
Atmospheric Transport and Dispersion (ATD) Qualification Report

Atmospheric Transport and Dispersion (ATD) Qualification Report

Version 2.0

A SIERRA Module

September 2026



Renaissance Code Development, LLC

310 NW 5th St., Suite 203

Corvallis, Oregon 97330

(541) 286-4428

<http://www.rcdsoftware.com>

Atmospheric Transport and Dispersion (ATD) Qualification Report

Atmospheric Transport and Dispersion (ATD) Qualification Report

Version 2.0

A SIERRA Module

September 2026

Preparer:	Jeffrey Luitjens cn=Jeffrey Luitjens, o=Renaissance Code Development, ou=Director - Software Division, email=jeff.luitjens@rcdsoftware.com, c=US 2026.09.17 15:47:01 -07'00'
Reviewer:	Mason Loidhamer DN: cn=Mason Loidhamer, o=Renaissance Code Development, ou=Associate Engineer, email=mason.loidhamer@rcdsoftware.c om, c=US Date: 2026.09.17 15:48:40 -07'00'
Approver:	David Hamby DN: cn=David Hamby, o=Renaissance Code Development, ou=Operations Manager, email=david.hamby@rcdsoftware.com, c=US Date: 2026.09.17 15:59:36 -07'00'

Atmospheric Transport and Dispersion (ATD) Qualification Report

Revision History

Revision	Description
0	Initial release.

Atmospheric Transport and Dispersion (ATD) Qualification Report

Table of Contents

1.0	Introduction.....	5
2.0	Definitions and Acronyms.....	6
3.0	General Development Practices and Guidelines	8
4.0	Requirements	9
5.0	Test Plans	16
5.1.	Global Input Verification Test	18
5.2.	UI Data Processing Test	18
5.3.	Save and Load Scenario File Test	19
5.4.	View Output File Test.....	20
5.5.	Global Results Verification Test	20
5.6.	Save Output Results to File Test.....	21
5.7.	Variable Input Unit Tests	22
5.8.	ATD Regression Testing	23
5.8.1.	Control Room Regression Tests.....	25
5.8.2.	Design Basis Accident Regression Tests	28
5.8.3.	Routine Release Regression Tests	31
6.0	Test Results	34
6.1.	Requirements Test Results	34
6.2.	Regression Test Results	35
6.2.1.	Control Room Regression Test Results.....	36
6.2.2.	Design Basis Regression Test Results	42
6.2.3.	Routine Release Regression Test Results	45
7.0	Summary/Conclusions.....	49
8.0	Electronic Files	50
9.0	References	51

Atmospheric Transport and Dispersion (ATD) Qualification Report Introduction

1.0 Introduction

This report captures the Verification and Validation activities for the Atmospheric Transport and Dispersion (ATD) module of SIERRA. It includes:

- identification of requirements,
- identification of verification methods to verify satisfaction of requirements, and
- verification results to document satisfaction of requirements.

This activity is performed in accordance with the SIERRA Software Project Plan [9.2].

The SIERRA ATD module is part of the Nuclear Regulatory Commission's (NRC's) SIERRA code system used for radiological consequence analysis. It models the dispersion of radioactive materials in the atmosphere during both routine operations and accident scenarios at nuclear facilities. SIERRA ATD replaces legacy codes like XOQDOQ, ARCON, and PAVAN by incorporating modernized atmospheric dispersion modeling aligned with NRC regulatory guides. Its primary applications include emergency preparedness, licensing reviews, and risk-informed decision-making, providing accurate dose and dispersion estimates for compliance and safety evaluations.

To modernize and integrate these and related codes, the NRC launched the Radiation Protection Computer Code Analysis and Maintenance Program (RAMP), which led to the development of SIERRA ATD. This new module consolidates and improves upon the technical basis of its predecessors, offering enhanced realism, broader applicability, and streamlined support under a unified platform.

Atmospheric Transport and Dispersion (ATD) Qualification Report
Definitions and Acronyms

2.0 Definitions and Acronyms

Term	Definition
ANS	American Nuclear Society – A professional organization that promotes nuclear science and technology.
ANSI	American National Standards Institute – A private nonprofit that oversees the development of voluntary consensus standards in the U.S.
API	Application Program Interface – The access points the front end uses to get data from the backend.
Assert	Check if a statement is true.
ATD	Atmospheric Transport and Dispersion
Backend	Java – The source code that manages where and how the data is stored and processed.
CFR	Code of Federal Regulations – The codified set of rules issued by U.S. federal agencies, including nuclear energy regulations under Title 10.
denormal flushing	Flushing denormals to zero replaces any floating-point value that underflows below the smallest normal representable magnitude with exactly zero, rather than preserving it as a reduced-precision.
Frontend	JavaScript, CSS, HTML – The source code which establishes and manages features of the UI.
GET	A database or API query that requests the retrieval of information of a source.
PATCH	A database or API query that requests a partial modification to an already existing source.
PNNL	Pacific Northwest National Laboratory – A U.S. Department of Energy research lab focused on energy, environment, and national security.
REQ	Requirement – used as designation in this document to identify a unique requirement.
RTM	Requirements Traceability Matrix – A document that maps and tracks requirements throughout the project lifecycle to ensure compliance.
UI	User Interface

Atmospheric Transport and Dispersion (ATD) Qualification Report
Definitions and Acronyms

Term	Definition
V&V	Verification and Validation – Processes to ensure a system meets design specifications (verification) and fulfills intended use (validation).

Atmospheric Transport and Dispersion (ATD) Qualification Report
General Development Practices and Guidelines

3.0 General Development Practices and Guidelines

Identified here are the development practices and guidelines that should be applied when developing this module. These are items that are identified as important for the overall usability of the program but are not necessarily expected to have explicit tests to demonstrate satisfaction of implementation.

1. Fortran compiler options should be implemented as specified by [9.3].
2. When input fields are not applicable to the user selected options or models, those inputs fields should be hidden from the user to provide focus on the applicable input fields.
3. The look and feel of the new ATD module should be consistent with that of the current release ATD module to provide program consistency. Fields may be moved around and group with other related inputs where it makes logical sense.
4. Tests should be developed to maximize source code coverage (i.e., activation of as much of the source code logic as possible). This may involve unit tests of specific sections of the code, expanding regression tests performing sensitivity-like analyses, or general integrated tests.
5. When implementing reference standard models, verification tests should be implemented to confirm proper implementation.
6. Standard error handling and protections should be implemented (e.g., divide by zero, file availabilities, etc.) and handled gracefully by the code.
7. General minimum and maximum bounds checking on input variables should be performed. When the user enters an input value that exceeds those bounds, the program should attempt to execute but the user should be notified when those bounds have been exceeded and that the results may not be reliable.
8. ATD version 1.0.3 only accepts SI units as inputs. Through development, input fields should be expanded to allow English units as well. When implementing requirements for the applicable input, they should be updated in Table 4-1.

Atmospheric Transport and Dispersion (ATD) Qualification Report Requirements

4.0 Requirements

Requirements for the SIERRA ATD module are derived from the following types of sources:

1. regulations and regulatory guidance [9.6, 9.7, 9.8]
2. standards or other references,
3. critical functionality of current/legacy code capabilities [9.4, 9.5],
4. user interaction with program, and/or
5. project sponsor identified.

The SIERRA Software Project Plan [9.2, Table 5-1] identifies references that may be useful in defining requirements. Revision 0 of this report heavily relied on [9.4, 9.5] to develop the initial requirements for the ATD module and thus, a majority of the listed requirements are a result of item 3 above.

Additional requirements may be identified for the software as part of the software lifecycle. Those identified modifications to the baseline are tracked and managed through the issue tracker in the form of feature requests. New features that are approved for implementation and identified as a new requirement will result in a revision to the requirements here to include the newly identified requirement.

To develop specific requirements, a walkthrough of [9.4, 9.5] and the executed code of SIERRA ATD version 1.0.3 was performed. Requirements were identified to ensure that the existing functionalities of the code were maintained when developing the SIERRA ATD module. The resulting requirements list is defined in Table 4-1. Each requirement is identified with:

- The unique ID of the requirement.
- The requirement statement.
- The section number of the test processes used to execute the test.
- The resulting acceptability of the of the requirement satisfaction based on the testing acceptance criteria after completion of test execution.

The test number of a specific test is the same as the requirement number for ease of traceability of requirement and test. Each requirement is noted to which sub-module(s) it applies to:

Atmospheric Transport and Dispersion (ATD) Qualification Report Requirements

- Control Room (CR) (legacy code ARCON),
- Design Basis Accident (DBA) (legacy code PAVAN), and/or
- Routine Release (RR) (legacy code XOQDOQ).

A requirement is noted as deferred when it is identified as a potential requirement for the future and not yet approved for the current scope of work. Requirements are written to be specific, measurable, achievable, relevant, and testable.

Requirements marked as Reserved are requirement numbers that are not currently used.

Atmospheric Transport and Dispersion (ATD) Qualification Report Requirements

Table 4-1. Requirements traceability matrix.¹

ID	Requirement Statement	CR	DBA	RR	Test Description Section #	PASS/FAIL
REQ-001	Allow selection of analysis type of Onsite Control Room Analysis.	x	-	-	5.1	PASS
REQ-002	Allow selection of analysis type of Offsite Design Basis Accident.	-	x	-	5.1	PASS
REQ-003	Allow selection of analysis type of Offsite Routine Release.	-	-	x	5.1	PASS
REQ-004	Allow saving of inputs to an input file.	x	x	x	5.3	PASS
REQ-005	Allow reading of saved input files.	x	x	x	5.3	PASS
REQ-006	Allow loading of NRC-formatted Meteorological Data File. (Meteorological file standard format defined by Regulatory Guide 1.23 [9.11])	x	x	x	5.1	PASS
REQ-007	Allow numerical input to define calm wind speed threshold in units of (m/s).	x	x	x	5.1	PASS
REQ-008	Allow selection of meteorological data display as lower or upper to view wind speed statistics.	x	x	x	5.2	PASS
REQ-062	Include window to display meteorological statistics from the NRC-formatted met. data file for total no. of hours, average wind speed (m/s), minimum wind speed (m/s), maximum wind speed (m/s), calm records, calm wind frequency (%), data availability (%), and the number of incomplete or missing records	x	x	x	5.2	PASS
REQ-009	Allow numerical input for surface roughness length in units of (m).	x	-	-	5.1	PASS
REQ-063	Allow input of meteorological data file containing only one elevation.	x	x	x	5.1	PASS

¹ A requirement is noted as deferred when it is identified as a potential requirement not yet approved for the current scope of work.

Atmospheric Transport and Dispersion (ATD) Qualification Report Requirements

ID	Requirement Statement	CR	DBA	RR	Test Description Section #	PASS/ FAIL
REQ-010	Allow selection of the NRC diffusion model (see REQ-012) with corrections to account for enhanced dispersion under low wind speed conditions and in building wakes described by Ramsdell and Fosmire (1995) consistent with models specified in NUREG CR-6331.	x	-	-	5.1	PASS
REQ-011	Allow selection of the NRC diffusion model defined in Regulatory Guide 1.145 Appendix A [9.7].	-	x	x	5.1	PASS
REQ-012	Allow DESERT_SIGMA diffusion model.	-	x	x	5.1	PASS
REQ-013	Allow ISC diffusion model.	-	-	x	5.1	PASS
REQ-014	Allow BRIGGS_RURAL diffusion model.	-	-	x	5.1	PASS
REQ-015	Allow BRIGGS_URBAN diffusion model.	-	-	x	5.1	PASS
REQ-016	Accept numerical input for diffusion coefficient sigma Y in units of (m).	x	-	-	5.1	PASS
REQ-017	Accept numerical input for diffusion coefficient sigma Z in units of (m).	x	-	-	5.1	PASS
REQ-018	Accept numerical input that specifies the acceptable missing data criterion when calculating average values in units of (%).	x	x	-	5.1	PASS
REQ-019	Accept numerical input that specifies the confidence threshold in units of (%).	x	-	-	5.1	PASS
REQ-020	Allow user to select/de-select Open Terrain Recirculation.	-	x	x	5.1	PASS
REQ-021	Allow activation of the Plume Rise model when Release Type is ELEVATED. It is enabled when any of the following are entered as non-zero values: Release Inside Diameter, Average Release Flow Rate, and Average Vent Heat Emission Rate.	-	x	-	5.1	PASS
REQ-022	Allow selection of Release Type as GROUND.	x	x	x	5.1	PASS

Atmospheric Transport and Dispersion (ATD) Qualification Report Requirements

ID	Requirement Statement	CR	DBA	RR	Test Description Section #	PASS/ FAIL
REQ-023	Allow selection of Release Type as ELEVATED.	x	x	x	5.1	PASS
REQ-024	Allow selection of Release Type as VENT.	-	-	x	5.1	PASS
REQ-025	Allow numerical input for RELEASE HEIGHT (m) when Release Type is ELEVATED.	x	x	x	5.1	PASS
REQ-026	Allow numerical input for STACK DIAMETER (m) when Release Type is ELEVATED.	x	x	x	5.1	PASS
REQ-027	Allow numerical input for STACK FLOW RATE (m3/s) when Release Type is ELEVATED.	x	x	x	5.1	PASS
REQ-028	Allow numerical input for PLANT GRADE ELEVATION ABOVE SEA LEVEL (m) when Release Type is ELEVATED.	x	x	x	5.1	PASS
REQ-029	Allow numerical input for VENT HEAT EMISSION RATE (cal/s) when Release Type is ELEVATED & Plume Rise is selected.	-	x	x	5.1	PASS
REQ-030	Allow selection of Site Type as INLAND or COASTAL when Release Type is ELEVATED.	-	x	-	5.1	PASS
REQ-031	Allow numerical input for BUILDING HEIGHT (m) when Release Type is GROUND.	-	x	x	5.1	PASS
REQ-032	Allow numerical input for BUILDING CROSS-SECTIONAL AREA (m2) when Release Type is GROUND.	x	x	-	5.1	PASS
REQ-033	Allow numerical input for PLANT GRADE ELEVATION ABOVE SEA LEVEL (m) when Release Type is GROUND.	x	-	-	5.1	PASS
REQ-034	Reserved.	-	-	-	-	N/A
REQ-035	Allow numerical input for RELEASE HEIGHT (m) when Release Type is VENT.	-	-	x	5.1	PASS
REQ-036	Allow numerical input for STACK DIAMETER (m) when Release Type is VENT.	-	-	x	5.1	PASS

Atmospheric Transport and Dispersion (ATD) Qualification Report Requirements

ID	Requirement Statement	CR	DBA	RR	Test Description Section #	PASS/FAIL
REQ-037	Allow numerical input for BUILDING HEIGHT (m) when Release Type is VENT.	-	-	x	5.1	PASS
REQ-038	Reserved.	-	-	-	-	-
REQ-039	Allow numerical input for STACK FLOW RATE (m3/s) when Release Type is VENT.	-	-	x	5.1	PASS
REQ-040	Allow numerical input for PLANT GRADE ELEVATION ABOVE SEA LEVEL (m) when Release Type is VENT.	-	-	x	5.1	PASS
REQ-041	Allow numerical input for VENT HEAT EMISSION RATE (cal/s) when Release Type is VENT & Plume Rise is selected.	-	-	x	5.1	PASS
REQ-042	Allow numerical input for single RECEPTOR DISTANCE (Control Room) (m).	x	-	-	5.1	PASS
REQ-043	Allow numerical input for BUILDING INTAKE HEIGHT (m).	x	-	-	5.1	PASS
REQ-044	Allow numerical input for TERRAIN HEIGHT AT RECEPTOR LOCATION (m).	x	-	-	5.1	PASS
REQ-045	Allow numerical input for WIND DIRECTION SPREAD ABOUT CENTERLINE DIRECTION (degrees).	x	-	-	5.1	PASS
REQ-046	Allow numerical input for DIRECTION FROM RECEPTOR TO SOURCE (degrees).	x	-	-	5.1	PASS
REQ-047	Accept multiple inputs to define multiple receptors including label, type, sector, and distance.	-	-	x	5.1	PASS
REQ-048	Allow defining range of EAB (Exclusion Area Boundary).	-	x	-	5.1	PASS
REQ-049	Allow selection range of LPZ (Low Population Zone)	-	x	-	5.1	PASS
REQ-050	Include fields to accept Sector Distances (m) and Elevations (m) for the standard 16 sectors (N, NNE, NE, ENE, E, ESE, SE, SSE, S, SSW, SW, WSW, W, WNW, NW, NNW)	-	x	x	5.1	PASS

Atmospheric Transport and Dispersion (ATD) Qualification Report
Requirements

ID	Requirement Statement	CR	DBA	RR	Test Description Section #	PASS/FAIL
REQ-051	Allow defining up to 10 range sets.	-	-	x	5.1	PASS
REQ-052	Allow viewing of output file.	x	x	x	5.4	PASS
REQ-053	Allow viewing of frequency file.	x	x	-	5.4	PASS
REQ-054	Allow viewing of hourly file.	x	x	x	5.4	PASS
REQ-055	Display Output Summary Data by Averaging Interval	x	x	-	5.5	PASS
REQ-056	Output Summary Data by Standard Time Interval	x	-	-	5.5	PASS
REQ-057	Allow selection of Output Summary Type to view as NO DECAY/UNDEPLETED.	-	-	x	5.5	PASS
REQ-058	Allow selection of Output Summary Type to view as 2.260 DAY DECAY/DEPLETED.	-	-	x	5.5	PASS
REQ-059	Allow selection of Output Summary Type to view as 8.000 DAY DECAY/DEPLETED.	-	-	x	5.5	PASS
REQ-060	Allow selection of Output Summary Type to view as RELATIVE DEPOSITION PER SQUARE-METER AREA.	-	-	x	5.5	PASS
REQ-061	Allowing saving of output results to file(s).	x	x	x	5.6	PASS
REQ-064	Allow user to specify SI or English inputs on the UI.	x	x	x	5.7	PASS

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

5.0 Test Plans

Verification and Validation Tests are developed to demonstrate satisfaction of software requirements with each test linked to the specific requirement it is intended to verify. Verification is performed to confirm the software meets specified requirements related to the design, code, or other items. This begins with defining requirements and then verifying the end software product meets those requirements. Validation is the process of demonstrating that a product or system fulfills its intended use when placed in its operational environment. This ensures the output is correct and consistent with the physical world or intended implemented models. Functional tests used for validating intended functionality are implemented into ATD in the same fashion as the requirements tests. Functional tests are additional tests added by the developer(s) and/or reviewer(s) at their discretion. These functional tests are not documented here explicitly but test reports are created for them, and they are reviewed. Functional tests will continue to grow with further development.

The methods that will be used to perform V&V and ensure requirements are satisfied include testing to provide quantitative proof of requirement satisfaction. Test methods/cases are defined in the following subsections.

It begins by identifying the requirement to be assessed, by referencing its unique identifier, and summarizing its purpose. The test description outlines the objective of the test and the expected behavior, output, or condition that will confirm that the requirement has been met.

The test description involves:

1. Arrange: Describe the test setup, including any necessary preconditions, configurations, or data inputs.
2. Act: Specify the steps to execute the test, ensuring they are detailed enough to be repeatable by others.
3. Assert: Identify the expected results for each step or for the overall test.

Finally, the acceptance criteria is identified to explain how these results demonstrate compliance with the requirement.

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

If applicable, note any tools, environments, or metrics used to evaluate success. Test descriptions are written with the intent to be unambiguous, focused, and provide a clear rationale for how it validates the requirement.

A Requirements Traceability Matrix (RTM) is a table that links requirements to their corresponding design specifications, implementation artifacts, and verification/validation activities. It helps track the status of requirements and ensures that all are addressed. A requirements traceability matrix is provided in Section 4.0 generated to track and confirm that requirements are satisfied.

Requirements satisfaction is implemented within GitLab by leveraging its requirements management framework, allowing developers to link requirements to a automated tests. Tests are executed for each merge (code change), and each test is assigned a pass or a fail. If a requirement is linked to a test and that test passes, then the requirement is met. This allows for live tracking of the status of requirement acceptance.

Multiple requirements may be linked to multiple tests due to repeated functionality existing throughout the code. The following subsections are generally broken up by categories defining the various test procedures which may be applied to demonstrating multiple requirements depending on the overall function of the test.

Tests marked as Reserved are test numbers that are not currently used.

Atmospheric Transport and Dispersion (ATD) Qualification Report
Test Plans

5.1. Global Input Verification Test

Test Description:

The goal of this test is to verify that user interaction with a variable in the UI will be reflected in the database, the input file to the Fortran, and the response from the API.

The Action:

Patch the API with a value.

The Assertions:

1. Check that the database updated the variable with the value from the action.
2. Check the API for the variable will return with the updated variable.
3. Check that the JSON going to Fortran contains the updated variable.
4. Check that the output file from Fortran contains the updated variable.

Acceptance Criteria:

The acceptance criteria for this test requires the simulated user interaction to successfully propagate through the assertions. These values are verified to be identically equivalent.

5.2. UI Data Processing Test

Test Description:

The goal of this test type is to verify that the database and API contain the same value for processed data. This test method typically applies to data that is available to the user in the UI for viewing and interpretation of inputs. This applies to the loading and viewing of a meteorological data file. The results from processing a meteorological data file (e.g., average wind speed) in the UI are not input to the calculational method and have no impact on the output results.

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

To confirm proper processing of values, reference values are determined through alternative means for comparisons through hand calculations, other codes, literature, etc.

The Action:

Call the API to do the action generating the processed data.

The Assertions:

1. Check that the database updated each corresponding variable to match the hand calculated/literature value.
2. Check that the API for each corresponding variable returned with the hand calculated/literature value.

Acceptance Criteria:

The acceptance criteria for this test requires the processed data be within the reference data with the absolute difference of 0.0001. This is set with the expectation that numeric results should be processed within near single-precision tolerance.

5.3. Save and Load Scenario File Test

Test Description:

The goal of this test is to verify that the user can save and load a scenario file and that the database reflects the loaded scenario file.

The Action:

1. Patch 3 different variables.
2. Call the API to save the scenario file.
3. Reset the database.
4. Load the scenario file.

The Assertions:

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

1. Assert that the database contains the original patched variables in Action 1.

Acceptance Criteria:

The acceptance criteria for this test requires that after the database is reloaded from file it contains the initially patched variables identically. This proves that both the saved and the load features are properly working.

5.4. View Output File Test

Test Description:

The goal of this test type is to verify that the user can view the files output by Fortran.

The Action:

Call the API to return the file.

The Assertions:

1. Check that the expected length of the file is the same as the actual.
2. Check every line of the file to verify that it is the same as the expected line of the file.

Acceptance Criteria:

The acceptance criteria for this test requires the returned file from the API is identical to the file generated by Fortran.

5.5. Global Results Verification Test

Test Description:

The goal of this test type is to verify that the results produced by the Fortran engine are loaded into Java, parsed, and returned by the API for display to the user. This is accomplished by performing a direct content comparison between the API response and the raw engine output file, confirming that no data is lost, altered, or misrepresented during the load and parsing process.

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

The Action:

1. Run the calculation.
2. Read ATD_ENGINE_OUT.JSON directly from disk and deserialize it.
3. Retrieve the API results.

The Assertions:

1. Compare the results API content with the content deserialized from disk.

Acceptance Criteria:

The acceptance criteria for this test requires that the results API contains the same information as the deserialized file generated by Fortran, with no differences in the values.

5.6. Save Output Results to File Test

Test Description:

The goal of this test is to verify that the expected output files are generated by the Fortran engine.

The Action:

1. Run the calculation.

The Assertions:

1. Asserts that the .OUT file does exist.
2. Assert that the .CFD file does exist.
3. Assert that the .ERR file does exist.
4. Assert that the .JFD file does exist.
5. Assert that the .PLT file does exist.
6. Assert that the .OUT file completed with "NORMAL PROGRAM COMPLETION" denoted within the output file.

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

Acceptance Criteria:

The acceptance criteria for this test requires that Fortran generated all the expected files and that the program completed normally. This is performed for each mode.

5.7. Variable Input Unit Tests

Test Description:

The processed file that is passed to the Fortran executable to perform calculations only accepts SI units. The user is allowed to enter either SI or English units within the UI and the UI automatically generates the correct SI input based json object.

This test verifies that the user can input equivalent variable values in the UI in either SI or English units and the generated json input for Fortran will be the same.

The Action:

1. Generate and save a Fortran json input object using SI units.
2. Switch each numeric variable to its English unit equivalent.
3. Generate and save the Fortran json input object processed using the UI specified English units.

The Assertions:

1. Assert that the Fortran json input generated by the SI scenario file and English scenario file are identical.

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

5.8. ATD Regression Testing

Test Description:

This section performs regression testing of the ATD module against the previous versions of itself. A parametric regression test suite was developed for each module: 40 Control Room test cases, 19 Design Basis Accident test cases, and 27 Routine Release test cases, for a total of 86 test cases. Output results from the previous version (baseline) are compared to the results of a new version developed for release. This is used to confirm that any modifications have not negatively impacted the technical solution in an unexpected way. When differences in the output results occur, they are evaluated for the cause, and a determination is made if the changes are acceptable. If the change is acceptable the regression suite baseline results are updated for regression testing of the next version.

There are no linked requirements for regression testing, as regression testing is a software quality assurance practice aimed at ensuring code stability and integrity across version updates rather than a verification of a specific system or performance requirement.

Each suite follows the same design. A core parametric set varies the release geometry inputs applicable to the module and release elevation mode (release height, diameter, flow rate, plant grade elevation, building area and height, and cross-sectional area) over two release elevations to provide broad regression coverage based on physical processes. This core set is supplemented by single-variation coverage cases, each of which changes one input per execution to exercise a specific portion of the Fortran engine, such as the alternative diffusion options, surface roughness ranges, recirculation factor distance bands, plume rise behavior, and the calm, missing data, and wind direction window handling. The one-year meteorological input file (MET_8387.nrc) contains all seven stability classes, calm hours, missing-data hours, and north-wrap wind directions. North-wrap wind directions are hours with winds from near due north (close to 0°/360°), which are required to exercise the Control Room wind-direction-window logic that splits the acceptance window into two segments when it crosses the 0°/360° boundary (e.g., direction to source = 10° or 350° with a 45° window)

The Action (For each module):

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

1. Select the module.
2. Load the test case scenario file containing the inputs.
3. Run the calculation.
4. Repeat for each test case defined for the module.

The Assertions:

1. Assert that the output is equal to the previous version's (baseline) output for each test case.

The branch coverage of each suite was estimated by static enumeration of the branch outcomes in the Fortran subprograms reachable by the module being tested (e.g., Control Room); branches reachable only by the other modules (e.g., Routine Release) are excluded. Coverage is expressed as branch outcomes, not lines of code, statements, or subroutines: each IF...THEN block contributes two outcomes (condition true and false), each ELSE IF adds one further outcome, a single-statement logical IF contributes two, and a SELECT CASE contributes one outcome per CASE value plus one for the default or fall-through; loop constructs and arithmetic are not counted. The denominator for each module counts only outcomes in subprograms reachable when that module is selected; outcomes reachable only by the other modules (e.g., Routine Release), outcomes selectable only through inputs the interface does not offer for that module (e.g., non-NRC diffusion options for Control Room), and known-dead code are excluded from coverage targets. Excluding interface-unreachable outcomes, the estimated full-suite branch coverage is approximately 80% for Control Room, 82% for Design Basis Accident, and 87% for Routine Release. Covered counts are static estimates derived by inspecting which input values and meteorological content drive each conditional; they are based on the Fortran source as of version 2.0, may drift as code changes occur, and may require future re-evaluation.

Acceptance Criteria: This test is acceptable when parity is established between the baseline reference results and the newly developed ATD module version results, or when the results of the newly developed ATD module version are considered expected for the changes made. Any differences are documented and evaluated for acceptability in Section 6.2.

The following subsections describe the specific regression tests performed for each module.

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

5.8.1. Control Room Regression Tests

Table 5-1 defines the Control Room module parameters and their associated ranges for the parametric test cases listed in Table 5-2. Table 5-2 identifies the inputs that define each test case as well as the base case to which change is applied.

Table 5-1. Control Room reference case.

Parameter	Ground Value	Release	Elevated Value	Release
Release Height (H) (m)	N/A		0, 15	
Release Diameter (D) (m)	N/A		0, 2	
Release Flow Rate (Q) (m ³ /s)	0, 2		0, 2	
Plant Grade Elevation (PGE) (m)	0, 20		0, 20	
Building Cross-sectional Area (BA) (m ²)	0, 100		N/A	
Receptor Distance (m)		20		
Intake Height (m)		5		
Terrain Height of Receptor (m)		10		
Wind Direction Window (°)		45		
Direction to Source (°)		270		
Met File		MET_8387.nrc		
Wind Speed Calm Threshold (m/s)		0.5		
Surface Roughness Length (z0) (m)		1		
Diffusion		NRC		
Initial Diffusion Sigma Y (σY_0) (m)		1		
Initial Diffusion Sigma Z (σZ_0) (m)		1		
Missing Data Criterion (%)		10		
User Defined Percentile (%)		99.5		

Table 5-2. Control Room regression test cases.

Test Case	Description
Test 1	Ground: Q=0, PGE=0, BA=0
Test 2	Ground: Q=0, PGE=0, BA=100

Atmospheric Transport and Dispersion (ATD) Qualification Report
Test Plans

Test Case	Description
Test 3	Ground: Q=0, PGE=20, BA=0
Test 4	Ground: Q=0, PGE=20, BA=100
Test 5	Ground: Q=2, PGE=0, BA=0
Test 6	Ground: Q=2, PGE=0, BA=100
Test 7	Ground: Q=2, PGE=20, BA=0
Test 8	Ground: Q=2, PGE=20, BA=100
Test 9	Elevated: H=0, D=0, Q=0, PGE=0
Test 10	Elevated: H=0, D=0, Q=0, PGE=20
Test 11	Elevated: H=0, D=0, Q=2, PGE=0
Test 12	Elevated: H=0, D=0, Q=2, PGE=20
Test 13	Elevated: H=0, D=2, Q=0, PGE=0
Test 14	Elevated: H=0, D=2, Q=0, PGE=20
Test 15	Elevated: H=0, D=2, Q=2, PGE=0
Test 16	Elevated: H=0, D=2, Q=2, PGE=20
Test 17	Elevated: H=15, D=0, Q=0, PGE=0
Test 18	Elevated: H=15, D=0, Q=0, PGE=20
Test 19	Elevated: H=15, D=0, Q=2, PGE=0
Test 20	Elevated: H=15, D=0, Q=2, PGE=20
Test 21	Elevated: H=15, D=2, Q=0, PGE=0
Test 22	Elevated: H=15, D=2, Q=0, PGE=20
Test 23	Elevated: H=15, D=2, Q=2, PGE=0
Test 24	Elevated: H=15, D=2, Q=2, PGE=20
Test 25	Reserved
Test 26	Reserved
Test 27	Reserved
Test 28	Reserved
Test 29	Test 24 with $z_0=0.01$, H=30
Test 30	Test 24 with $z_0=0.05$, H=30
Test 31	Test 24 with $z_0=0.5$, H=30
Test 32	Test 8 with receptor distance = 150

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

Test Case	Description
Test 33	Test 8 with receptor distance = 1200, $\sigma_{y0}=5$, $\sigma_{z0}=5$
Test 34	Test 8 with $\sigma_{y0}=5$, $\sigma_{z0}=5$
Test 35	Test 24 with user-defined percentile omitted from input file
Test 36	Test 24 with missing data criterion = 0
Test 37	Test 24 with missing data criterion = 100
Test 38	Test 24 with wind speed calm threshold = 1.5
Test 39	Test 24 with wind speed calm threshold = 0.05 (engine resets to 0.5)
Test 40	Test 24 with wind direction window = 360
Test 41	Test 24 with direction to source = 10
Test 42	Test 24 with direction to source = 350
Test 43	Reserved
Test 44	Test 24 with release height = 110 (upper met level selection)
Test 45	Test 24 with release flow rate = 20

Table 5-3. Estimated branch coverage of Control Room.

Module	Possible Branch Outcomes	Reached Branch Outcomes
ARCON.f90	6	6 (100%)
XOQ.f90 (concentration functions)	5	3 (60%)
SIGMAS.f90	19	16 (84%)
MO_RAMSDCELL.f90	19	17 (89%)
PROC_HOURLY.f90	12	12 (100%)
PROC.f90 + CalmsDistribution	17	17 (100%)
MET.f90	53	47 (89%)
POSTPROC.f90 (ARCON + utilities)	47	44 (94%)
USER_INPUTS.f90	67	45 (67%)
JSON_QA/FILES/JFD/MESSAGES/ATD_ENGINE (I/O, parsing, messages)	55	33 (60%)
Total (Control Room reachable)	300	240 (80%)

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

5.8.2. Design Basis Accident Regression Tests

Table 5-4 defines the Design Basis Accident parameters and their associated ranges for the parametric test cases listed in Table 5-5. Table 5-5 identifies the inputs that define each test case as well as the base case to which each change is applied. The interface selects the plume rise option automatically when any of release diameter, release flow rate, or vent heat emission rate is entered as non-zero (and deselects it when all three are zero). The engine computes plume rise only for an elevated release with the option selected and a non-zero release diameter; a non-zero heat emission rate selects the buoyant-rise formulation (flow rate is then not used), otherwise the flow rate provides momentum rise.

Table 5-4. Design Basis Accident reference case.

Parameter	Ground Release Value	Elevated Release Value
Building Cross-sectional Area (BA) (m ²)	0, 2000	N/A
Building Height (BH) (m)	0, 30	N/A
Release Height (H) (m)	N/A	30, 100
Release Diameter (D) (m)	N/A	0
Release Flow Rate (Q) (m ³ /s)	N/A	0
Vent Heat Emission Rate (Qh) (cal/s)	N/A	0
Plant Grade Elevation (PGE) (m)	N/A	0
Land Type	N/A	Inland, Coastal
Met file	MET_8387.nrc	
Wind speed calm threshold (m/s)	0.5	
Diffusion	NRC	
Recirculation factor (RF)	OFF	
Missing data criterion (%)	10	
EAB distance (m, all sectors)	800	
LPZ distance (m, all sectors)	4800	
Terrain (16 sectors x 2)	all 0 (flat)	

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

Table 5-5. Design Basis Accident regression test cases.

Test Case	Description
Test 1	Ground: BA = 0, BH = 0
Test 2	Ground: BA = 0, BH = 30
Test 3	Ground: BA = 2000, BH = 0
Test 4	Ground: BA = 2000, BH = 30
Test 5	Elevated: H=30, inland
Test 6	Elevated: H=30, coastal
Test 7	Elevated: H=100, inland
Test 8	Elevated: H=100, coastal
Test 9	Identical to Test 7 (plume rise explicitly disabled with D=0, Q=0); retained as a repeat of the base case
Test 10	Test 7 with D=1, Q=0, Qh = 1e6 (plume rise with buoyancy only)
Test 11	Test 7 with D=1, Q=2, (plume rise with momentum only)
Test 12	Test 7 with diffusion model= desert sigma
Test 13	Test 7 with recirculation factor on
Test 14	Test 7 with recirculation factor on, LPZ distance = 12000
Test 15	Test 7 with recirculation factor on, LPZ distance = 20000
Test 16	Reserved
Test 17	Reserved
Test 18	Test 10 with H=320
Test 19	Test 7 with sector varying EAB/LPZ distances and terrain rising from 0 to 50 m
Test 20	Test 7 with missing data criterion = 0
Test 21	Test 7 with missing data criterion = 100

Table 5-6. Estimated branch coverage of DBA.

Module	Possible Branch Outcomes	Reached Branch Outcomes
PAVAN_V2.f90	15	15 (100%)
BUILDCORR_NRC.f90	18	15 (83%)
SIGMAS.f90	20	19 (95%)

Atmospheric Transport and Dispersion (ATD) Qualification Report
Test Plans

Module	Possible Branch Outcomes	Reached Branch Outcomes
PROC_HOURLY.f90 (incl. RISE, TERR)	42	39 (93%)
PROC.f90 + CalmsDistribution	36	33 (92%)
MET.f90 (incl. fumigation)	42	38 (90%)
POSTPROC.f90 (PAVAN + RF1)	37	36 (97%)
JFD.f90	12	12 (100%)
USER_INPUTS.f90	70	48 (69%)
JSON_QA/FILES/MESSAGES/ATD_ENGINE (I/O, parsing, messages)	44	22 (50%)
XOQ.f90 (concentration functions)	5	3 (60%)
Total (DBA reachable)	341	280 (82%)

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

5.8.3. Routine Release Regression Tests

Table 5-7 defines the Routine Release parameters and their associated ranges for the parametric test cases listed in Table 5-8. Table 5-8 identifies the inputs that define each test case as well as the base case to which each change is applied.

Table 5-7. Routine Release reference case.

Parameter	Ground Release Value	Elevated Release Value	Vent Release Value
Building Cross-sectional Area (BA) (m ²)	0, 2000	N/A	N/A
Building Height (BH) (m)	0, 30	N/A	N/A
Release Height (H) (m)	N/A	10, 60	10
Release Diameter (D) (m)	N/A	2	0, 2
Release Flow Rate (Q) (m ³ /s)	N/A	2	0, 2
Vent Heat Emission Rate (Qh) (cal/s)	N/A	0, 1E6	0
Plant Grade Elevation (PGE) (m)	N/A	0	0
Met file	MET_8387.nrc		
Wind speed calm threshold (m/s)	0.5		
Diffusion	NRC		
Recirculation factor (RF)	OFF		
Discrete receptor sites	Table 5-9		
Terrain Elevation (m)	all 0 (flat)		
Terrain distance (m)	500/1k/2k/5k/10k		

Every Routine Release test case includes the same three fixed discrete receptor sites listed in Table 5-9. The discrete receptor inputs are optional to the engine: omitting them produces a warning and skips only the discrete receptor outputs; specifying sector and distance information is required only when sites are defined. Because the fixed distance grid begins at 402 m, the close-in depletion branches below approximately 400 m are reachable only through discrete receptor

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

distances. Tests 26 through 29 therefore vary the discrete inputs to cover the close-in bands.

Table 5-8. Routine Release regression test cases.

Test Case	Description
Test 1	Ground: BA = 0, BH = 0
Test 2	Ground: BA = 0, BH = 30
Test 3	Ground: BA = 2000, BH = 0
Test 4	Ground: BA = 2000, BH = 30
Test 5	Vent: Q=0, D=0
Test 6	Vent: Q=0, D=2
Test 7	Vent: Q=2, D=0
Test 8	Vent: Q=2, D=2
Test 9	Elevated: H=10, Qh = 0
Test 10	Elevated: H=10, Qh = 1e6
Test 11	Elevated: H=60, Qh = 0
Test 12	Elevated: H=60, Qh = 1e6
Test 13	Test 12 with diffusion model = ISC
Test 14	Test 12 with diffusion model = Briggs Rural
Test 15	Test 12 with diffusion model = Briggs Urban
Test 16	Test 12 with diffusion model = Desert Sigma
Test 17	Test 12 with recirculation factor on
Test 18	Test 12 with H = 30
Test 19	Test 12 with H = 100
Test 20	Test 12 with H = 320
Test 21	Test 12 with Vent, Q = 10
Test 22	Test 12 with terrain elevation rising from 0 to 50 m
Test 23	Reserved
Test 24	Test 12 with no terrain distances defined (ndist = 0)
Test 25	Reserved
Test 26	Test 12 with discrete receptor sites at 150 and 350 m, H=30, Qh = 0
Test 27	Test 12 with discrete receptor sites at 150 and 350 m, H=60, Qh = 0

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Plans

Test Case	Description
Test 28	Test 12 with discrete receptor sites at 150 and 350 m, H=100, Qh = 0
Test 29	Test 12 with discrete receptor count set to zero (nsites = 0)

Table 5-9. Fixed discrete receptor sites for Routine Release.

Site	Title	Sector	Distance (m)
1	Site boundary	S	805
2	Milk cow	NNW	1931
3	Residence	SSE	6437

Table 5-10. Estimated branch coverage of Routine Release.

Module	Possible Branch Outcomes	Reached Branch Outcomes
XOQDOQ.f90 (incl. RF1, DEPL, DEP)	112	111 (99%)
BUILDCORR_NRC.f90 (SAXOQ only)	4	4 (100%)
SIGMAS.f90	48	46 (96%)
PROC_HOURLY.f90 (incl. RISE, TERR)	41	39 (95%)
PROC.f90 + CalmsDistribution	37	34 (92%)
MET.f90	38	34 (89%)
POSTPROC.f90 (XOQDOQ part)	29	29 (100%)
JFD.f90	12	12 (100%)
USER_INPUTS.f90	80	54 (68%)
JSON_QA/FILES/MESSAGES/ATD_ENGINE (I/O, parsing, messages)	48	26 (54%)
XOQ.f90 (concentration functions)	3	2 (67%)
Total (Routine Release reachable)	452	391 (87%)

Atmospheric Transport and Dispersion (ATD) Qualification Report
Test Results

6.0 Test Results

6.1. Requirements Test Results

The requirements test report 'TEST-com.rcd.atd.reqTests.xml' documents the summary PASS/FAIL report for the requirements identified in Section 4.0 with the implementing tests defined in Sections 5.1 through 5.7. This report is stored as an electronic file with this document (Section 8.0).

Status of requirements can also be viewed live and interactively at:

https://gitlab.com/RCD-1/SIERRA/ATD/-/requirements_management/requirements

Requirements that have Passes are denoted as “satisfied” in the GitLab UI. Of the 62 requirements, all 62 are satisfied. This demonstrates that all requirements identified in Section 4.0 are satisfied as demonstrated through the testing process outlined in Sections 5.1 through 5.7.

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Results

6.2. Regression Test Results

This section summarizes the regression test results applying the regression testing plans in Section 5.8. Regression result differences are associated with each of the discrete changes made to the Fortran source code. The changes described below, scoped only to the Fortran source code, are isolated from other changes that resolve additional issues. That is, a single change is made to a reference baseline (base) to create a modified Fortran executable (mod). Output results between base and mod are then compared to assess how a specific change impacted the output. This allows for isolating the impact of that specific change. This is opposed to comparing an initial baseline to the final modified product where some changes may cause answers to increase and other changes to cause answers to decrease making it impossible to isolate the impact of a specific change.

Table 6-1 presents the Fortran executable version starting with the baseline (v1.0.3) with each subsequent row adding an incremental change. For example, the changes to address Issue 137 are compared to the previous baseline defined by Issue 119. The change is noted by the description with commit ID capturing the version. The commit IDs (the squash commit of each merge request) were gathered from the GitLab commit history, each commit was checked out, and the Fortran source incrementally compiled and named as identified in the table. The first increment (v1.0.3 to ATD_Issue127.exe) also carries the Fortran source clean-up and the compiler option changes of merge request !12 (local arrays and saved scalars are zero-initialized in the Release build); that build change, not issue #127 itself, is the origin of last-digit rounding and Routine Release Test 24 differences discussed below. Each later increment contains a single-issue resolution.

GitLab Commit History Link: https://gitlab.com/RCD-1/SIERRA/ATD/-/commits/Develop-ATD-Module/fortran/x64/Release/ATD_Fort.exe

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Results

Table 6-1. Fortran executable history.

Issue	Merge Request	Description	Commit ID	Exe Name
N/A	N/A	Initial Baseline (v1.0.3)	N/A ²	ATD_v1.0.3.exe
#127	!25	Fortran Notice Banner Update	f98246f1	ATD_Issue127.exe
#119	!32	Output File Denotes Specified Model and not Actual Model Used	867afef6	ATD_Issue119.exe
#137	!40	Fortran Output Field Overflow	e46835e9	ATD_Issue137.exe
#145	!39	Echo of User Inputs in Output File	8870ef0f	ATD_Issue145.exe
#14	!41	Control Room Accounting of Number of Calm Records	ceaaa39e	ATD_Issue14.exe
#113	!43	Control Room Stack-Flow Correction is Computed and then Overwritten	6c6e1c73	ATD_Issue113.exe
#26	!44	Routine Release Application of Decay Half-Life Error	c08fda96	ATD_Issue26.exe
N/A	N/A	Final Version (version 2.0.0)	6385f172	ATD_Fort.exe

6.2.1. Control Room Regression Test Results

Regression tests for the Control Room module are performed as described in Section 5.8.1. This section documents and addresses the differences between regression testing performed on ATD version 1.0.3 and version 2.0. It is noted that file paths and dates are expected to be different in outputs and these are not further addressed. The provided change descriptions are isolated to the specific change applied as opposed to the cumulative changes made to the Fortran source code to add clarity on what causes a specific difference in the result. The

² There is no commit ID associated with this, this is the executable as delivered with the as-received version of SIERRA ATD install package.

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Results

following additional items are noted and may differ in all cases with cases specific differences noted in Table 6-2 as it applies:

ATD output file (*.OUT):

- Informational banner is updated with the latest code and development information. (issue #127)
- Input echo of 'Surface Roughness (m)' is added. (issue #145)
- Input echo of 'Sigma-y initial diffusion (m)' is added. (issue #145)
- Input echo of 'Sigma-z initial diffusion (m)' is added. (issue #145)
- Input echo of 'Additional Percentile (%)' is added. (issue #145)
- Input echo of 'Missing Criteria (%)' is added. (issue #145)
- Input echo of receptor 'Label' is added. (issue #145)
- Input echo of 'Wind direction window (deg)' updated to include 1 decimal place of precision. (issue #14)
- Calculation of 'Hours direction in window' and 'Hours direction not in window' updated based on error correction. (issue #14)

ATD CFD file (*.CFD):

- Fractional change in the statistical binned χ/Q values. The CFD prints a cumulative frequency distribution of hourly χ/Q in percent tallying how often each level of air concentration occurred across a year of hourly weather. The small differences are the result of two factors: the old and new program versions round small floating-point numbers slightly differently, which occasionally nudges an hour from one bin to the neighboring one. As a result of one of the changes, in the corresponding test case, the program now correctly counts four hours of wind blowing toward the air intake that the old version had mistakenly thrown out. Those hours are now binned. (issue #14)

ATD ERR file (*.ERR):

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Results

- No technical change to the printed output. The program compilation has been added for enhanced traceability.

ATD JFD file (*.JFD):

- No changes.

ATD PLT file (*.PLT):

- Calculation of 'Hours direction in window' and 'Hours direction not in window' was updated based on error correction. As a result, the count of hours within a window may be smaller in the cases the meteorological file reported a wind direction for wind speeds that are evaluated as calm which by definition have no definitive direction. (issue #14)
- Hourly values that version 1.0.3 printed as 0.00E+00 are printed as (small) numbers, for example 4.90E-44, because the version 2.0 release build no longer flushes denormal numbers to zero. These values are numerically zero. A small number of hourly values (Tests 2 and 6, 21 values each) and single CFD bins differ in the last printed digit (0.23 % or 0.01–0.02 percentage points) from floating-point differences between the v1.0.3 and v2.0 builds (merge request !12).

ATD Output JSON file (*.JSON):

- Both versions print the JSON values with 17 significant digits. Differences appear in the seventh significant digit and beyond (relative differences below 0.002 %) as a result of floating-point differences between the v1.0.3 and v2.0 builds (merge request !12); results are otherwise identical except where noted in Table 6-2 (issues #14 and #113).

Table 6-2. Control Room regression test results.

Test Case	Results Description
Test 1	No case-specific differences.
Test 2	No case-specific differences.
Test 3	No case-specific differences.

Atmospheric Transport and Dispersion (ATD) Qualification Report
Test Results

Test Case	Results Description
Test 4	No case-specific differences.
Test 5	No case-specific differences.
Test 6	No case-specific differences.
Test 7	No case-specific differences.
Test 8	No case-specific differences.
Test 9	No case-specific differences.
Test 10	No case-specific differences.
Test 11	This case activates the stack-flow (finite-flow) correction with $Q=2 \text{ m}^3/\text{s}$ at an effective release height of 0 m. The correction was previously computed and then discarded and is now applied, reducing χ/Q . The maximum hourly centerline χ/Q falls from $2.41\text{E}+00$ to $4.14\text{E}-01 \text{ s/m}^3$ (-83%) and the maximum sector-average χ/Q from $5.54\text{E}-01$ to $2.63\text{E}-01 \text{ s/m}^3$ (-53%); the 95th-percentile results decrease by up to 59% and the CFD distribution shifts to lower χ/Q by up to 16 percentage points in individual bins. (issue #113)
Test 12	This case activates the stack-flow (finite-flow) correction with $Q=2 \text{ m}^3/\text{s}$ at a 20 m plant grade elevation (effective release height 5 m). The maximum hourly centerline χ/Q falls from $4.73\text{E}-03$ to $4.68\text{E}-03 \text{ s/m}^3$ (-1.1%) and the maximum sector-average χ/Q from $2.75\text{E}-03$ to $2.74\text{E}-03 \text{ s/m}^3$ (-0.4%). The 95th-percentile results change by less than 6.5% (the 8- to 24-hour value increases slightly because it is derived by differencing the 8- and 24-hour percentiles) and CFD bins move by at most 1.7 percentage points. (issue #113)
Test 13	No case-specific differences.
Test 14	No case-specific differences.
Test 15	This case activates the stack-flow (finite-flow) correction with $Q=2 \text{ m}^3/\text{s}$ at an effective release height of 0 m. The correction was previously computed and then discarded and is now applied. (issue #113)
Test 16	This case activates the stack-flow (finite-flow) correction with $Q=2 \text{ m}^3/\text{s}$ at an effective release height of 5 m. The correction was previously computed and then discarded and is now applied, reducing χ/Q . (issue #113)
Test 17	No case-specific differences.
Test 18	No case-specific differences.
Test 19	This case activates the stack-flow (finite-flow) correction with $Q=2 \text{ m}^3/\text{s}$ at an effective release height of 0 m. The correction was

Atmospheric Transport and Dispersion (ATD) Qualification Report
Test Results

Test Case	Results Description
	previously computed and then discarded and is now applied, reducing χ/Q . (issue #113)
Test 20	No case-specific differences.
Test 21	No case-specific differences.
Test 22	No case-specific differences.
Test 23	This case activates the stack-flow (finite-flow) correction with $Q=2$ m ³ /s at an effective release height of 0 m. The correction was previously computed and then discarded and is now applied, reducing χ/Q . (issue #113)
Test 24	No case-specific differences.
Test 25	Reserved
Test 26	Reserved
Test 27	Reserved
Test 28	Reserved
Test 29	No case-specific differences.
Test 30	No case-specific differences.
Test 31	No case-specific differences.
Test 32	No case-specific differences.
Test 33	No case-specific differences.
Test 34	No case-specific differences.
Test 35	No case-specific differences.
Test 36	No case-specific differences.
Test 37	No case-specific differences.
Test 38	With the calm threshold raised to 1.5 m/s, 'Hours direction in window' falls from 1854 to 1740 and the window flag changes for 114 hours in the hourly file, because hours now classified as calm are no longer counted in the window. χ/Q results are unchanged. (issue #14)
Test 39	No case-specific differences.
Test 40	With a 360 degree window, version 1.0.3 reported the window as '90 - 90' with 8759 hours in window and -114 hours not in window. Version 2.0 reports '0.0 - 360.0' with 8645 and 0, correcting the negative count; the window flag changes for the 114 calm hours in the hourly file. χ/Q results are unchanged. (issue #14)

Atmospheric Transport and Dispersion (ATD) Qualification Report
Test Results

Test Case	Results Description
Test 41	The window wraps through 0 degrees (direction to source 10 degrees). 'Hours direction in window' falls from 848 to 824 and the window flag changes for 32 hours (28 calm hours are removed from the window, and 4 hours whose wind direction is recorded as 370 degrees, i.e., 10 degrees, are now correctly counted inside it). Because fewer hours are averaged, reported χ/Q rises by up to 2.9 % and CFD bin percentages change by up to 2.6 percentage points. (issue #14)
Test 42	The window wraps through 0 degrees (direction to source 350 degrees). 'Hours direction in window' falls from 1268 to 1240 and the window flag changes for 28 calm hours in the hourly file. χ/Q results are unchanged. (issue #14)
Test 43	Reserved
Test 44	'Hours direction in window' falls from 1543 to 1532 and the window flag changes for 11 calm hours at the 122 m measurement level selected for this release height. χ/Q results are unchanged. (issue #14)
Test 45	No case-specific differences. The stack-flow correction ($Q=20$ m ³ /s) has no effect here because the elevated release ($H=15$ m, $PGE=20$ m) gives χ/Q below the $1E-10$ s/m ³ threshold at which the correction is applied.

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Results

6.2.2. Design Basis Regression Test Results

Regression tests for the Design Basis Accident module are performed as described in Section 5.8.2. This section documents and addresses the differences between regression testing between ATD version 1.0.3 and version 2.0. It is noted that file paths and dates are expected to be different in outputs and these are not further addressed. Change descriptions described are isolated to the specific change applied as opposed to the integral change of all changes put together to add clarity on what causes a specific change. The following additional items are noted and may differ in all cases, with case-specific differences noted in Table 6-3 as it applies:

ATD output file (*.OUT):

- Informational banner is updated with the latest code and development information. (issue #127)
- Input echo of 'Plume Rise' is added regardless of if active or not; version 1.0.3 printed this line only when plume rise was enabled (true). (issue #145)
- Input echo of 'Missing Criteria (%)' is added. (issue #145)
- Input echo of 'Release Location' now reports the option the engine applied, in upper case (INLAND or COASTAL), rather than the text as entered. (issue #119)
- Input echo field widths are widened to prevent write overflows so that large entries print as numbers rather than asterisks. This applies to 'Vent heat emission rate (cal/s)' and the boundary distance column of the by-sector summary tables. No calculated value changes. (issue #137)

ATD CFD file (*.CFD):

- The 'Boundary Distance' header field is widened to prevent write overflows so that large entries print as numbers rather than asterisks. (issue #137)

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Results

- Fractional change in the statistical binned χ/Q values. Bin percentages move by at most 0.03 percentage points, which is one to three hours of the 8,760-hour meteorological record crossing a bin boundary as a result of floating-point differences between the v1.0.3 and v2.0 builds (merge request !12).

ATD ERR file (*.ERR):

- No technical change to the printed output. The program compilation date has been added for enhanced traceability.

ATD JFD file (*.JFD):

- No changes.

ATD PLT file (*.PLT):

- Hourly values that version 1.0.3 printed as 0.00E+00 are printed as denormalized numbers, for example 4.90E-44, because the version 2.0 release build no longer flushes denormals to zero. These values are numerically zero.

ATD Output JSON file (*.JSON):

- Both versions print the JSON values with 17 significant digits. Differences appear in the seventh significant digit and beyond (relative differences below 0.01%) as a result of floating-point differences between the v1.0.3 and v2.0 builds (merge request !12).

Table 6-3. Design Basis Accident regression test results.

Test Case	Results Description
Test 1	No case-specific differences.
Test 2	No case-specific differences.
Test 3	No case-specific differences.
Test 4	No case-specific differences.
Test 5	No case-specific differences.
Test 6	No case-specific differences.
Test 7	No case-specific differences.

Atmospheric Transport and Dispersion (ATD) Qualification Report
Test Results

Test Case	Results Description
Test 8	No case-specific differences.
Test 9	No case-specific differences.
Test 10	Numerous χ/Q values in the hourly file differ in the last printed digit (0.3 %) from floating-point differences between builds in the plume-rise arithmetic; the reported results agree within 0.0005 %.
Test 11	No case-specific differences.
Test 12	No case-specific differences.
Test 13	No case-specific differences.
Test 14	No case-specific differences.
Test 15	No case-specific differences.
Test 16	Reserved
Test 17	Reserved
Test 18	No case-specific differences.
Test 19	One value in the W sector row of the exclusion area boundary table changes from 4.44E-06 to 4.45E-06 (0.23%) from floating-point differences between builds carried through the terrain interpolation and rounding of the final printed value.
Test 20	Two CFD bins change by 0.01 and 0.03 percentage points, and one value in the S sector row of the low population zone table changes from 1.84E-07 to 1.85E-07 (0.5%), from floating-point differences between builds and rounding of the final printed value.
Test 21	No case-specific differences.

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Results

6.2.3. Routine Release Regression Test Results

Regression tests for the Routine Release module are performed as described in Section 5.8.3. This section documents and addresses the differences between regression testing between ATD version 1.0.3 and version 2.0. It is noted that file paths and dates are expected to be different in outputs and these are not further addressed. Change descriptions described are isolated to the specific change applied as opposed to the integral change of all changes put together to add clarity on what causes a specific change. The following additional items are noted and may differ in all cases, with case-specific differences noted in Table 6-4 as it applies:

ATD output file (*.OUT):

- Informational banner is updated with the latest code and development information. (issue #127)
- Input echo of 'Plume Rise' is added regardless of if it is activated or not; version 1.0.3 printed this line only when plume rise was enabled (true). (issue #145)
- The discrete receptor summary table has a new leading 'LABEL' column carrying the receptor label from the input file, and the remaining columns shift right. (issue #145)
- Input echo field width of 'Vent heat emission rate (cal/s)' is widened to prevent write overflow errors printing values instead of *****. No calculated value changes. (issue #137)
- The 2.26-day decay tables decrease because the 2.26-day half-life is now applied where the previous version applied the 8-day value. The faster decay lowers χ/Q by an amount that grows with travel distance. The annual-average sector values fall by less than 1% at 0.25 mile and by 10–20% at 50 miles, and the discrete-receptor values fall accordingly. The no decay and 8-day decay tables and the deposition (D/Q) values are unchanged. (issue #26)

ATD CFD file (*.CFD):

Atmospheric Transport and Dispersion (ATD) Qualification Report Test Results

- Neither version writes a cumulative frequency distribution for Routine Release. The file contains the informational banner only, so the banner is the only difference.

ATD ERR file (*.ERR):

- No technical change to the printed output. The program compilation date has been added for enhanced traceability.

ATD JFD file (*.JFD):

- No changes.

ATD PLT file (*.PLT):

- Hourly values that version 1.0.3 printed as 0.00E+00 are printed as denormalized numbers, for example 4.90E-44, because the version 2.0 release build no longer flushes denormals to zero. These values are numerically zero.
- The 2.26-day decay column decreases in every case because the 2.26-day half-life is now applied where the previous version applied the 8-day value; individual hourly values fall by 0.1% at 0.25 mile to as much as 34% at 50 miles. The no decay and 8-day decay columns and the deposition (D/Q) column are unchanged. (issue #26)

ATD Output JSON file (*.JSON):

- A 'label' entry is added for each discrete receptor, matching the new output file column.
- Both versions print the JSON values with 17 significant digits. Apart from the 2.26-day decay change, results agree within 0.05% (seventh significant digit; floating-point differences between the v1.0.3 and v2.0 builds, merge request !12) in every case except Test 24; see the table below for details.
- The 2.26-day decay entries decrease as described for the output file (less than 1% at 0.25 mile to 10–20% at 50 miles); the no decay, 8-day decay and D/Q entries are unchanged. (issue #26)

Atmospheric Transport and Dispersion (ATD) Qualification Report
Test Results

Table 6-4. Routine Release regression test results.

Test Case	Results Description
Test 1	No case-specific differences.
Test 2	No case-specific differences.
Test 3	No case-specific differences.
Test 4	No case-specific differences.
Test 5	No case-specific differences.
Test 6	No case-specific differences.
Test 7	No case-specific differences.
Test 8	No case-specific differences.
Test 9	No case-specific differences.
Test 10	No case-specific differences.
Test 11	No case-specific differences.
Test 12	No case-specific differences.
Test 13	No case-specific differences.
Test 14	No case-specific differences.
Test 15	No case-specific differences.
Test 16	No case-specific differences.
Test 17	No case-specific differences.
Test 18	No case-specific differences.
Test 19	No case-specific differences.
Test 20	No case-specific differences.
Test 21	No case-specific differences.
Test 22	No case-specific differences.
Test 23	Reserved
Test 24	With no terrain stations defined (ndist = 0) version 1.0.3 still performed the terrain lookup and applied an uninitialized value to every hour and every receptor. The version 2.0 release build zero-initializes local storage (merge request !12), so no terrain correction is applied, which is the intended result for this input; annual-average χ/Q values change by up to 73% and individual hourly values by more. The Fortran engine still has no explicit test for ndist = 0, so the correct result depends on a build setting rather than on the source code; this is recommended for resolution. (issue #146)

Atmospheric Transport and Dispersion (ATD) Qualification Report
Test Results

Test Case	Results Description
Test 25	Reserved
Test 26	No case-specific differences.
Test 27	No case-specific differences.
Test 28	No case-specific differences.
Test 29	No case-specific differences.

Atmospheric Transport and Dispersion (ATD) Qualification Report Summary/Conclusions

7.0 Summary/Conclusions

The Verification and Validation (V&V) activities for the SIERRA ATD module confirm that the modernization and packaging of the ARCON96, PAVAN, and XOQDOQ legacy code into the SIERRA framework preserving legacy functionality while meeting newly-defined requirements. A comprehensive Requirements Traceability Matrix (RTM) has been established, linking each requirement to specific test cases and acceptance criteria. Verification tests covered input handling, unit consistency, legacy file compatibility, and computational accuracy.

Regression testing against legacy codes demonstrated technical equivalence for the Control Room, DBA, and Routine Release analysis modules, ensuring that modernization efforts did not compromise analytic integrity.

Automated testing integrated using GitLab provides continuous compliance tracking for all requirements. Future work will include regression testing across subsequent SIERRA ATD module releases.

Overall, the module satisfies its intended design and operational objectives, providing a validated and reliable tool.

Atmospheric Transport and Dispersion (ATD) Qualification Report
Electronic Files

8.0 Electronic Files

Table 8-1. Electronic files.

File Name	Checksum (SHA512)
RCD-25-339-0.zip	f803ba8b620679ad4b110d0200b4226c

Atmospheric Transport and Dispersion (ATD) Qualification Report
References

9.0 References

- 9.1. RCD-19-0157, RCD Software Program Manual.
- 9.2. RCD-25-0283, SIERRA Software Project Plan.
- 9.3. RCD-25-0346, Use of Fortran Guidelines.
- 9.4. PNNL-36688, Revision 1, Software Integration for Environment Radiological Release Assessments (SIERRA), Atmospheric Transport and Diffusion Module User's Guide, March 2025.
- 9.5. PNNL-30355 (DRAFT), Revision 1, Software Requirements Document for an Atmospheric Dispersion Engine (Section 4.0), September 2020.
- 9.6. U.S. Nuclear Regulatory Commission. (1977). Regulatory Guide 1.111: Methods for Estimating Atmospheric Transport and Dispersion of Gaseous Effluents in Routine Releases from Light-Water-Cooled Reactors (Rev. 1). Washington, DC: U.S. NRC. Retrieved from <https://www.nrc.gov/docs/ML0037/ML003740354.pdf>
- 9.7. U.S. Nuclear Regulatory Commission. (1983). Regulatory Guide 1.145: Atmospheric Dispersion Models for Potential Accident Consequence Assessments at Nuclear Power Plants (Rev. 1). Washington, DC: U.S. NRC. Retrieved from <https://www.nrc.gov/docs/ML0037/ML003740205.pdf>
- 9.8. U.S. Nuclear Regulatory Commission. (2003). Regulatory Guide 1.194: Atmospheric Relative Concentrations for Control Room Radiological Habitability Assessments at Nuclear Power Plants. Washington, DC: U.S. NRC. Retrieved from <https://www.nrc.gov/docs/ML0315/ML031530505.pdf>
- 9.9. PNNL-36715, SIERRA-STP-001, Revision 2, Software Integration for Environmental Radiological Release Assessments (SIERRA), Atmospheric Transport and Diffusion Module Test Plan, March 2025.
- 9.10. PNNL-36758, SIERRA-STR-001, Revision 2, Software Integration for Environmental Radiological Release Assessments (SIERRA), Atmospheric Transport and Diffusion Module Software Test Record, March 2025.

Atmospheric Transport and Dispersion (ATD) Qualification Report
References

- 9.11. Regulatory Guide 1.23, Revision 1, Meteorological Monitoring Programs for Nuclear Power Plants. U.S. Nuclear Regulatory Commission. Washington, DC. March 2007. (ADAMS Accession No. ML070350028)