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SOFTWARE QUALITY ASSURANCE FOR EMERGENCY RESPONSE CONSEQUENCE ASSESSMENT MODELS AT DOE'S SAVANNAH RIVER SITE

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The Savannah River National Laboratory's (SRNL) Atmospheric Technologies Group develops, maintains, and operates computer-based software applications for use in emergency response consequence assessment at DOE's Savannah River Site. These applications range from straightforward, stand-alone Gaussian dispersion models run with simple meteorological input to complex computational software systems with supporting scripts that simulate highly dynamic atmospheric processes. A software quality assurance program has been developed to ensure appropriate life-cycle management of these software applications. This program was designed to meet fully the overall structure and intent of SRNL's institutional software QA programs, yet remain sufficiently practical to achieve the necessary level of control in a cost-effective manner. A general overview of this program is described.

I. INTRODUCTION

The Savannah River Site (SRS) is an 800 square kilometer (km) reservation in south central South Carolina, approximately 40 kilometers (km) east of Augusta, Georgia. From the 1950s through the early 1990s, the mission of the SRS was the production of nuclear materials for national defense. This mission was fulfilled primarily through the operation of up to five nuclear reactors, two large chemical processing plants, and numerous support facilities.

Although production at most of these facilities has ceased, considerable quantities of high-level nuclear and mixed hazardous wastes that were generated by these production processes remain stored at SRS in large underground tanks. Current operations at SRS include management and disposition of these legacy wastes, as well as activities associated with the maintenance of the nation's tritium stockpiles.

Emergency Planning Hazards Assessments (EPHAs) conducted for SRS operational facilities and production processes indicate that potential releases of radiation and other hazardous materials to the atmosphere could pose a significant hazard to workers and the general public from both the plume exposure and ingestion pathways. To provide an appropriate response to such an event, the SRS has developed a mature emergency planning and preparedness infrastructure[1].

II. CURRENT CAPABILITIES FOR CONSEQUENCE ASSESSMENT

The Weather INformation and Display (WIND) System, developed and operated by the Savannah River National Laboratory (SRNL), provides a comprehensive resource for conducting quantitative assessments of environmental consequence during all phases of emergency response at SRS[2]. The backbone of the WIND System is a cluster of UNIX workstations that are used to gather and archive data from a regional network (mesonet) of meteorological monitoring stations. A suite of transport and dispersion models, developed or adapted by SRNL and available on designated PCs, are run with current observations from the mesonet, and forecasts from the operational runs of a prognostic mesoscale model, to generate real-time predictions of downwind consequences.

Local Meteorological Measurements. The observational mesonet consists of: (1) Towers adjacent to each of the eight major operations areas at SRS that are instrumented to measure winds, turbulence, temperature, and moisture at an elevation of 60 meters above ground level; (2) a TV transmission tower near the SRS that is instrumented to measure wind, temperature, and moisture at several levels through a height of 360 meters above ground level; and (3) four monitoring stations in Augusta/Richmond Co. (GA) that were established under mutual aid agreements with local governments. Every 15 minutes, field observations are transmitted to the UNIX cluster and archived, as noted above.

Meteorological Forecasts. SRNL has adapted and configured a prognostic atmospheric mesoscale model, the Regional Atmospheric Modeling System (RAMS), to generate operational three-dimensional forecasts of meteorological conditions throughout the Central Savannah River area and much of the Southeast U.S.[3] Two real-time forecast data sets are generated: (1) A 6-hour high resolution (2 km grid) forecast of wind speed, direction, turbulence, and other meteorological variables generated every 3 hours for a region encompassing the local Central Savannah River area; and (2) A 36-hour forecast produced every 12 hours for a regional area that includes much of Georgia and South Carolina (10 km grid). Both of the operational model runs use regional observations and upper air data, as well as gridded output from National Weather Service (NWS) operational numerical weather prediction models, for initial and boundary conditions.

Atmospheric Transport and Consequence Assessment Models. A suite of transport and dispersion models are available for assessing consequences of hazardous materials released to the environment. These models, developed or adapted by SRNL, are tailored to support a broad range of assessment needs during the early to intermediate phase of response. All of the consequence assessment models are run from a PC and are configured to automatically access meteorological observations and forecasts. The two principal models used in consequence assessment during emergency response are summarized below.

(1) *Puff/Plume* is a segmented trajectory Gaussian dispersion model that provides a reasonably conservative initial estimate of potential downwind hazards from airborne exposure to chemical or radiological release via inhalation. Puff or plume release trajectories are constructed for up to 12 hours of observed and RAMS forecast winds with results available in less than a minute. Lateral dispersion is based on direct input of turbulence intensity; dispersion in the vertical is based on discrete expressions as a function of stability class. Deposition is determined using a surface depletion model. The model assumes uniform terrain. Model output consists of tabular and graphical displays of concentration, dose and deposition along the release centerline. Dose includes exposure from inhalation and shine from the passing contaminant cloud, as applicable.

(2) The *Lagrangian Particle Dispersion Model (LPDM)* provides refined analyses of transport and dispersion on local to regional scales. LPDM utilizes the full three-dimensional winds forecast by RAMS to account for complex wind patterns due to the effects of terrain or other mesoscale atmospheric phenomena[4]. The position of particles used to represent the release is tracked by solving the Langevin stochastic differential equations of subgrid-scale turbulent velocities, and atmospheric diffusion if modeled by a Markov chain process. Modifications to the original code have been made to incorporate mass removal via radioactive decay and deposition. Output consists of static and animated graphical displays of concentration, dose, and deposition throughout the region surrounding the SRS. Most significantly, the LPDM output provides custom displays of areas exceeding derived response levels (DRL) of isotopic-specific deposition. The DRLs are used for initial assessments of potential impacts via ingestion pathway.

III. SOFTWARE QUALITY ASSURANCE FOR EMERGENCY RESPONSE MODELS

III.A. Overview

Software quality assurance for WIND System software is based on company-level requirements[5] and corresponding SRNL implementing procedures[6]. These requirements, drawn from DOE Orders and Guides[7] and national consensus standards, such as NQA-1, identify the appropriate elements of software life-cycle management, and the implementation of each of these elements, in a graded approach.

All distinct WIND System software (tower data acquisition, database, data display, and consequence and meteorological modeling systems, and accompanying scripts) were subject to initial review and classification with respect to four levels of software significance. Part of the classification process includes an assessment of the software's safety significance, which, in turn, determines one of two distinct tracks that are followed for final classification. Each software application requiring quality control is assigned a unique software identification number and entered into an electronic software inventory database. Database entries include the current software version number, the classification level, the applicable software quality assurance plan (SQAP) document number and a list of software users. Most of the individual WIND System software components included in the review (more than 50) received a classification that required no special controls beyond those identified in a generic SQAP.

Results generated by the Puff/Plume consequence assessment model, described above, are used as primary input for decisions related to emergency classification and initial protective actions for workers and the public from plume exposure; as a result, this software was declared safety significant (as defined in DOE Order 414.1C, safety management and administrative controls) and placed in an SRS electronic inventory list for safety software. As a distinct, stand-alone software package, Puff/Plume is amenable to control through the traditional approaches to software QA that are implemented by these corporate requirements.

Conversely, LPDM results do not have a primary role in decisions having an immediate affect on health and safety. While model output provides useful, early identification of areas potentially exceeding ingestion pathway thresholds (DRLs), comprehensive decisions regarding protective actions and disposition of contaminated food products require confirmatory results from field monitoring; therefore, LPDM was not classified as safety significant. The LPDM software is part of a complex software system that includes RAMS, and numerous scripts supporting execution of RAMS and LPDM through the processing of input and output data streams. The inherent complexity of these types of software systems, both in terms of the number of interrelated software components and the dynamic, complex physical processes simulated by the algorithms, requires a more holistic approach to software QA than is traditionally prescribed.

III.B. SQA for Puff/Plume

Puff/Plume is legacy software developed at SRNL that was subsequently incorporated into the current software QA structure as existing code. An application-specific SQAP was developed to establish an application baseline and manage the code through the 'operations and maintenance' phase of the software life cycle[8].

Code Baseline. The Puff/Plume baseline consisted of a thorough model evaluation and code verification for up to seven performance criteria including centerline location of a puff or plume, concentration (peak and average), and (two-sigma) width of the puff or plume.[9] Evaluations for each of these performance criteria were conducted for:

1. A comparison of model results against analytic solutions to verify that the theoretical puff or plume characteristics are being calculated by the code correctly.[10]
2. A comparison of model results to field data collected during a series of sulfur-hexaflouride tracer experiments conducted at SRS to define a performance basis under actual meteorological conditions. [11]
3. A comparison of model results against other widely-accepted dispersion models. [12]
4. A comparison of model results against field monitoring data collected during past off-normal releases from SRS operational facilities.

An additional series of comparisons were conducted for the Windows-OS compiled version the code (with graphical user interface) with versions run on earlier operating systems (i.e., VMS)[13].

Configuration Management. The production version of the code is maintained: (1) electronically in a location managed by a designated Software Administrator for installation on client PCs; and (2), on a CD that resides in a change control history file. The CDs that are archived in the history file for each version of the code permit earlier versions of the code to be recovered, as needed. The history file also documents the hierarchical structure of all directories and files that comprise the installed version of the code. An user manual is also maintained, although most users at SRS have significant experience with the code's operation.

Proposed modifications to the code are formally approved by a responsible technical lead and assigned a modification reference number that is placed on the software modification package cover sheet. The code to be modified is provided to the developer by the Software Administrator. This transaction is documented and placed in the change control history file. Once the modification is approved, a new production version is assigned and entered into the SRNL software inventory database.

Ongoing Lifecycle Activities. Major revisions to the code are documented in the QA history file. Test and evaluation plans identify code modules and variables affected by the modification, summarize the results of tests to ensure the modifications were applied appropriately, and summarize the impact of the changes on model results. Test runs are targeted in a way that demonstrates the adequacy of the specific changes. Additional generic runs are performed to ensure the changes did not have unintended impacts on previous baseline results.

III.C. SQA for RAMS/LPDM

Both RAMS and LPDM software was obtained as 'commercial off-the-shelf' (COTS) software from the Aster Division of Mission Research Corporation. Quality assurance of this software system has been achieved primarily through establishing a thorough operational baseline for specific system components (e.g., RAMS or LPDM) that includes a documented in-depth analysis of the governing equations and code framework[14,15], and verification of acceptable performance of the modeling system through sustained operational use.

The performance baseline for the SRNL implementation of RAMS/LPDM software system has been demonstrated as follows:

(1) In addition to utilizing operational RAMS forecasts for emergency response, model output has been used extensively since 1998 to prepare daily weather forecasts supporting SRS operations and prescribed fire planning for surrounding woodland areas. As part of the forecast process, RAMS output is routinely assessed with respect to forecasts from NWS numerical weather prediction models and local observations. Such routine use has provided a high level of confidence that RAMS output is reliable for a wide range of meteorological situations, and allows for identification of situations where RAMS performance may be enhanced through improved parameterizations.

(2) A formal statistical comparison of RAMS forecasts to NWS and onsite tower observations.[16] This study, based on a comparison period of up to two years, concluded that RAMS provided realistic results with skill, including turbulence quantities used as input for LPDM.

(3) Application of RAMS to reproduce successfully unique mesoscale wind phenomenon such as sea breeze fronts that penetrate inland over South Carolina and have significant affect on local transport and dispersion. [17, 18]

(4) Application of RAMS/LPDM in tracer studies sponsored by the European Union (ETEX and Ensemble)[19,20]. An example of SRNL's modeling system performance is illustrated in Figure 1, which depicts results from an Ensemble experiment for a simulated release of Cs-137 over a 6 hour period from Nantes in northwestern France. Eleven modeling systems from nine countries were run in real time. Results illustrated in Fig. 1 depict the percent of models that predicted a time-integrated surface concentration equal or above the threshold of 1 Bq/m3. The SRNL results, shown by the red cross-hatch, indicate performance that agrees very well with the model ensemble consensus.

Configuration Management. Executables for operational execution of RAMS and LPDM and the scripts used to (1) initiate model runs (2) process input data (regional surface observations and NWS forecast model GRIB files), and (3) process data for output and display, have been cataloged and placed in a documented directory structure on designated operational computer systems.[21] These scripts are designed to minimize references to specific computer names and drive letters which provides easier transition to changes in computer systems.

Modifications to production versions of the operating codes and scripts are performed by one of two designated technical leads for operations. These individuals are responsible for testing the changes to ensure successful implementation of the modification and placing the modified software into operational directories.

IV. CONCLUSIONS

SRNL has developed a software quality assurance program to ensure appropriate life-cycle management of software applications used for consequence assessment during emergency response. These applications range from straightforward, stand-alone Gaussian dispersion models run with simple meteorological input to complex computational software systems with supporting scripts that simulate highly dynamic atmospheric processes. As a result the SQA program was tailored to the practical attributes of the particular application, yet conforms to the overall structure and intent of SRNL's institutional software QA programs in a reasonably cost-effective manner.

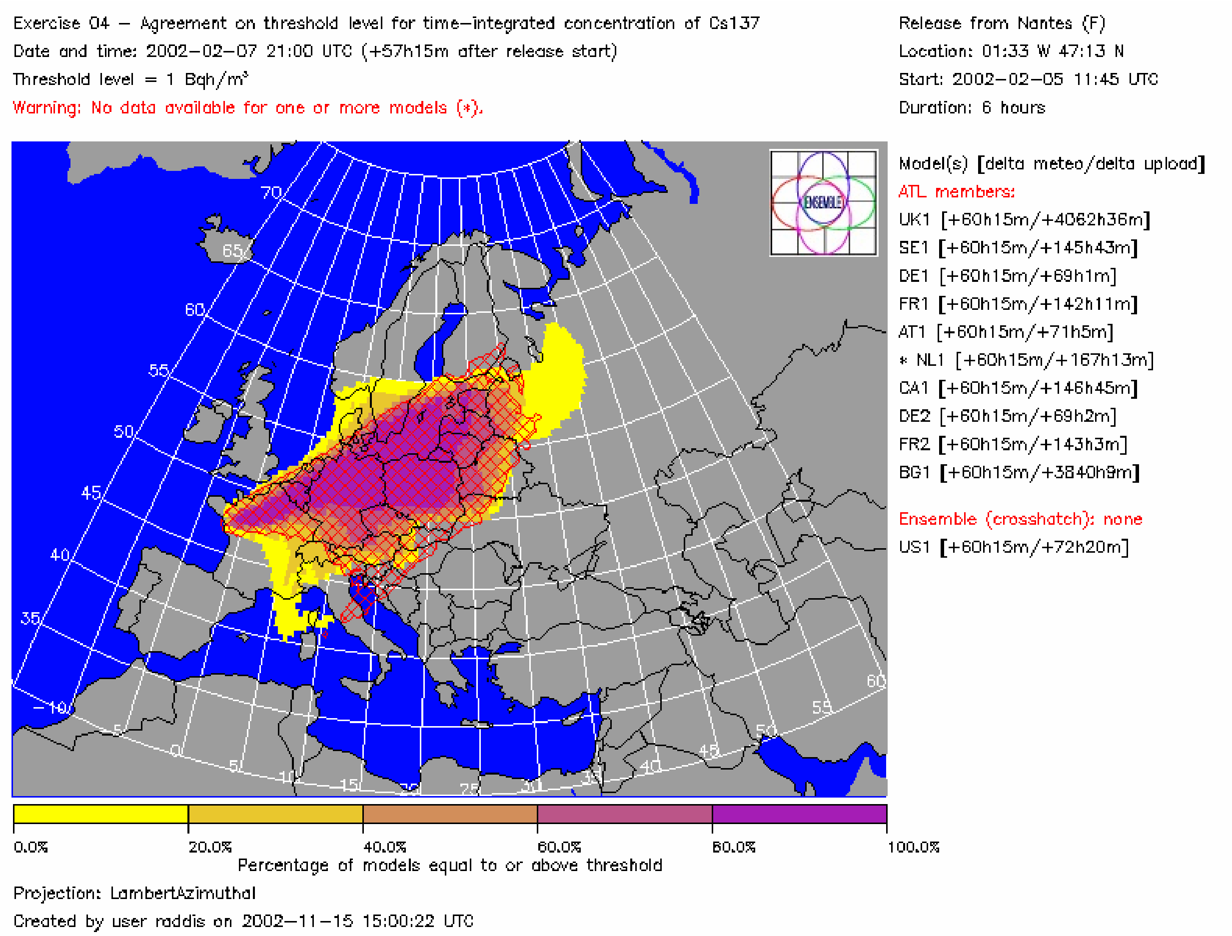

Fig. 1. Ensemble results for a release of Cs-137 from Nantes, France on November 15, 2002. Color contours show the percent of models producing an time integrated concentration of 1 Bq/m3. The SRNL run of RAMS/LPDM is indicated by the red hatching.

V. REFERENCES

1. Washington Savannah River Company, *Savannah River Site Emergency Plan,* WSRC-SCD-7, Aiken, SC (2007).

2. C. H. Hunter, *The Weather INformation and Display System,* Publication 05A00978-01, Westinghouse Savannah River Company, Aiken SC (2005).

3. R. A. Pielke, et al., *A Comprehensive Meteorological Modeling System – RAMS*, Meteor. Atmos. Phys., 49, 69-91 (1992).

4. M. Uliasz, *The Atmospheric Mesoscale Dispersion Modeling System*, J.Appl. Meteor., 32, 139-149 (1993)

5. Washington Savannah River Company, *Software Quality Assurance*, Manual 1Q – Procedure 20-1, Aiken SC (2003).

6. Savannah River National Laboratory, *Software Classification Guidance Document*, SRNL-ESB-2006-00008, Washington Savannah River Company, Aiken SC (2006).

7. U. S. Department of Energy, *Safety Software Guide for use with 10 CFR Part 830 Subpart A, Quality Assurance Requirements, and DOE Order 414.1C, Quality Assurance*, DOE G 414.1-4 (Draft), Washington DC (2007)

8. C. H. Hunter, *Software Quality Assurance Plan for the Puff/Plume Software Package*, C-SQP-G-00073, Westinghouse Savannah River Company, Aiken SC (2002).

9. J. D. Fast, *Evaluation Protocol for the WIND System Atmospheric Models*, WSRC-RP-91-426, Westinghouse Savannah River Company, Aiken SC (1991).

10. J. D. Fast, Evaluation of the WIND System Models: An Analytic Approach, WSRC-RP-91-1208, Westinghouse Savannah River Company, Aiken SC (1991).

11. J. D. Fast, *A Comparison of the WIND System Atmospheric Models and MATS Data*, WSRC-RP-91-1209, Westinghouse Savannah River Company, Aiken SC (1991).

12. J. D. Fast, *A Comparison of the WIND System Atmospheric Models and RASCAL*, WSRC-RP-91-894, Westinghouse Savannah River Company, Aiken SC (1991).

13. R. J. Kurzeja, *Puff/Plume, the SRTC Atmospheric Deposition Model: Baseline Documentation for WINDOWS NT*, WSRC-TR-98-00360, Westinghouse Savannah River Company, Aiken SC (1998).

14. K. Chen, *Regional Atmospheric Modeling System (RAMS) Technical Description*, WSRC-TR-2005-00499, Washington Savannah River Company, Aiken SC (2005).

15. K. Chen, *Lagrangian Particle Dispersion Model (LPDM) Technical Description*, WSRC-STI-2006-00058, Washington Savannah River Company, Aiken SC (2006).

16. R. L. Buckley, et. al., *Statistical Comparison of Regional Atmospheric Modeling System Forecast Meteorology with Observations*, WSRC-TR-2001-00563, Westinghouse Savannah River Company, Aiken SC (2001).

17. R. L. Buckley and R. J. Kurzeja, *An Observational and Numerical Study of the Nocturnal Sea Breeze. Part I: Structure and Circulation*, Journal of Applied Meteorology, 36(12), 1577-1589 (1997).

18. R. L. Buckley and R. J. Kurzeja, *An Observational and Numerical Study of the Nocturnal sea Breeze. Part II: Chemical Transport,* J Appl. Meteor., 36(12), 1577-1589 (1997).

19. S. Galmarini, et. al., *Ensemble Dispersion Forecasting, Part I: Concept, Approach, and Indicators*, Atmospheric Environment, 38, 4607-4617 (2004).

20. S. Galmarini, et. al., *Ensemble Dispersion Forecasting, Part II: Application and Evaluation,* Atmospheric Environment, 38, 4607-4617 (2004).

21. R. L. Buckley, *Utilization of Automated Scripts in the Atmospheric Technologies Group Meteorological Forecasting Program*, WSRC-IM-2002-00015, Westinghouse Savannah River Company (2002).