Development of the Simplified Radionuclide Transport (SRT) Code Version 2.0 for Versatile Test Reactor (VTR) Mechanistic Source Term Calculations

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DEVELOPMENT OF THE SIMPLIFIED RADIONUCLIDE TRANSPORT (SRT) CODE VERSION 2.0 FOR VERSATILE TEST REACTOR (VTR) MECHANISTIC SOURCE TERM CALCULATIONS

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Abstract

The Versatile Test Reactor (VTR) is a fast spectrum test reactor currently being developed in the United States under the direction of the US Department of Energy (USDOE), Office of Nuclear Energy. The mission of the VTR is to enable accelerated testing of advanced reactor fuels and materials required for advanced reactor technologies. The conceptual design of the 300 MW(th) sodium-cooled metallic-fueled pool-type fast reactor has been led by US National Laboratories in collaboration with General Electric-Hitachi and Bechtel National Inc.

The VTR is utilizing a risk-informed performance-based approach for authorization by the USDOE. As part of this approach, the development of a mechanistic source term (MST), or a realistic evaluation of radionuclide transport and release for specific transient scenarios, is central to developing an accurate representation of reactor risk. A new version of the Argonne National Laboratory Simplified Radionuclide Transport (SRT) code has been developed to support VTR MST analyses.

The SRT code is an integral sodium fast reactor radionuclide transport analysis tool, which assesses radionuclide movement from the reactor fuel to the environment. The code includes models for phenomena associated with radionuclide behavior within the fuel pins, release from failed fuel, migration through the sodium pool, and behavior in the cover gas region and containment. SRT is purposefully designed to facilitate sensitivity and uncertainty analyses with offsite consequences as the metric of interest.

For VTR, version 2.0 of the code was established to fulfill quality assurance requirements associated with the project. These efforts included updating and expanding the suite of verification and validation test cases, extension of the code models for the demonstration of code accuracy, and revisions to code software quality assurance documentation. This paper provides a summary of these activities along with a sample of analysis cases utilizing the new version of the code. The work reported in this summary is the result of studies supporting a VTR conceptual design, cost, and schedule estimate for DOE-NE to make a decision on procurement. As such, it is preliminary.

1. INTRODUCTION

The development of a mechanistic source term (MST), which is the assessment of potential radionuclide (RN) release to the environment utilizing realistic phenomena, models, and data, is central to understanding the possible consequences of reactor transient scenarios. As part of recent efforts centered on the development of an MST for sodium fast reactors (SFRs), Argonne National Laboratory (Argonne) developed the Simplified Radionuclide Transport (SRT) code with support from the US Department of Energy (USDOE) and TerraPower. The goal of SRT is to perform MST analyses for SFRs, while also providing the capabilities to execute rapid uncertainty and sensitivity analyses to identify influential phenomena and inputs.

Currently, SRT is being utilized to perform MST analyses as part of the design and authorization of the Versatile Test Reactor (VTR) being developed by the US Department of Energy (USDOE) Office of Nuclear Energy. As an important tool in the establishment of the VTR safety basis, several improvements were made to SRT to increase capabilities and expand code verification and validation. Based on these enhancements, a new version of the code (version 2.0) was established and released [1]. The following sections contain a brief description of important SFR source term phenomena, before providing an overview of SRT, its models, recent improvements, and an example analysis.

2. BACKGROUND

In regard to advanced reactor licensing, the US Nuclear Regulatory Commission (USNRC) has repeatedly stated an expectation that MST analyses will be part of future application submittals [2, 3]. As the MST analysis is likely to play a central role in future SFR licensing, Argonne conducted several studies into SFR MST analyses in recent years [4-6]. The focus of these investigations was on metal-fuel pool-type SFRs, as those are the most common designs among US industry. There were several key findings from these studies. First, SFRs have multiple barriers to the release of RNs, which can essentially be assessed in series. Figure 1 provides a conceptual overview of the barriers to RN release for a core damage event, including the RN transport and retention phenomena at each stage. The second major finding was that the US currently had no single computational tool capable of assessing RN behavior from the point of fuel damage to potential release to the environment. Lastly, the studies identified uncertainties related to RN transport and retention phenomena, which could be reduced with future research, but the importance of the uncertainties could be dependent on the specific reactor design.

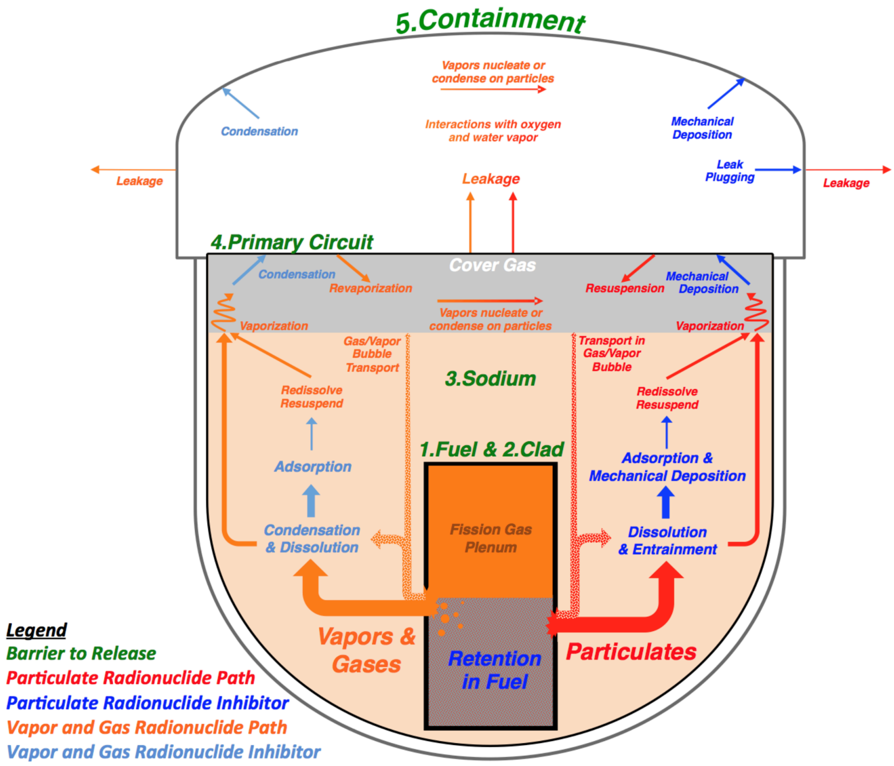

FIG. 1. SFR Radionuclide Barriers and Transport and Retention Phenomena [4]

As a result of these findings and the immediate needs of projects at the time, such as the modernization of the GE-Hitachi PRISM probabilistic risk analysis [7, 8], a computational tool (SRT) was developed that provides an integral analysis of RN release and transport for metal-fuel pool-type SFRs. In addition, SRT was designed to facilitate uncertainty and sensitivity analyses, as part of the identification of influential uncertainties. Initial versions were developed for internal Argonne use, while subsequent support from TerraPower allowed the creation of a version for external release. SRT is licensed by Argonne and questions regarding code licensing can be addressed to the authors.

3. SRT OVERVIEW AND CALCULATION PROCESS

SRT assesses RN release and transport for metal-fuel pool-type SFR systems and metal fuel microreactor designs (with a focus on the SFR modeling capabilities for the current work). As the purpose of the SRT code is to rapidly perform uncertainty/sensitivity analyses to determine the importance of RN transport factors, the models utilized to assess RN transport and retention phenomena are highly customizable and heavily dependent on user input. As shown in Figure 2, SRT does not model reactor transient behavior. Therefore, the timing of fuel pin failure and the conditions associated with failure, such as fuel temperature, percentage of molten fuel, and sodium pool/reactor vessel temperature, must be supplied by the user. This information can be based on the results of other analysis codes, such as SAS4A/SASSYS-1 [9], or created by the user. SRT utilizes this information to determine the magnitude and timing of RN release from the fuel and the impact on RN transport/retention. The main outputs of SRT are the time-dependent RN inventories within the reactor system and the environment and associated dose values.

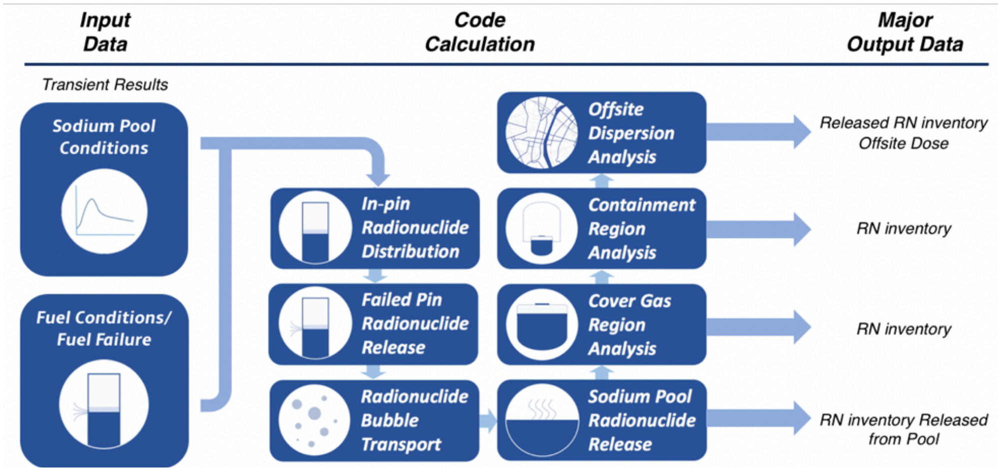

FIG. 2. Overview of SRT Input, Calculation, and Output for SFR Calculation [1]

SRT performs a time-dependent RN transportation calculation utilizing a user-specified timestep. At its core, SRT is a compartment model that simulates the transport and retention of RNs within different volumes coupled with additional models to assess RN release from fuel and transport within a sodium pool. User-supplied information regarding fuel and sodium pool/reactor vessel conditions is used to perform the calculation. The code is capable of tracking 770 isotopes of the 32 elements outlined in Table 1. This includes stable isotopes, as they may impact chemical behavior through the RN transport and retention process. SRT accounts for radioactive decay of all RN isotopes and the birth of daughter products for certain short-lived noble gases.

TABLE 1. Elements Tracked by SRT

Elements		
Kr	Eu	Pr
Xe	Ru	Sm
I	Rh	Y
Br	Pd	Cm
Cs	Mo	Am
Rb	Tc	Ce
Te	Co	Np
Sb	La	Pu
Se	Zr	U
Ba	Nd	Na
Sr	Pm	

To facilitate uncertainty and sensitivity analyses, almost all inputs to SRT can be identified as uncertainties with specified distributions (uniform, log-uniform, normal, lognormal, and binomial). The user can then select for the code to perform multiple iterations, which are repeat calculations utilizing newly sampled values from the uncertainty distributions. Figure 3 outlines the inputs, outputs, and execution structure of SRT, including the creation of multiple iterations and outputs describing both individual iterations and summary data. As part of the summary data, SRT conducts importance measure calculations on the input uncertainties, including Kendall and Pearson correlation coefficients.

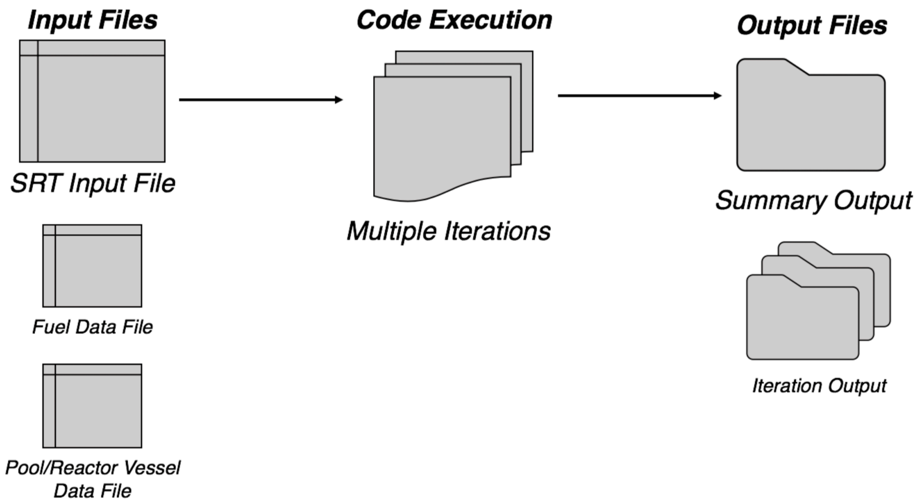

Fig. 3. SRT Input, Output, and Code Iteration Structure [1]

SRT is written in the R programming language, which is an interpreted language that does not require compiling. Selection of the R language was based on several factors. First, R is primarily a statistical analysis tool, which contains many built-in statistical and graphical data analysis tools. Second, the use of an interpreted language allows users to access source code, including the individual code functions, which permits modifications and the development of new models by the user. SRT utilizes text input files and can be executed from the command line.

4. SRT MODELS AND CODE IMPROVEMENTS

As highlighted in Section 3, SRT is an integral MST analysis tool that contains models for RN release, transport, and retention from the reactor fuel to the environment. Table 2 outlines the main phenomena modeled by the code. The following subsections describe the main solution methodology of the code and the individual phenomena models. This includes improvements to the code made as part of the release of version 2.0.

TABLE 2. Phenomena Modeled by SRT

Phenomena	**Description**
In-pin RN migration	Migration of RNs from the fuel matrix to the bond sodium and fission gas plenum during irradiation
RN release from failed fuel	RN release from the fuel pin (fuel matrix, bond sodium, and fission gas plenum) with cladding breach
RN bubble transport	RN transport through the sodium pool within vapor/gas bubbles
RN vaporization from sodium pool	RN vaporization from the sodium hot pool to the cover gas region
RN behavior in cover gas region	RN vapor/gas and aerosol behavior in the cover gas region
RN behavior in containment	RN vapor/gas and aerosol behavior in the containment
Offsite dispersion and dose	Offsite dispersion of RNs and the predicted dose to individuals

4.1. Solution Methodology

SRT is primarily a compartment model that simulates RN transport and retention within different volumes. A time-dependent solution to the compartment model is solved using a time-step specified by the user, which can vary from one second to one hour. SRT first determines RN releases from the fuel before performing the compartment model calculation. This methodology is possible as RN release from the fuel is not impacted by RN behavior in the rest of the reactor system. Both analytical and numerical solvers to the system of ordinary differential equations are included within the code to assist with code verification. In addition, the numerical solver allows additional RN release modeling flexibility but is generally slower than the analytical solver. For example, using the analytical model RN releases from the fuel are assumed to occur instantaneously at the start of the time-step (a bolus input in compartment modeling terminology), while the numerical model also permits the utilization of a distributed release throughout the time-step.

4.2. In-Pin Radionuclide Migration and Fuel Pin Radionuclide Release

The first phenomenon addressed by SRT is RN migration within the fuel pin during irradiation and prior to cladding failure. The migration of RNs is important as it determines the RN inventory within the fuel pin fission gas plenum and bond sodium, which are likely available for release with cladding failure. In SRT, RN migration is assumed to be directly dependent on fuel burnup level, as this was identified as a major factor during a recent Argonne study on metal fuel RN release [5]. The extent of RN migration from the fuel matrix to the bond sodium/fission gas plenum is determined based on linear interpolation utilizing user input for each element and designated fuel burnup levels.

With the occurrence of cladding failure, RN release from failed fuel pins depends on three factors: RN migration fraction during irradiation, fuel temperature, and the molten percentage of the fuel. First, when fuel pin failure occurs, it is assumed that all RNs that have migrated to the bond sodium/fission gas plenum are instantaneously released. However, additional RN releases from the fuel matrix may also occur, either at the same time as fuel pin failure or at a later time. The RN release from the fuel matrix depends on the fuel temperature and the molten percentage. These calculations also depend on user-supplied tables concerning RN release with temperature. These modeling choices were also made based on the findings of the recent Argonne study on metal fuel RN release [5].

4.3. Bubble Transport

RNs released from failed fuel may form a vapor/gas bubble within the primary sodium coolant. In addition to RN vapors/gases, other RN aerosols may become entrained within the bubbles and could be transported to the cover gas region, effectively bypassing the sodium pool. Within the code, a bubble is assumed to be created only during initial cladding breach of the fuel pin, when the largest concentration of noble gas release is likely to occur. All subsequent RN releases from a failed fuel pin are assumed to directly enter the sodium pool. There are two bubble transport models available in the code: the simple model and the detailed model. In the simple model, the user specifies a bubble decontamination factor (DF), which is the ratio of aerosol mass entering the bubble to the aerosol mass exiting the bubble once it reaches the cover gas region. The detailed bubble model performs a mechanistic calculation of aerosol removal based on classical pool scrubbing theories and includes condensation, Brownian diffusion, inertial deposition, and gravitational sedimentation. Additional information on the calculation performed by the detailed bubble model can be found in ref [10].

4.4. Pool Vaporization

RNs may also enter the cover gas region due to vaporization from the sodium pool. Perfect mixing is assumed for RNs within the sodium pool. Specifically, thermodynamic equilibrium is assumed to be achieved between the cover gas region and the sodium pool for each timestep of the calculation. This is thought to be a conservative assumption, as equilibrium will likely maximize the amount of RNs present in the cover gas region but typically takes an extended period of time to occur. As part of this assumption, the cover gas temperature is conservatively assumed to be at the same temperature as the sodium pool.

SRT utilizes RN vaporization response surfaces that were developed utilizing HSC Chemistry [11]. Based on the temperature of the sodium pool/cover gas region and the mass of the sodium pool, the response surfaces determine the fraction of each element that should be present within the cover gas region as a gas/vapor, assuming thermodynamic equilibrium. Different response surface functions are utilized for different temperature ranges. The HSC Chemistry calculations utilized a custom thermodynamic database that was developed by Argonne as part of past SFR source term efforts [6].

4.5. Cover Gas Region and Containment

Within the cover gas region and containment, RNs may exist as a gas/vapor or as aerosols. Based on user-specified options, RNs may transition between the two classes. For example, NaI aerosols may exist within the cover gas region but may dissociate to sodium oxide aerosol and iodine gas within the containment due to the presence of oxygen. Maximum flexibility is provided to the user to explore the impact of such phenomena.

Those RNs in the aerosol class may deposit on the sodium pool (in the cover gas region) or other surfaces. Exponential decay is utilized to model aerosol deposition, with multiple options available to the user for the determination of removal rates (decay constants). First, constant removal rates can be specified by the user, with different removal rates possible for each element modeled by the code. Second, a customizable power function can be used to calculate removal rates based on the aerosol mass concentration within the volume. Lastly, the "Henry" correlation is available, which determines removal rates using correlations developed for sodium oxide aerosols based on the results of the ABCOVE sodium fire experiments [12, 13]. In addition, minimum aerosol concentrations can be specified, below which aerosol deposition is halted.

To determine the transport of RNs from the cover gas region to containment and from containment to the environment, user-specified volumetric leakage rates are used. As perfect mixing is assumed to occur within both the cover gas region and containment, the volumetric leakage rates directly translate to RN mass leakage rates.

4.6. Consequence Modeling

SRT provides two options for the assessment of onsite or offsite consequence. First, the RN masses released to the environment are provided as outputs by SRT and can be utilized within detailed consequence codes such as MACCS [14]. In addition, SRT provides an internal dose calculation utilizing user-specified χ/Q and breathing rate values. Based on this information, SRT calculates whole body dose, thyroid dose, and total effective dose equivalent (TEDE) utilizing dose conversion factors (DCFs) from US Federal Guidance Reports 11 and 12 [15, 16] (the user may also specify custom DCFs).

4.7. Software Quality Assurance

A major part of the development of SRT version 2.0 has been the expansion and improvement of SRT's software quality assurance (SQA) program to align with the expectations of the VTR authorization (USDOE). This has included the transition to a formal version control and change approval system and significant updates to the code's SQA documentation. The latter task has involved the creation of detailed code verification and validation documents. The SRT requirements verification document provides an assessment of the code's capabilities versus the designated software requirements. In addition, a verification test suite has been created that performs verification calculations for each function within the code and integral code tests. The verification test suite is available to SRT licensees and can be used as a regression test when the code is installed on new systems or when changes are made to the source code (as is possible since SRT is distributed in an interpreted programming language).

Significant effort has also been made in establishing the validation case for the code. As SRT simulates a variety of phenomena, with models ranging from mechanistic to user input-driven, the validation case is complex. For some models, validation focuses on supporting the appropriateness of the underlying assumptions, such as the use of burnup-dependent functions for the determination of in-pin RN migration. Other models include quantitative comparisons to experimental results, as is done with the detailed bubble transport model [17]. The validation of the individual code models/functions is especially important given the general lack of a suitable integral validation case.

5. EXAMPLE ANALYSIS

As a demonstration of the capabilities of SRT, an example analysis is provided here. It is important to note that this example is not representative of the VTR design or potential VTR transient sequences but is included here simply as a display of the code's functionality and outputs. The problem is not the result of a detailed transient analysis but a postulated fuel failure and melting transient.

The description of the example reactor system is presented in Table 3. The core is divided into four fuel batches at different burnup levels, with 217 pins per assembly. The postulated transient is described in Table 4 and involves a rapid heat-up of the core fuel, exceeding the fuel melting point. The cover gas and containment leakage rates are treated as uncertainties, as are many RN transport characteristics not outlined in the table, such as in-pin migration fractions, fuel pin release fractions, bubble characteristics, and aerosol deposition options. For this example, the "Henry" aerosol deposition model was selected. To assess these uncertainties, 250 code iterations were performed.

TABLE 3. Example Problem Reactor Description

Parameter	Value
Reactor Power	500MWth
Reactor Fuel	U-Pu-Zr
Core Fuel Batches and Burnup	4 Batches (60 assemblies per batch), Burnup: 2,4,6,8%
Fuel Pins Per Assembly	217
Pool Depth	~5m (Pool top to top of active core)
Cover Gas Volume	50m^3
Containment Volume	1000m^3
Sodium Pool Volume	250m^3

TABLE 4. Example Problem Transient Description

Parameter	Value or Description
Transient	Postulated fuel failure and melting scenario (not based on a realistic event sequence)
Fuel Batch Failure Times (and Max Temperatures)	1: No Failure 2: 3.5 minutes (~1350 °C) 3: 1.5 minutes (~1250 °C) 4: 0.5 minutes (~1200 °C)
Max Pool Temperature	650°C at time = 5 minutes
Cover Gas Leakage Rate	Normal Distribution (μ, σ): (0.1, 0.05) vol % per day
Containment Leakage Rate	Normal Distribution (μ, σ): (1.0, 0.5) vol % per day
χ/Q	1E-4 sec/m^3
Code iterations	250
Other input uncertainties	RN in-pin migration and release fractions, bubble characteristics, RN vaporization multipliers, aerosol deposition options, RN dissociation characteristics (physical class changes)

Figure 4 presents summary results for the 250 code iterations in the form of a TEDE cumulative distribution function (CDF). The analysis resulted in a mean TEDE value of 5.2E-4 rem, with 5%/95% values of 6.9E-5 and 1.2E-3 rem. Figure 5 contains an example output from one of the code iterations. This plot contains the time-dependent RN inventory within the cover gas region, including both vapor/gases and aerosols. As the plot shows, many of the RN elements are in the aerosol form and quickly deposit back into the sodium pool or onto other structures within the cover gas region. This process rapidly reduces their inventory in the cover gas region. For the RN elements that are present in the vapor/gas state (at least partially), such as Kr, I, and Cs, they remain within the cover gas region and are available for further transport to the containment through reactor head leakage.

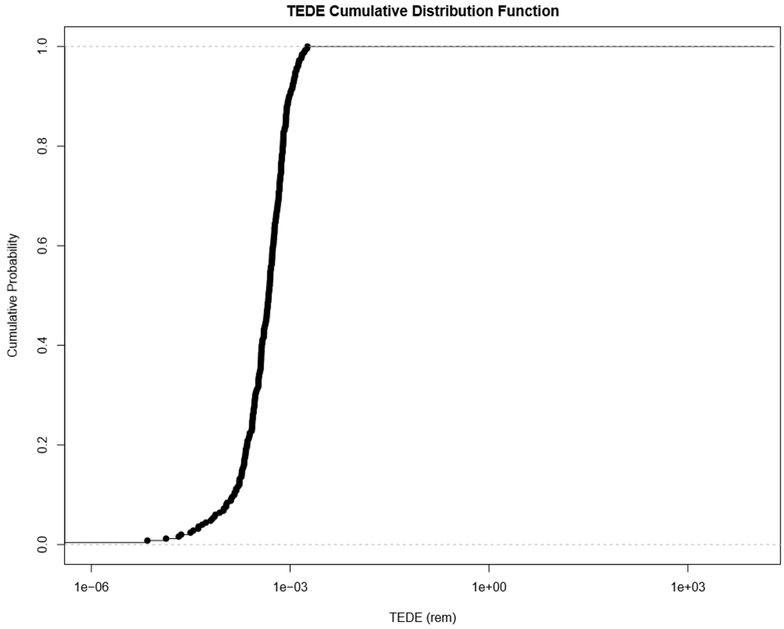

Fig. 4. Example SRT Analysis – TEDE CDF

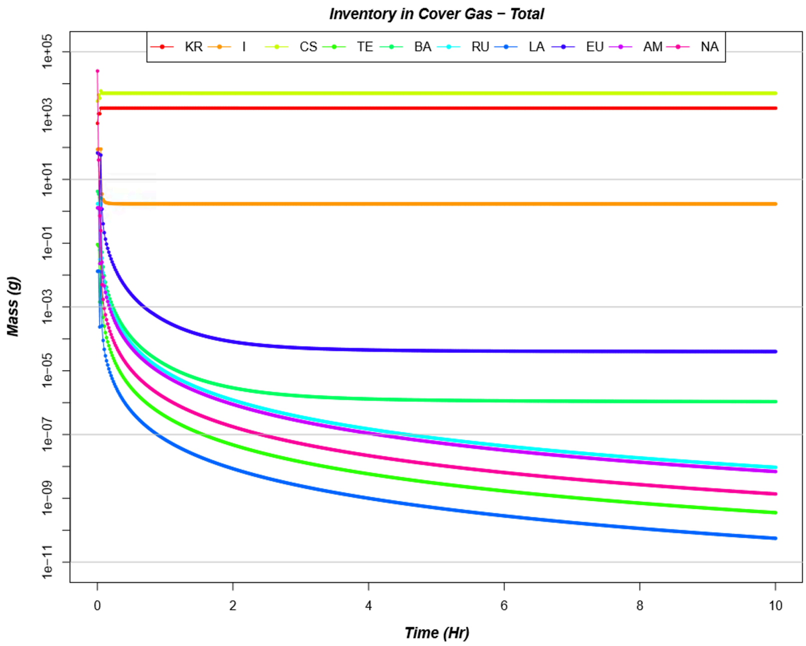

Fig. 5. Example SRT Analysis – Inventory in Cover Gas for Specific Iteration

Figure 6 contains another example output from one of the code iterations, which highlights the fractional release of individual isotopes. This plot illustrates the inventory of the RN isotope available at each stage of the RN transport process. Such information is useful in determining what phenomena were most influential in RN retention. For example, cesium isotopes were largely retained within the primary sodium pool and cover gas region. For this plot, surrogate TEDE values are utilized for each phase using point source χ/Q values to provide a point of comparison to the final location of interest (referenced as “offsite dose” in the figure).

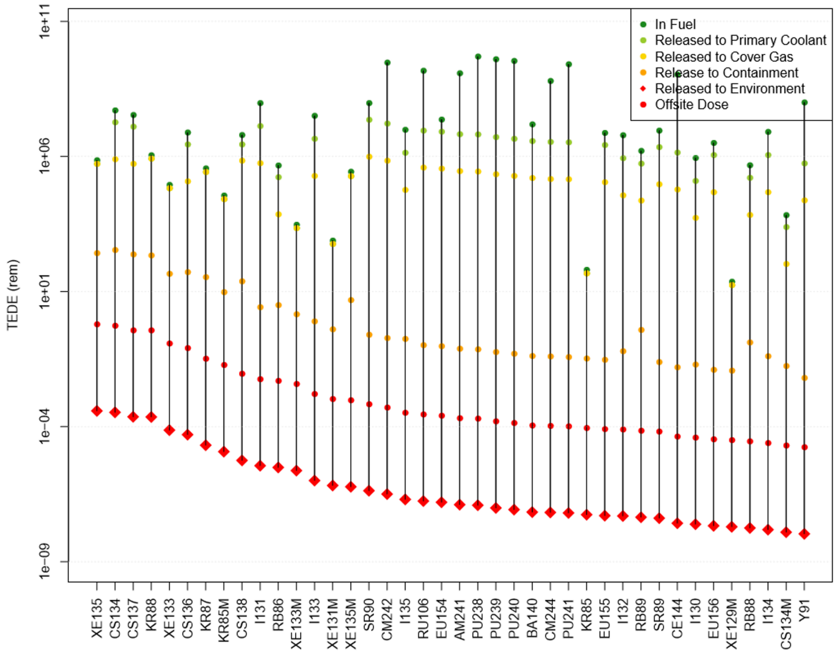

Fig. 6. Example SRT Analysis – Fractional Release Plot for Specific Iteration

Figure 7 contains Pearson correlation coefficient values for all 250 iterations. This analysis examines the correlation between offsite TEDE and the uncertain input values. As the results show, the greatest correlation was found to be with the cover gas region and containment leakage values (*leakage.cg* and *leakage.cont*). Other potentially impactful input variables were the assumed aerosol fall height in containment (*aerosol.height.cont*), the aerosol particle diameter within fission product bubbles in the sodium (*d.par*), and fraction of cesium and rubidium that was in the vapor/gas form when entering containment (*vapor.unc[Cs/Rb]*). As the Pearson correlation coefficient is a measure of linear correlation, Kendall rank correlation coefficients are also provided by the code to assist in identifying non-linear correlations.

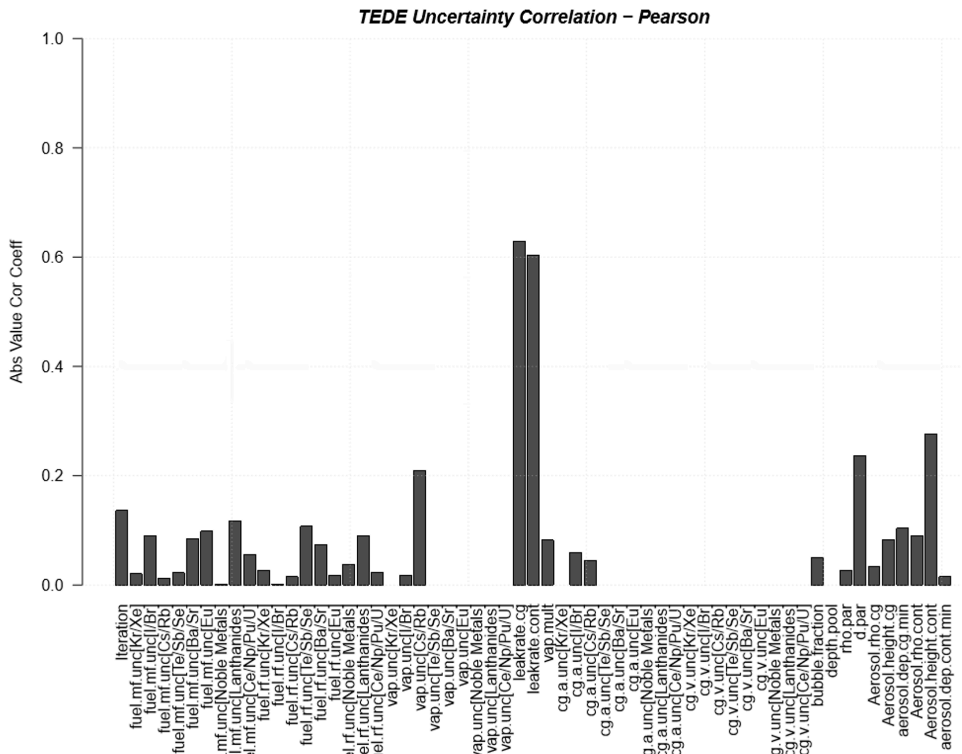

Fig. 7. Example SRT Analysis – Pearson Correlation Coefficient Values

6. CONCLUSIONS

Mechanistic source term evaluations are an important part of advanced reactor development, such as with the USDOE VTR design, due to their role within risk-informed design and authorization processes. For VTR, the SRT code developed by Argonne is utilized for the source term assessment of potential core damage event sequences. As part of its role within the VTR authorization safety case, improvements have been made to SRT, including model development and enhancements to the code's SQA program. SRT version 2.0 has now been formally released and is available to licensees of the code.

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