900 \left[1 - \left(1 + \frac{45}{10\sqrt{1900}} \right) \exp\left(\frac{-45}{10\sqrt{1900}} \right) \right] = -22.2$$

 $\sigma_{z2}^2 = 1.17 \times 10^{-2} \times 1^2 \times 1900 \left[1 - \left(1 + \frac{45}{10\sqrt{1900}} \right) \exp\left(\frac{-45}{10\sqrt{1900}} \right) \right] = -5$

Then, the composite wake diffusion coefficients from Equation 5 in (Ramsdell and Simonen 1997) are computed.

Equation 5 Calcs: $\Sigma_y = (4.5^2 + 897.1 - 22.2)^{1/2} = 30$

$$\Sigma_z = (2.5^2 + 50.3 - 5)^{1/2} = 7.2$$

Finally, the relative concentration for a ground-level release from Equation 3 in (Ramsdell and Simonen 1997) is computed. The primary source of the difference between the value that resulted from the hand calculation and the value presented in Table B.2 is the approximation of the diffusion coefficients from the figures in RG 1.194. Based on the approximations, the resultant sigma-y was 30 m, compared with 30.31 m from the exact values, and the resultant sigma-z was 7.2 m, compared with 7.45 m from the exact values.

Equation 3 Calc:
$$\chi/Q = 1/(3.14 \times 30 \times 7.2 \times 1) \times \exp[-0.5 \times (0/30)^2] = 1.47 \times 10^{-3}$$

Wind Speed (m/s)	Stability Class	Distance (m)	ATD σ _y (m)	ATD σ _z (m)	ATD Centerline χ/Q (s⋅m⁻³)	ATD Sector Avg χ/Q (s⋅m⁻³)	ARCON2 Centerline χ/Q (s·m ⁻³)	ARCON2 Sector Avg χ/Q (s⋅m⁻³)
1	А	45	32.05	9.81	1.0×10 ⁻³	5.9×10 ⁻⁴	1.0×10 ⁻³	5.9×10 ⁻⁴
2	А	45	18.95	7.80	1.1×10 ⁻³	6.3×10 ⁻⁴	1.1×10 ⁻³	6.3×10 ⁻⁴
3	А	45	15.35	7.32	9.4×10 ⁻⁴	5.5×10 ⁻⁴	9.4×10 ⁻⁴	5.5×10 ⁻⁴
1	D	45	30.31	7.45	1.4×10 ⁻³	8.2×10 ⁻⁴	1.4×10 ⁻³	8.2×10 ⁻⁴
2	D	45	15.83	4.48	2.2×10⁻³	1.3×10⁻³	2.2×10⁻³	1.3×10 ⁻³
3	D	45	11.27	3.59	2.6×10 ⁻³	1.5×10⁻³	2.6×10 ⁻³	1.5×10⁻³
1	G	45	30.00	7.14	1.5×10⁻³	8.7×10 ⁻⁴	1.5×10⁻³	8.7×10 ⁻⁴
2	G	45	15.23	3.94	2.7×10⁻³	1.6×10 ⁻³	2.7×10⁻³	1.6×10⁻³
3	G	45	10.41	2.88	3.5×10⁻³	2.1×10⁻³	3.5×10⁻³	2.1×10 ⁻³

Table B.2. ATD and ARCON2 calculations of hourly χ/Q values for a ground-level release with synthetic meteorological data. The 1 m/s D stability case in bold font represents the results of the example "hand calculation."

ARCON = computer code for Atmospheric Relative CONcentration in Building Wakes; ATD = atmospheric transport and diffusion; m = meter(s); m/s = meter(s) per second; $s \cdot m^{-3} = second(s)$ per cubic meter.

B.1.1.2 Elevated Release

In the elevated release case, the release height was set to 60 m, and a receptor was prescribed at a 210 m distance with a 0 m height. Though 6.25% of winds are within the wind direction window, only 2.08% of occurrences with an elevated plume were calculated in the source–receptor direction. These calculations were consistent between the two codes. Table B.3 presents the centerline and sector-averaged χ/Q values calculated from ATD and ARCON2 for the synthetic data conditions. As noted previously, the diffusion coefficients are available from the ATD model, while they are not reported by ARCON2. The χ/Q values presented in Table B.3 are identical between the two codes. The χ/Q values were calculated as zero by both codes under extremely stable conditions (stability class G).

A "hand calculation" was performed for a wind speed of 1 m/s and stability category D. The P-G diffusion coefficients were approximated from Figures 4 and 5 in RG 1.194 (NRC 2003). Since the exit velocity is zero (no flow rate), the downwash and finite flow correction can be ignored in this calculation. The relative concentration for an elevated release from Equation 12 of the ARCON96 documentation (Ramsdell and Simonen 1997) is computed. As was the case for the ground-level release, the hand calculation result is similar but not identical to the corresponding value in Table B.3 because of the approximation of the diffusion coefficients.

Equation 12 Calc: $\chi/Q = 1/(3.14 \times 20 \times 9 \times 1) \times \exp[-0.5 \times (0/20)^2] \times \exp\left[-0.5\left(\frac{60-0}{9}\right)^2\right] = 4.8 \times 10^{-13}$

WS @ Release Height (m/s)	Stability Class	Distance (m)	ATD σ _y (m)	ATD σ _z (m)	ATD Centerline χ/Q (s·m⁻³)	ATD Sector Avg χ/Q (s·m⁻³)	ARCON2 Centerline χ/Q (s·m⁻³)	ARCON2 Sector Avg χ/Q (s⋅m⁻³)
0.96	А	210	45.76	30.5	3.4×10 ⁻⁵	2.0×10⁻⁵	3.4×10⁻⁵	2.0×10⁻⁵
1.92	А	210	45.76	30.5	1.7×10 ⁻⁵	1.0×10 ⁻⁵	1.7×10⁻⁵	1.0×10⁻⁵
2.88	А	210	45.76	30.5	1.2×10 ⁻⁵	6.7×10 ⁻⁶	1.2×10⁻⁵	6.7×10 ⁻⁶
0.92	D	210	18.40	9.01	5.0×10 ⁻¹³	2.8×10 ⁻¹³	5.0×10 ⁻¹³	2.8×10 ⁻¹³
1.84	D	210	18.40	9.01	2.5×10 ⁻¹³	1.4×10 ⁻¹³	2.5×10 ⁻¹³	1.4×10 ⁻¹³
2.75	D	210	18.40	9.01	1.7×10 ⁻¹³	9.3×10 ⁻¹⁴	1.7×10 ⁻¹³	9.3×10 ⁻¹⁴
0.51	G	210	6.02	2.51	0.0	0.0	0.0	0.0
0.95	G	210	6.02	2.51	0.0	0.0	0.0	0.0
1.42	G	210	6.02	2.51	0.0	0.0	0.0	0.0

Table B.3. ATD and ARCON2 calculations of hourly χ/Q values for an elevated release with synthetic meteorological data. The 0.92 m/s D stability case in bold font represents the results of the example "hand calculation."

ARCON = computer code for Atmospheric Relative CONcentration in Building Wakes; ATD = atmospheric transport and diffusion; m = meter(s); m/s = meter(s) per second; $s \cdot m^{-3} = second(s)$ per cubic meter; WS = wind speed.

B.2 SIERRA ATD Offsite Design Basis Accident Analysis Comparison with PAVAN

RG 1.145 provides the regulatory basis for potential accident consequence assessments and an acceptable methodology to determine site-specific χ/Q at the exclusion area boundary (EAB) and low population zone (LPZ). RG 1.145 requires meteorological data as input for a consequence assessment that represent hourly averages, as defined in RG 1.23 (NRC 2007). The U.S. Nuclear Regulatory Commission (NRC) developed PAVAN (Bander 1982) to implement the guidance and regulatory positions in RG 1.145. PAVAN was developed in Fortran 77 and uses a JFD of the wind speed and stability along 16 directions as the meteorological input. The SIERRA ATD engine reengineered the implementation of RG 1.145 to use hourly meteorological data. Both SIERRA ATD and NRC PAVAN have the same governing equations and diffusion parameters and implement the regulatory basis that users would need for dose calculations for Title 10 of *Code of Federal Regulations*, Part 100 (10 CFR Part 100) and 10 CFR Part 50. The statistical routines within SIERRA ATD are updated to process hourly data directly, rather than a conversion from the JFD. The SIERRA ATD model meets the objectives of the offsite design basis consequence analyses as outlined in RG 1.145 (NRC 1982):

- 3. compute χ/Q on a directional basis
- 4. compute χ/Q on an overall site basis
- 5. choose χ/Q values to be used in evaluations to meet RG 1.3 and RG 1.4.

RG 1.145 requires the calculation of peak χ/Q values for a 2-hour period at the EAB and longer time periods for the LPZ including 8, 16, 72, and 624 hours. The maximum values for these time periods are selected from the maximum sector χ/Q or the 5 percent overall site χ/Q , whichever

is higher. RG 1.145 also requires the determination of 2-hour and annual average χ/Q values at the LPZ.

In the following sections, the SIERRA ATD model output is presented, along with outputs from PAVAN. To illustrate the factors that contribute to the differences in the numerical results from these models, synthetic data and site-specific data were employed.

B.2.1 Assessments with Synthetic Meteorological Data

An offsite design basis accident analysis was performed using the synthetic data described in Table B.1. These data were primarily utilized to compare the short-term χ/Q (0–2 h) calculations from SIERRA ATD and PAVAN. The CHIQ subroutine within NRC PAVAN computes these short-term values with JFD meteorological data as input using the Gaussian plume formulations provided in Equations 6 through 11 in the PAVAN user manual (Bander 1982). SIERRA ATD implements the same equations to compute the short-term χ/Q at each hour. These calculations precede the statistical interpolations and therefore provide an understanding of how the SIERRA ATD model captures the plume equations, including factors such as building corrections and elevated releases. For the simulations in this analysis, the EAB and LPZ distances were set to 800 and 3000 m, respectively. Simulations with a ground-level release and with an elevated release are described in the following subsections.

B.2.1.1 Ground-Level Release with No Adjacent Building

The lateral (σ_y) and vertical (σ_z) dispersion coefficients for the ground-level release are calculated using NRC P-G formulae. The hourly χ/Q values computed with ATD are similar to the short-term χ/Q values computed by the CHIQ subroutine within PAVAN. The sigmas are slightly lower for the G stability category from the ATD output; therefore, the consequent χ/Q values are also slightly higher compared to those from PAVAN. The normalized mean bias of the short-term χ/Q values is +8.6%. The resultant χ/Q values are slightly conservative; however, this difference is still negligible compared to the potential differences in statistical processing, as presented below. Note that the vertical dispersion is limited to 1000 m in both ATD and PAVAN. For ground-level releases, both PAVAN's CHIQ and the ATD model calculate the meander and building corrections by comparing three equations for χ/Q [Equations 6 through 8 in the PAVAN user manual, (Bander 1982)]. The similarities in χ/Q calculations (Table B.4 and Figure B.1) show that ATD captures the meander calculations from these three equations correctly.

The post-processing of centerline and sector averages is performed by PAVAN using the JFD with interpolations. The statistical calculations are inherently different between the ATD and PAVAN codes due to the differences in the meteorological data (hourly data for ATD and JFD data for PAVAN). ATD calculates the annual average using the frequency distribution from the hourly results of the sector-average equations presented in Equations 2 and 3 of the PAVAN manual (Bander 1982) as 4.33×10^{-6} for 800 m and 4.86×10^{-7} for 3000 m, while the PAVAN calculation results in 5.88×10^{-6} for 800 m and 6.58×10^{-7} for 3000 m. Figure B.2 and Figure B.3 show portions of the PAVAN output file for the 800 and 3000 m results presented in Table B.4.

The PAVAN calculation for the annual average is slightly higher than the value produced by the ATD model. This can be attributed to the fact that PAVAN (and XOQDOQ) calculates sector averages using the midpoint value of the wind-speed classes (e.g., 0.5 m/s for the 0–1 m/s bin, 3 m/s for the 2–4 m/s bin). Based on the JFD wind-speed class definitions in this case, the resultant χ/Q values are slightly higher than those calculated by ATD, which uses the actual measured wind speed at every hour. Both ATD and PAVAN use the maximum of the sector-

based annual averages as the "site limit" values. The PAVAN-computed annual averages can vary with different combinations of wind-speed distributions and is thus sensitive to the definition and distribution of the JFD data. The overall site 5% values calculated by the ATD model are slightly lower compared to those calculated by PAVAN.

The PAVAN model calculated the maximum sector value for the 0–2 h 0.5% χ/Q as 2.8×10⁻⁴ at 800 m while the ATD model computed a sector maximum of 4.02×10^{-4} at 800 m. The PAVAN ENVLOP routine interpolates (or extrapolates) the 0.5% and 5% results based on the occurrences of the x/Q values on a lognormal plot. Since the ATD model uses hourly data, it has many more occurrences than the PAVAN code, which uses combinations of wind speed and stability. The ENVLOP routine within PAVAN computes a slope from the highest χ/Q to 10 lower values on the cumulative frequency distribution plot and uses the lowest slope (closest to horizontal) to interpolate the 0.5% (sector) or 5% (overall site) χ/Q value. If the frequency has a starting value greater than 0.5% (or 5%), ENVLOP extrapolates the first slope. The algorithm in the ATD model generates a cumulative distribution of hourly χ/Q values in a particular direction. Since the ATD model uses hourly data and has many occurrences, it utilizes the slope between the frequencies where the 0.5% (or 5%) falls. If the frequency is greater than 0.5% (or 5%), then the ATD model back-extrapolates based on the slope between the highest and second-highest χ/Q values in the cumulative distribution, like PAVAN. Since the distributions are inherently different between the PAVAN and ATD models, the interpolations (or extrapolations) could be significantly different. Section 4.11 of the PAVAN documentation (Bander 1982) notes the following:

The values calculated in ONEOUT must be considered as approximations only. The enveloped frequency distributions generated in Subroutine ENVLOP may not always be reasonable. These should <u>always</u> be checked, and the values listed by ONEOUT adjusted accordingly.

Moreover, ENVLOP calculations are very sensitive to the wind-speed distribution bins within the JFD input; therefore, the site limit can significantly vary based on the JFD. This could be demonstrated with sensitivity analyses of PAVAN to different wind-speed distributions (i.e., JFD). More investigation on this aspect is warranted, which is key to generate the design value for regulatory purposes.

The PAVAN ONEOUT subroutine computes χ/Q for intermediate time periods by interpolating the 0–2 h values and annual average values for each sector and overall site. In contrast, ATD uses moving averages of hourly data to compute χ/Q for each of the intermediate time periods and then computes the 0.5% and 5% values in a manner similar to the calculation of the short-term χ/Q values. RG 1.145, Section 2.2.1, states the following:

For a given sector, the average χ/Q values for the various time periods may be approximated by a logarithmic interpolation between the 2-hour sector χ/Q and the annual average (8760-hour) χ/Q Alternate methods should also be consistent with these studies and should produce results that provide a monotonic decrease in average χ/Q in time.

Since SIERRA ATD takes as input hourly data, the averages for various time periods are directly computed using moving (rolling) averages of the hourly data, and no logarithmic interpolation implemented. The moving averages generate a monotonic decrease in χ/Q values for longer time periods.

Table B.5 presents a summary of the statistical outputs from the ATD and PAVAN models at 800 and 3000 m. As described above, the two models necessarily treat the calculation of these statistics differently, and the resultant values differ by 15% to 60%.

WS Stability Class 1 A 2 A 3 A 1 D 2 D 3 D 1 G 3 D 3 D 3 G 3 G 1 A	Distance (m) 800 800 800	ATD σ _y (m) 153.1 153.1	ATD σ _z (m) 294.0	ATD Centerline $\chi/Q (s \cdot m^{-3})$ 7.07×10 ⁻⁶	ATD Sector Avg χ/Q (s·m ⁻³) 8.65×10 ⁻⁶	PAVAN σ_y (m)	PAVAN σ _z (m)	PAVAN χ/Q (s·m⁻³)
1 A 2 A 3 A 1 D 2 D 3 D 1 G 2 G 3 G 1 A	800 800 800	153.1 153.1	294.0	7.07×10⁻ ⁶	8.65×10⁻ ⁶	152 1		
2 A 3 A 1 D 2 D 3 D 1 G 2 G 3 G 1 A	800 800	153.1	20/ 0			155.1	294.0	7.07×10 ⁻⁶
3 A 1 D 2 D 3 D 1 G 2 G 3 G 1 A	800		234.0	3.54×10 ⁻⁶	4.32×10 ⁻⁶	153.1	294.0	3.53×10 ⁻⁶
1 D 2 D 3 D 1 G 2 G 3 G 1 A		153.1	294.0	2.36×10 ⁻⁶	2.88×10⁻ ⁶	153.1	294.0	2.36×10 ⁻⁶
2 D 3 D 1 G 2 G 3 G 1 A	800	61.6	26.6	9.74×10⁻⁵	9.57×10⁻⁵	61.6	26.6	9.73×10 ⁻⁵
3 D 1 G 2 G 3 G 1 A	800	61.6	26.6	4.87×10⁻⁵	4.79×10⁻⁵	61.6	26.6	4.87×10 ⁻⁵
1 G 2 G 3 G 1 A	800	61.6	26.6	4.19×10⁻⁵	3.19×10⁻⁵	61.6	26.6	4.19×10 ⁻⁵
2 G 3 G 1 A	800	20.1	7.1	3.71×10⁻⁴	3.58×10 ⁻⁴	20.9	7.5	3.37×10 ^{−4}
3 G 1 A	800	20.1	7.1	1.85×10 ⁻⁴	1.79×10⁻⁴	20.9	7.5	1.69×10 ⁻⁴
1 A	800	20.1	7.1	2.40×10 ⁻⁴	1.19×10 ⁻⁴	20.9	7.5	2.18×10 ⁻⁴
	3000	505.2	1000.0	6.30×10 ⁻⁷	6.78×10 ⁻⁷	505.2	1000.0	6.30×10 ⁻⁷
2 A	3000	505.2	1000.0	3.15×10⁻ ⁷	3.39×10⁻ ⁷	505.2	1000.0	3.15×10⁻ ⁷
3 A	3000	505.2	1000.0	2.10×10 ⁻⁷	2.26×10 ⁻⁷	505.2	1000.0	2.10×10 ⁻⁷
1 D	3000	203.1	65.4	1.84×10⁻⁵	1.04×10 ⁻⁵	203.1	65.4	1.84×10⁻⁵
2 D	3000	203.1	65.4	9.19×10 ⁻⁶	5.18×10 ⁻⁶	203.1	65.4	9.19×10 ⁻⁶
3 D	3000	203.1	65.4	6.85×10⁻⁵	3.45×10⁻ ⁶	203.1	65.4	6.84×10 ⁻⁷
1 G	3000	66.4	16.6	1.15×10 ⁻⁴	4.09×10 ⁻⁵	68.8	17.7	1.04×10 ⁻⁴
2 G	3000	66.4	16.6	5.75×10⁻⁵	2.05×10 ⁻⁵	68.8	17.7	5.21×10 ⁻⁵
3 G	2000	66.4	16.6	5.90×10 ⁻⁵	1.36×10⁻⁵	68.8	17.7	5.34×10 ⁻⁵

Table B.4.	ATD and PAVAN calculations of hourly χ/Q values for a ground-level release with
	synthetic meteorological data.

ATD = atmospheric transport and diffusion; m = meter(s); m/s = meter(s) per second;

PAVAN = computer code for ground-level χ/Q for accidental release; s m^{-3} = second(s) per cubic meter; WS = wind speed.



Figure B.1. Comparison of χ/Q values from ATD and the PAVAN CHIQ subroutine for a ground-level release without a building.

A set of "hand calculations" were performed for a case with a wind speed of 1 m/s and for stability category D. The χ/Q values were computed at 800 m following the PAVAN documentation (Bander 1982). First, the first two χ/Q equations for a ground-level release presented in Equations 6 and 7 of the PAVAN documentation (Bander 1982) are computed.

Equation 6 Calc: $\chi/Q = \{1.0 \times [3.14 \times 61.6 \times 26.6 + 0.5 \times 0]\}^{-1} = 1.94 \times 10^{-4}$

Equation 7 Calc: $\chi/Q = \{3 \times 1.0 \times 3.14 \times 61.6 \times 26.6\}^{-1} = 6.48 \times 10^{-5}$

Next, the meander factor from the MEANDR subroutine, which refers to RG 1.145, Figure 3, is computed. *M* is equal to 2 for wind speeds less than or equal to 2 m/s.

$$M\sigma_{\nu} = 61.6 + [2 - 1] \times 61.6 = 123.2$$

Then, the meander factor is incorporated into the third χ/Q equation, Equation 8 in the PAVAN documentation (Bander 1982).

Equation 8 Calc: $\chi/Q = \{1.0 \times 3.14 \times 123.1 \times 26.6\}^{-1} = 9.72 \times 10^{-5}$

The PAVAN manual suggests that the larger value from Equation 6 and Equation 7 is compared with the value from Equation 8, and the smaller value is selected as the appropriate χ/Q value. For this "hand calculation," the Equation 6 result is larger than the Equation 7 result, and the Equation 8 result is smaller than the Equation 6 result, so the Equation 8 result should be the final result. Table B.4 shows that the meander-based χ/Q value matches both the ATD and PAVAN results.

STABILIT CLASS	Y WINDSPEED METER/SEC AT 10.0 MM	FREQUENCY PERCENT ETERS	DISTANCE METERS	TERRAIN HT METERS	EFF PLUME HT METERS	SIGMA-Y METERS	SIGMA-Z METERS	MEANDER-SY METERS	** CHI/Q VALU MEANDER C/	JES (SEC/CUB BLDG WAKE A= 0.SQ.ME	IC METER) USED TERS
A	1.0	3.33	800.	0.	0.	153.1	294.0	153.1	7.071E-06	7.071E-06	7.071E-06
A	2.0	10.00	800.	0.	0.	153.1	294.0	153.1	3.535E-06	3.535E-06	3.535E-06
A	3.0	20.00	800.	0.	0.	153.1	294.0	153.1	2.357E-06	2.357E-06	2.357E-06
D	1.0	3.33	800.	0.	0.	61.6	26.6	123.1	9.734E-05	1.947E-04	9.734E-05
D	2.0	10.00	800.	0.	0.	61.6	26.6	123.1	4.867E-05	9.734E-05	4.867E-05
D	3.0	20.00	800.	0.	0.	61.6	26.6	95.3	4.191E-05	6.489E-05	4.191E-05
G	1.0	3.33	800.	0.	0.	20.9	7.5	125.2	3.374E-04	2.024E-03	3.374E-04
G	2.0	10.00	800.	0.	0.	20.9	7.5	125.2	1.687E-04	1.012E-03	1.687E-04
G	3.0	20.00	800.	0.	0.	20.9	7.5	64.6	2.179E-04	6.747E-04	2.179E-04

Figure B.2. CHIQ output at 800 m from PAVAN for a ground-level release.

STABILIT CLASS	Y WINDSPEED METER/SEC AT 10.0 ME	FREQUENCY PERCENT ETERS	DISTANCE METERS	TERRAIN HT METERS	EFF PLUME HT METERS	SIGMA-Y METERS	SIGMA-Z METERS	MEANDER-SY METERS	** CHI/Q VALU MEANDER CA	JES (SEC/CUB BLDG WAKE A= 0.SQ.ME	IC METER) USED TERS
A A	1.0 2.0	3.33 10.00	3000. 3000.	0. 0.	0. 0.	505.2 505.2	1000.0 1000.0	505.2 505.2	6.301E-07 3.151E-07	6.301E-07 3.151E-07	6.301E-07 3.151E-07
А	3.0	20.00	3000.	0.	0.	505.2	1000.0	505.2	2.100E-07	2.100E-07	2.100E-07
D D	1.0 2.0	3.33 10.00	3000. 3000.	0. 0.	0. 0.	203.1 203.1	65.4 65.4	264.7 264.7	1.837E-05 9.187E-06	2.394E-05 1.197E-05	1.837E-05 9.187E-06
D	3.0	20.00	3000.	0.	0.	203.1	65.4	236.9	6.843E-06	7.981E-06	6.843E-06
G G	1.0 2.0	3.33 10.00	3000. 3000.	0. 0.	0. 0.	68.8 68.8	17.7 17.7	173.1 173.1	1.041E-04 5.206E-05	2.619E-04 1.310E-04 8 731E 05	1.041E-04 5.206E-05
LUSNRC CO	MPUTER CODE-	-PAVAN, VEI	RSION 2.0	RI	JN DATE AND TI	ME: 06-03	-2024 13	3:44:23	J.JJ0L-0J	0.7512-05	5.5562-05

Figure B.3. CHIQ output at 3000 m from PAVAN for a ground-level release.

Table B.5 shows that the statistical results from both ATD and PAVAN are similar. While the hourly values are nearly identical, as shown in Table B.4, there are larger differences in the various comparisons presented in Table B.5. This is due to the differences in the statistical processing of the data. Annual averages obtained with ATD are slightly lower than those obtained by PAVAN. This is primarily because the actual hourly wind speed is used by the ATD model, while PAVAN uses the midpoint averages of the wind-speed classes.

Table B.5. Comparison of the key statistics relevant to regulatory applications from a ground-level release.

Distance	800 m	800 m	3000 m	3000 m
Model	ATD	PAVAN	ATD	PAVAN
Annual Average	4.33×10⁻ ⁶	5.88×10 ⁻⁶	4.87×10⁻ ⁷	6.58×10 ⁻⁷
Sector Max 0–2 h 0.5%	4.12×10 ⁻⁴	2.80×10 ⁻⁴	1.33×10 ⁻⁴	8.17×10⁻⁵
Overall Site 0–2 h 5%	2.78×10 ⁻⁴	3.13×10⁻⁴	6.0×10 ⁻⁵	9.48×10 ⁻⁵

ATD = atmospheric transport and diffusion; h = hour(s); m = meter(s); PAVAN = computer code for ground-level χ/Q for accidental release.

B.2.1.2 Elevated Release

The subroutines within PAVAN and ATD for an elevated release calculate χ/Q over predetermined grid distances from the EAB or LPZ boundary to a maximum of 90,000 m. The maximum of these χ/Q values is the 0–2 h χ/Q value for a given sector. This iterative calculation is recommended in the PAVAN documentation to ensure that the dispersion model captures the high ground-level concentrations at farther downwind distances where the elevated plume meets the ground, which is of particular concern at locations with elevated terrain. While PAVAN has predetermined 27 grid points from 100 m to 90,000 m, ATD uses a power law equation to use a finer grid near the source and more coarse resolution farther from the source, as given below. Figure B.4 shows the grid distances within PAVAN and ATD for an EAB of 800 m. The grid distances are adjusted by the ATD subroutine according to the boundary, unlike PAVAN, which has predetermined distances.

$$X_{k=2,n} = X_{\rm b} + 10^{\frac{\log_{10}(90000 - X_{\rm b})}{n} \times k}$$
(B.1)



Figure B.4. Comparison of the downwind distances set within ATD and PAVAN for an EAB of 800 m.

Short-term χ/Q calculations for an elevated release from the two codes are shown in Table B.6 and Figure B.5. The normalized mean bias (NMB) of the short-term χ/Q values is +8.5%. The maximum χ/Q calculations and respective grid distances are similar between ATD and PAVAN. There is slight difference due to distance estimation where the peak was simulated by the two codes. ATD computed the maximum χ/Q at 1,328 m for the EAB with stability category D, while PAVAN calculated the maximum χ/Q at 2,000 m for the same stability and atmospheric condition. Table B.6 also shows that the ATD model can compute χ/Q values with stability category G when fumigation occurs. In contrast, PAVAN does not incorporate fumigation χ/Q values within statistical routines but prints them separately for the user. Since ATD uses all hourly values for statistical calculations, the fumigation hours are also included. The wind-speed corrections from the measurement height of 100 m to the release height of 60 m were exactly the same between the ATD model and NRC PAVAN code. Figure B.6 and Figure B.7 show portions of the PAVAN output file for the 800 and 3000 m results presented in Table B.6.

ł	WS @ release neight (m/s)	Stability Class	Boundary	ATD Distance (m)	ATD σ _y (m)	ATD σ _z (m)	ATD Centerline χ/Q (s⋅m⁻³)	ATD Sector Avg χ/Q (s∙m⁻³)	PAVAN Distance (m)	PAVAN σ _y (m)	PAVAN σ _z (m)	PAVAN χ/Q (s∙m⁻³)
	0.9	А	EAB	800	153.1	294.0	7.87×10⁻ ⁶	9.61×10⁻⁵	800	153.1	294.0	7.87×10⁻ ⁶
	1.8	А	EAB	800	153.1	294.0	3.93×10 ⁻⁶	4.81×10 ⁻⁶	800	153.1	294.0	3.93×10 ⁻⁶
	2.6	А	EAB	800	153.1	294.0	2.62×10 ⁻⁶	3.2×10⁻ ⁶	800	153.1	294.0	2.62×10 ⁻⁶
	0.9	D	EAB	1328	97.3	38.5	2.87×10 ⁻⁵	8.46×10 ⁻⁶	2000	140.9	50.6	2.51×10⁻⁵
	1.8	D	EAB	1328	97.3	38.5	1.43×10⁻⁵	4.23×10⁻ ⁶	2000	140.9	50.6	1.26×10⁻⁵
	2.6	D	EAB	1328	97.3	38.5	9.56×10 ⁻⁶	2.82×10 ⁻⁶	2000	140.9	50.6	8.38×10 ⁻⁶
	0.8	G	EAB	16937	317.1	33.3	7.67×10 ⁻⁶	1.53×10 ⁻¹⁹	10000	204.1	27.4	6.67×10 ⁻⁶
	1.6	G	EAB	16937	317.1	33.3	3.84×10 ⁻⁶	7.64×10 ⁻²⁰	10000	204.1	27.4	3.34×10 ⁻⁶
	2.3	G	EAB	16937	317.1	33.3	2.56×10⁻ ⁶	5.09×10 ⁻²⁰	10000	204.1	27.4	2.22×10 ⁻⁶
	2.3	G	EAB ¹	16937	317.1	33.3	5.63×10 ⁻⁵	5.09×10 ⁻²⁰	N/A	N/A	N/A	N/A
	0.9	А	LPZ	3000	505.2	1000.0	7.15×10 ⁻⁷	1.68×10⁻ ⁷	3000	505.2	1000.0	7.15×10 ⁻⁷
	1.8	А	LPZ	3000	505.2	1000.0	3.57×10⁻ ⁷	8.41×10⁻ ⁸	3000	505.2	1000.0	3.57×10⁻ ⁷
	2.6	А	LPZ	3000	505.2	1000.0	2.38×10 ⁻⁷	5.61×10 ⁻⁸	3000	505.2	1000.0	2.38×10 ⁻⁷
	0.9	D	LPZ	3000	203.1	65.4	1.79×10⁻⁵	7.72×10⁻ ⁶	3000	203.1	65.4	1.79×10⁻⁵
	1.8	D	LPZ	3000	203.1	65.4	8.93×10 ⁻⁶	3.86×10⁻ ⁶	3000	203.1	65.4	8.94×10 ⁻⁶
	2.6	D	LPZ	3000	203.1	65.4	5.96×10 ⁻⁶	2.57×10⁻ ⁶	3000	203.1	65.4	5.96×10 ⁻⁶
	0.8	G	LPZ	11946	231.4	29.5	7.6×10⁻ ⁶	7.46×10⁻ ⁸	10000	204.1	27.4	6.67×10⁻ ⁶
	1.6	G	LPZ	11946	231.4	29.5	3.8×10⁻ ⁶	3.73×10⁻ ⁸	10000	204.1	27.4	3.34×10 ⁻⁶
	2.3	G	LPZ	11946	231.4	29.5	2.53×10⁻ ⁶	2.49×10⁻ ⁸	10000	204.1	27.4	2.22×10 ⁻⁶
	2.3	G	LPZ ¹	11946	231.4	29.5	1.79×10⁻⁵	2.49×10⁻ ⁸	N/A	N/A	N/A	N/A

Table B.6. ATD and PAVAN calculations of hourly χ/Q values for an elevated release with synthetic meteorological data.

¹ Fumigation condition. For fumigation conditions, PAVAN provides a cumulative distribution function (CDF) rather than a specific value. ATD = atmospheric transport and diffusion; m = meter(s); m/s = meter(s) per second; PAVAN = computer code for ground-level χ/Q for accidental release; s·m⁻³ = second(s) per cubic meter; WS = wind speed.



Figure B.5. Comparison of χ/Q values from ATD and PAVAN's CHIQ subroutine for an elevated release.

A "hand calculation" was performed for a case with a wind speed of 1 m/s (0.88 m/s at 10 m) and for stability category D. The χ/Q values were computed at 800 m following the PAVAN documentation (Bander 1982). The χ/Q equation for an elevated release for nonfumigation conditions presented in Equation 10 of the PAVAN documentation (Bander 1982) was computed.

Equation 10 Calc:	$X/Q = \exp\left\{-0.5 \times \left[\frac{60}{50.6}\right]^2\right\}$	${3.14 \times 0.88 \times 140.9 \times 50.6} = 2.51 \times 10^{-5}$
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STABILIT CLASS	Y WINDSPEED METER/SEC AT 60.0 ME	FREQUENCY PERCENT ETERS	DISTANCE METERS	TERRAIN HT METERS	EFF PLUME HT METERS	SIGMA-Y METERS	SIGMA-Z METERS	MEANDER-SY METERS	** CHI/Q VALU MEANDER CA	JES (SEC/CUB BLDG WAKE A= 0.SQ.ME	IC METER) USED TERS
А	0.9	3.33	800.	0.	60.	153.1	294.0	0.0	0.000E+00	0.000E+00	7.868E-06
Α	1.8	10.00	800.	0.	60.	153.1	294.0	0.0	0.000E+00	0.000E+00	3.934E-06
Α	2.6	20.00	800.	0.	60.	153.1	294.0	0.0	0.000E+00	0.000E+00	2.623E-06
D D D	0.9 1.8 2.6	3.33 10.00 20.00	2000. 2000. 2000.	0. 0. 0.	60. 60. 60.	140.9 140.9 140.9	50.6 50.6 50.6	0.0 0.0 0.0	0.000E+00 0.000E+00 0.000E+00	0.000E+00 0.000E+00 0.000E+00	2.513E-05 1.256E-05 8.377E-06
G G G	0.8 1.5 2.3	3.33 10.00 20.00	10000. 10000. 10000.	0. 0. 0.	60. 60. 60.	204.1 204.1 204.1	27.4 27.4 27.4	0.0 0.0 0.0	0.000E+00 0.000E+00 0.000E+00	0.000E+00 0.000E+00 0.000E+00	6.670E-06 3.335E-06 2.223E-06

Figure B.6. CHIQ output at 800 m from PAVAN for an elevated release.

STABILIT CLASS	Y WINDSPEED METER/SEC AT 60.0 ME	FREQUENCY PERCENT ETERS	DISTANCE METERS	TERRAIN HT METERS	EFF PLUME HT METERS	SIGMA-Y METERS	SIGMA-Z METERS	MEANDER-SY METERS	** CHI/Q VAL MEANDER C	UES (SEC/CUB BLDG WAKE A= 0.SQ.ME	IC METER) USED TERS
A	0.9 1.8	3.33 10.00	3000. 3000.	0. 0.	60. 60.	505.2 505.2	1000.0 1000.0	0.0	0.000E+00 0.000E+00	0.000E+00 0.000E+00	7.147E-07 3.573E-07
A	2.6	20.00	3000.	0.	60.	505.2	1000.0	0.0	0.000E+00	0.000E+00	2.382E-07
D D D	0.9 1.8 2.6	3.33 10.00 20.00	3000. 3000. 3000.	0. 0. 0.	60. 60. 60.	203.1 203.1 203.1	65.4 65.4 65.4	0.0 0.0 0.0	0.000E+00 0.000E+00 0.000E+00	0.000E+00 0.000E+00 0.000E+00	1.787E-05 8.935E-06 5.957E-06
G G G	0.8 1.5 2.3	3.33 10.00 20.00	10000. 10000. 10000.	0. 0. 0.	60. 60. 60.	204.1 204.1 204.1	27.4 27.4 27.4	0.0 0.0 0.0	0.000E+00 0.000E+00 0.000E+00	0.000E+00 0.000E+00 0.000E+00	6.670E-06 3.335E-06 2.223E-06

Figure B.7. CHIQ output at 3000 m from PAVAN for an elevated release.

Table B.7 shows the statistical calculations from both ATD and PAVAN. Though atmospheric conditions were kept same in all directions, PAVAN computed different 0.5% χ/Q values for few directions (Figure B.8). This demonstrates that the ENVLOP routine can generate slightly erroneous values compared to hand calculations. Overall, ATD shows lower statistical values than PAVAN, though the hourly values are similar. This again demonstrates the difference in the statistical processing. Annual averages computed with ATD are always slightly lower than those computed by PAVAN. This is primarily due to the use of the actual hourly wind speed in the ATD model, while PAVAN uses the midpoint averages of the wind-speed classes.

Table B.7. Comparison of key statistics used for regulatory purposes from an elevated release.

Distance Model	800 m ATD	800 m PAVAN	3000 m ATD	3000 m PAVAN
Annual Average	1.70×10⁻ ⁷	2.41×10 ⁻⁷	8.04×10 ⁻⁸	1.15×10⁻ ⁷
Sector Max 0–2 h 0.5%	3.95×10⁻⁵	4.93×10 ⁻⁵	2.45×10 ⁻⁵	2.30×10 ⁻⁵
Overall Site 0–2 h 5%	1.59×10⁻⁵	2.45×10⁻⁵	9.01×10 ⁻⁶	1.55×10⁻⁵

ATD = atmospheric transport and diffusion; h = hour(s); m = meter(s); PAVAN = computer code for ground-level χ/Q for accidental release.

				AVERAGING	G TIME		0-2	HR X/Q IS	
DOWNWIND	DISTANCE							EXCEEDED	DOWNWIND
SECTOR	(METERS)	0-2 HOURS	0-8 HOURS	8-24 HOURS	1-4 DAYS	4-30 DAYS	ANNUAL AVERAGE	IN SECTOR	SECTOR
S	800.	1.71E-05	8.46E-06	5.95E-06	2.77E-06	9.24E-07	2.41E-07	3.2	S
SSW	800.	1.71E-05	8.46E-06	5.95E-06	2.77E-06	9.24E-07	2.41E-07	3.2	SSW
SW	800.	1.71E-05	8.46E-06	5.95E-06	2.77E-06	9.24E-07	2.41E-07	3.2	SW
WSW	800.	2.06E-05	1.01E-05	7.07E-06	3.27E-06	1.08E-06	2.77E-07	5.3	WSW
W	800.	2.98E-05	1.45E-05	1.01E-05	4.60E-06	1.49E-06	3.75E-07	13.1	W
WNW	800.	4.93E-05	2.38E-05	1.65E-05	7.47E-06	2.40E-06	5.96E-07	43.7	WNW
NW	800.	1.71E-05	8.46E-06	5.95E-06	2.77E-06	9.24E-07	2.41E-07	3.2	NW
NNW	800.	1.71E-05	8.46E-06	5.95E-06	2.77E-06	9.24E-07	2.41E-07	3.2	NNW
N	800.	1.71E-05	8.46E-06	5.95E-06	2.77E-06	9.24E-07	2.41E-07	3.2	N
NNE	800.	1.71E-05	8.46E-06	5.95E-06	2.77E-06	9.24E-07	2.41E-07	3.2	NNE
NE	800.	1.71E-05	8.46E-06	5.95E-06	2.77E-06	9.24E-07	2.41E-07	3.2	NE
ENE	800.	1.71E-05	8.46E-06	5.95E-06	2.77E-06	9.24E-07	2.41E-07	3.2	ENE
E	800.	1.71E-05	8.46E-06	5.95E-06	2.77E-06	9.24E-07	2.41E-07	3.2	E
ESE	800.	1.71E-05	8.46E-06	5.95E-06	2.77E-06	9.24E-07	2.41E-07	3.2	ESE
SE	800.	1.71E-05	8.46E-06	5.95E-06	2.77E-06	9.24E-07	2.41E-07	3.2	SE
SSE	800.	1.71E-05	8.46E-06	5.95E-06	2.77E-06	9.24E-07	2.41E-07	3.2	SSE
MAX X/Q		4.93E-05				TOTAL HO	OURS AROUND SITE	: 104.4	
SRP 2.3.4	4 800.	6.19E-05	2.87E-05	1.96E-05	8.51E-06	2.57E-06	5.96E-07		
SITE LIM	ET	2.45E-05	1.33E-05	9.76E-06	5.01E-06	1.92E-06	5.96E-07		

Figure B.8. PAVAN output showing the statistical results for χ/Q values at 800 m computed using the ENVLOP and ONEOUT routines.

B.3 SIERRA ATD Routine Release Analysis Comparison with XOQDOQ

Part 50 of 10 CFR requires NPPs to limit radioactive releases to the atmosphere as low as is reasonably achievable (ALARA) and provides numerical guidance in Appendix I to meet these design objectives. RG 1.111 provides procedures and models to implement the numerical guidance in Appendix I. This RG describes the basic features of the model calculations and assumptions to facilitate estimates of the atmospheric transport and dispersion of gaseous effluents in routine releases. RG 1.111 highlights that the recommended procedures and models will be subject to continuing review by the NRC staff, providing flexibility to the applicant in meeting the requirements of Appendix I. The XOQDOQ code (Sagendorf et al. 1982) implements RG 1.111 and is used by NRC staff in their independent evaluation of routine or intermittent releases from nuclear power reactors. It is not intended to evaluate the consequences of accidental releases.

The XOQDOQ code computes the relative atmospheric dispersion (χ/Q) and deposition factors (D/Q) for 22 specific distances to 50 miles from the site for each directional sector. XOQDOQ implements a straight-line Gaussian plume model with plume depletion due to dry deposition and radioactive decay and also accounts for plume recirculation. Meteorological data are input into the program as a JFD that includes the stability class, wind direction, and wind-speed class. The "Routine Release" algorithm within ATD implements RG 1.111 in a method like XOQDOQ, with the primary difference of incorporating hourly meteorological data rather than a JFD. The sections below present a comparison of the annual average outputs from the ATD model with those of XOQDOQ.

B.3.1 Assessments with Synthetic Meteorological Data

A routine release analysis was performed using the synthetic data described in Table B.1. These data were primarily utilized to compare the annual average calculations from SIERRA ATD and XOQDOQ. For the simulations in this analysis, the recirculation factor was turned off, and the stack flow was set to zero so that no plume rise was calculated.

B.3.1.1 Ground-Level Release with No Adjacent Building

The annual average χ/Q values from XOQDOQ and ATD for a ground-level release are presented in Figure B.9. For the XOQDOQ simulation, two variants of the JFD that represent the same meteorological data were evaluated. One JFD file used bin definitions of 1, 2, and 3 m/s to match the hourly meteorological data. A second JFD file used bin definitions of 2 and 4 m/s. The ATD calculation shows better agreement with the XOQDOQ simulation that used the JFDs with bins defined at 2 and 4 m/s. The XOQDOQ model uses the average wind speed within each bin to compute the annual average x/Q. As a result, when the bins are defined as 1. 2, and 3 m/s, XOQDOQ uses the average wind speeds of 0.5, 1.5, and 2.5 m/s for the three wind-speed classes. This results in higher χ/Q values due to the use of lower wind speeds compared with the actual measured wind speed. In contrast, the simulation with bins defined at 2 and 4 m/s uses average wind speeds of 1 and 3 m/s, which aligns more closely to the true wind speeds and compares more favorably with the χ/Q values from the ATD model. This simulation demonstrates the impacts of JFD bin selection on the output of models that use a JFD, such as PAVAN and XOQDOQ. SIERRA ATD uses hourly data directly, which eliminates the issue of approximations to the wind and is therefore an improvement to the simulation results.

The annual average χ/Q values from XOQDOQ and ATD for a ground-level release with 8-day decay and depletion are presented in Figure B.9. ATD implemented the plume depletion and deposition curves from Figures 2 through Figure 9 of RG 1.111 (NRC 1977).





A "hand calculation" was performed for a case with a wind speed of 1 m/s and for stability category D. The χ/Q values were computed for a hypothetical receptor at 0.44 miles (715 m) for no decay and depletion. The χ/Q equation for a ground-level release presented in Equation 2 of the XOQDOQ documentation (Sagendorf et al. 1982) is computed.

Equation 2 Calc:
$$X/Q = \frac{2.032}{715} \times 1 \times$$

$$\left[\left(\frac{0.208}{100} \times \frac{1}{1.0} + \frac{0.625}{100} \times \frac{1}{2.0} + \frac{1.25}{100} \times \frac{1}{3.0} \right) \left(\left\{ \left(238.2^2 + 0.5 \times \frac{0^2}{3.14} \right)^{\frac{1}{2}} \right\}^{-1} + \left\{ \left(24.35^2 + 0.5 \times \frac{0^2}{3.14} \right)^{\frac{1}{2}} \right\}^{-1} + \left\{ \left(6.5^2 + 0.5 \times \frac{0^2}{3.14} \right)^{\frac{1}{2}} \right\}^{-1} \right\} = 5.3 \times 10^{-6}$$

Table B.8 shows the χ/Q and D/Q values at the receptor located 0.44 miles downwind for both ATD and XOQDOQ and the ground-level release case. Note that the D/Q values do not vary with the wind-speed classes since its calculation does not consider the wind-speed. As shown in Figure B.9, the XOQDOQ simulation that employed the three wind-speed bins at 1, 2, and 3 m/s had slightly higher normalized concentration results compared with the simulation that employed two wind-speed bins at 2 and 4 m/s. The ATD normalized concentration result was more closely aligned with the XOQDOQ result with the two wind-speed bins because those bins more closely align with the true wind-speed values prescribed in the synthetic dataset. At this distance, the No Decay and 2.26 Day decay values are identical.

Table B.8.Routine release calculations at a receptor point located 0.44 miles (715 m) from a
ground-level release (10 m).

Calculation	ATD	XOQDOQ (WS = 1, 2, 3 m/s)	XOQDOQ (WS = 2, 4 m/s)
χ/Q (No Decay, Undepleted)	5.29×10 ⁻⁶	7.20×10 ⁻⁶	4.50×10 ⁻⁶
χ/Q (2.26 Day, Undepleted)	5.29×10 ⁻⁶	7.20×10 ⁻⁶	4.50×10 ⁻⁶
χ/Q (8 Day Decay, Depleted)	4.87×10 ⁻⁶	6.60×10 ⁻⁶	4.10×10 ⁻⁶
D/Q	1.48×10 ^{−8}	1.50×10 ⁻⁸	1.50×10 ⁻⁸

ATD = atmospheric transport and diffusion; m/s = meter(s) per second; WS = wind speed; XOQDOQ = computer code for evaluation of routine effluent releases at commercial nuclear power stations.

B.3.1.2 Elevated Release

The annual average χ/Q values from XOQDOQ and ATD for an elevated release at 60 m are presented in Figure B.10. As described in the previous section, two different wind-speed bin selections were employed for the XOQDOQ simulations to illustrate the impact of bin selection.




A "hand calculation" was performed for a case with a wind speed of 1 m/s and for stability category D. The χ/Q values were computed for a hypothetical receptor at 0.44 miles (715 m) for no decay and depletion. The χ/Q equation for an elevated release presented in Equation 1 of the XOQDOQ documentation (Sagendorf et al. 1982) is computed.

Equation 1 Calc:
$$\chi/Q = \frac{2.032}{715} \times 1 \times$$

$$\begin{split} \left[\left(\frac{0.208}{100} \times \frac{1}{0.88} + \frac{0.625}{100} \times \frac{1}{1.8} + \frac{1.25}{100} \times \frac{1}{2.6} \right) \left(\frac{1}{238.2} \times \exp\left\{ -0.5 \left(\frac{60^2}{238.2^2} \right) \right\} \\ &+ \frac{1}{24.34} \times \exp\left\{ -0.5 \left(\frac{60^2}{24.34^2} \right) \right\} + \frac{1}{6.5} \times \exp\left\{ -0.5 \left(\frac{60^2}{6.5^2} \right) \right\} \right) \right] = 1.83 \times 10^{-7} \end{split}$$

Table B.9 shows the results for the χ/Q and D/Q values at the receptor located 0.44 miles downwind for both XOQDOQ and ATD and the elevated release case. As noted previously, the D/Q values do not vary with the wind-speed classes since its calculation does not consider the wind-speed. As demonstrated in Figure B.10, the XOQDOQ simulation that employed the three wind-speed bins at 1, 2, and 3 m/s had slightly higher normalized concentration results compared with the simulation that employed two wind-speed bins at 2 and 4 m/s. For this elevated case, the ATD normalized concentration result was just slightly more closely aligned with the XOQDOQ result for the case with two wind-speed bins because those bins more closely align with the true wind-speed values prescribed in the synthetic dataset. At this distance, the No Decay, 2.26 Day Decay, and 8 Day Decay values are identical for the ATD simulation, and the 8 Day Decay value is only slightly lower than the No Decay result. As noted in Figure B.10, these values diverge slightly at greater distances.

Table B.9.Routine release calculations at a receptor point located 0.44 miles (715 m) from an
elevated release (60 m).

Calculation	ATD	XOQDOQ (WS = 1, 2, 3 m/s)	XOQDOQ (WS = 2, 4 m/s)				
χ/Q (No Decay, Undepleted)	2.16×10 ⁻⁷	2.70×10 ⁻⁷	1.70×10 ⁻⁷				
χ/Q (2.26 Day, Undepleted)	2.16×10 ⁻⁷	2.70×10 ⁻⁷	1.70×10 ⁻⁷				
χ/Q (8 Day Decay, Depleted)	2.14×10 ⁻⁷	2.70×10 ⁻⁷	1.70×10 ⁻⁷				
D/Q	4.18×10 ⁻⁹	4.20×10 ⁻⁹	4.20×10 ⁻⁹				

ATD = atmospheric transport and diffusion; m/s = meter(s) per second; WS = wind speed; XOQDOQ = computer code for evaluation of routine effluent releases at commercial nuclear power stations.

B.4 References

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Appendix C – Legacy Code Input File Examples

1
C:\Projects\Sierra\Testing\Meteorology\Meteorological Data Formatted JPR\Levy\arcon\Levy0709.arn
10.00
60.00
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1
0.00
1900.00
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326 90
45.00
15.00
0.00
C:\Projects\Sierra\Testing\Outputs\ControlRoom\ARCON\Levy0709\Scenario_GR.cfd
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Example GR
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ARLUN Z.U EXAMPLE I - GTOUDD-LEVEL RELEASE

Figure C.1. Example of an ARCON .rsf file used in the site-specific meteorological comparative analysis. This file is for the Levy site and represents the ground-level release scenario.

Figure C.2. Example of a PAVAN .inp file used in the site-specific meteorological comparative analysis. This file is for the Levy site and represents the ground-level release scenario. The calms are evenly distributed in the 0.5 m/s wind-speed bin.

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4	5	6	6	5	3	4	3	3	1	1	6	3	6	7	4
16	30	27	24	30	15	5	5	3	6	30	38	44	17	20	26
14	19	39	58	50	24	6	10	8	7	56	138	137	13	16	23
7	13	21	46	54	13	1	1	4	24	42	90	66	6	7	18
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0	0	0	2	0	1	0	0	0	4	0	1	3	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0 8	2	4	7	12	2	6	4	10	11	5	0	8	10	3	9
11	17	11	11	20	14	14	8	11	11	14	13	18	11	11	18
28	35	29	52	51	30	21	18	14	14	31	54	72	18	12	21
6	11	44	54	41	24	10	10	7	9	17	44	69	3	5	9
3	4	19	28	23	10	3	2	2	9	9	12	18	3	0	5
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4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4
20	9	17	16	20	12	13	13	15	16	15	15	10	9	13	8
38	36	44	26	24	25	32	25	27	20	34	35	24	23	31	26
100	113	211	105	143	33	31	20	16	26	39	135	195	33	29	32
45	72	115	102	112	43	36	18	22	70	38	87	67	10	22	24
17	29	47	63	49	25	9	8	30	45	26	27	17	11	9	7
0	1	13	16	19	9	1	1	13	25	11	11	17	2	0	3
16	16	1	16	16	16	16	16	4	10	16	16	10	16	16	16
22	56	67	72	62	41	53	50	27	23	32	35	34	50	35	17
35	78	130	149	134	82	51	35	37	24	47	48	39	31	21	25
38	50	123	135	125	54	44	14	37	19	18	26	30	15	28	30
58	75	83	113	122	52	40	16	29	29	6	17	23	10	34	29
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42	42	42	42	42	42	42	42	42	42	42	42	42	42	42	42
16	29	69	99	92	38	24	25	15	14	21	13	22	25	18	17
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147	147	147	147	147	147	147	147	147	147	147	147	147	147	147	147
19	14	29	94	79	44	20	13	10	7	2	3	3	4	22	16
8	2	8	42	32	10	2	3	2	1	1	1	3	2	3	8
3	0	0	5	3	2	0	0	0	1	0	0	0	0	1	1
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100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100
800	800	800	800	800	800	800	800	800	800	800	800	800	800	800	800
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Figure C.3. Example of a XOQDOQ .inp file used in the site-specific meteorological comparative analysis. This file is for the Levy site and represents the ground-level release scenario. The calms are evenly distributed in the 0.5 m/s wind-speed bin.

Pacific Northwest National Laboratory

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