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DEMONSTRATION OF MACCS CAPABILITIES FOR ADVANCED REACTORS: NORMALIZED DOSE ASSESSMENT AND RADIONUCLIDE SENSITIVITY ANALYSIS FOR A HIGH TEMPERATURE GAS REACTOR MECHANISTIC SOURCE TERM

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ABSTRACT

Consequence analysis for non-LWR accidents is an evolving field and is dependent on the fidelity of mechanistic source term models. This study examines an approach to perform an initial dose assessment over distance, which could then be further analyzed to determine health and economic consequences as the fidelity of mechanistic source term models for non-LWRs further evolve. This study utilizes a preliminary mechanistic source term for a Pebble Bed Modular Reactor developed in MELCOR, and subsequently models the atmospheric transport and dispersion of the released material using the MELCOR Accident Consequence Code System (MACCS). Normalized results for scaled reactor core inventories are compared with the effects of evacuation, and the key contributors and sensitivities of the dose assessment are described in terms of chemical groups. It is the goal of this work to contribute to consequence analysis methods for non-LWRs, inform priorities for mechanistic source term models in terms of the relative importance of the chemical groups, and inform government regulations for non-LWRs.

Key Words: MACCS, Source Term, HTGR

1. INTRODUCTION

As advanced reactor designs are maturing and their designers are embarking on the licensing process within the United States and across the world, there is great interest in characterizing severe accident scenarios associated with non-Light Water Reactor (LWR) designs and their associated consequences. Using state of the art computer codes, this paper outlines an approach to performing an initial dose assessment and radionuclide sensitivity analysis for a High Temperature Gas Reactor (HTGR) mechanistic source term. This approach can be applied to a broad range of non-LWR designs, accident scenarios, mitigating safety features, location characteristics, and health and economic consequence outcomes. MELCOR and MELCOR Accident Consequence Code System (MACCS) are the computer codes used in this approach, both of which are developed by Sandia National Laboratories (SNL) on behalf of the United States Nuclear Regulatory Commission (U.S. NRC). This paper details source term input generated by MELCOR along with areas of potential uncertainty, the modeling framework in MACCS to include specifics on input parameter selection, and a method for analyzing the dose assessment data in terms of specific chemical group contributions. The source terms generated by MELCOR reflect efforts to develop and demonstrate accident progression and source term modeling and simulation capabilities. While MELCOR modeling and simulation capabilities are available for characterizing non-LWR accident progression and source terms, these source terms represent generic reactor designs developed from publicly available information. The modeling is also influenced by the current state-of-knowledge regarding critical phenomena and processes; e.g., fission product speciation in and diffusion through a TRISO particle, which will evolve with improved characterization of fundamental fission product thermochemistry and diffusion

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in these novel fuel forms. Since the studies reported in this paper are focused on understanding relative significance of a range of effects to overall consequences, these fundamental knowledge gaps can also be assessed with respect to their contribution to consequence evaluations of relevance to regulatory decision-making. This approach could, furthermore, be used to compare current Emergency Planning Zone requirements for LWRs (e.g., SMRs), and proposed updates to these requirements.

2. MELCOR

The MELCOR code is composed of an executive driver and several major modules (commonly referred to as packages) that together model systems, structures and components (SSCs) as well as processes and phenomena relevant to safety. The range of SSCs and processes modeled by MELCOR are essential to characterizing off-normal and accident response of a range of nuclear power and non-power production facilities. The range of behavior treated by MELCOR includes:

- Thermal-hydraulic response of the primary reactor coolant system, reactor cavity, containment, and confinement buildings
- Thermal-mechanical[1] and thermal-chemical[2] response of structures in the reactor core, including the fuel in the case of solid fuel systems
- Response of the reactor vessel structure under severe challenges imposed in the course of in-vessel damage progression
- Relocation of in-reactor vessel structural material (including fuel) into the enclosure volume surrounding the vessel
- Interaction of relocated debris with the structural material of the reactor enclosure (including core-concrete interaction)
- Flammable gas production due to high-temperature oxidation of reactor structures, followed by gas transport and possible combustion
- Fission product release (aerosol and vapor), transport, and deposition
- Behavior of radioactive aerosols in the reactor enclosure building, including scrubbing in water pools and aerosol dynamics in the containment atmosphere, such as agglomeration and deposition
- Impact of engineered safety features on thermal-hydraulic and radionuclide behavior

The various code packages have been written using a carefully designed modular structure with well-defined interfaces between them. This allows the exchange of complete and consistent information so that all phenomena are explicitly coupled at every step. The structure also facilitates maintaining and upgrading the code.

Initially, the MELCOR code was envisioned as being predominantly parametric with respect to modeling complicated physical processes. MELCOR has evolved to become largely best estimate in its characterization of processes and phenomena. Most MELCOR models are mechanistic, with capabilities

[1] This includes a range of processes that lead to loss of structural integrity and coolable geometry in the case of solid fuel systems.
[2] In the case of solid fuel systems, high-temperature conditions could lead to oxidation of fuel cladding and other metals in the core. At high temperatures, additional material interactions can occur that lead to the early liquefaction of core structures. This is explicitly treated in MELCOR models as it represents an important condition leading to early loss of core coolable geometry.

consistent with the most detailed, systems codes. In some cases, more parametric models are still provided to address uncertainties related to state-of-knowledge and extrapolation to reactor scale. Parametric models also remain the primary means to quantitatively evaluate a range of issues where consensus on appropriate mechanistic models does not exist.

While MELCOR has increased the fidelity of a range of models, it has maintained significant levels of computational efficiency and is able to achieve rapid code execution times. This is essential to characterize the impact of a broad range of uncertainties in an integral accident analysis. Achieving enhanced fidelity while maintain execution times for simulations has been supported by the continuous evolution of computer systems.

Current applications of MELCOR often include sensitivity and uncertainty studies. MELCOR simulations can evaluate these uncertainties since optional adjustable parameters describing many of MELCOR's mechanistic model can be modified by analysts. This does not affect the mechanistic nature of the modeling, but it does allow the analyst to easily address questions of how uncertainties in particular modeling parameters affect the course of a calculated transient. Parameters of this type, as well as numerical parameters that control convergence criteria and iteration limits, are coded in MELCOR as sensitivity coefficients, which may be modified through optional code input.

MELCOR modeling is general and flexible, making use of a "control volume" approach in describing the plant system. No specific nodalization of a system is forced on the user, which allows a choice of the degree of detail appropriate to the modeling requirements. Reactor-specific geometry is imposed only in modeling the reactor core. Even for this case, one basic model suffices for representing either a boiling water reactor (BWR) or a pressurized water reactor (PWR) core, and a wide range of levels of modeling detail is possible. For example, MELCOR has been successfully used to model East European reactor designs such as the Russian VVER, and RMBK-reactor classes. It has more recently been readily extended to characterize accident progression and source terms for water-moderated SMRs as well as non-LWR concepts. Its extension to the modeling of non-LWRs includes the pebble bed and prismatic High-Temperature Gas-cooled Reactor (HTGR), Molten Salt Reactor (MSR), pebble bed Fluoride-salt-cooled High-temperature Reactor (FHR), and liquid metal reactors such as Heat Pipe Reactors (HPRs).

2.1 MELCOR Accident Consequence Code System (MACCS)

Source term information obtained by MELCOR is then input into the MELCOR Accident Consequence Code System (MACCS) to conduct the consequence analysis portion of the study. The MACCS code suite has been created by SNL for the U.S. NRC in order to perform calculations of health and economic consequences following a release of radioactive material in the atmosphere. MACCS accomplishes this by modeling the atmospheric dispersion, deposition, and consequences of the release, which depend on several factors. These include the source term, weather, population, economic, and land-use characteristics of the impacted geographical area. For the purposes of MACCS modeling, the source term generated by MELCOR is typically characterized into a set of distinct temporal release phases defined in terms of radionuclide release rates, elevations, and energies. From these inputs, MACCS determines the characteristics of the plume, as well as ground and air concentrations as a function of time and tracked radionuclide.

Users may select an atmospheric transport model based on a simpler straight-line Gaussian plume segment model or a more detailed hybrid Lagrangian/Eulerian method. This latter model is an enhancement added in June 2020 that couples MACCS with HYSPLIT, an atmospheric transport and dispersion modeling system developed by NOAA. Along with atmospheric dispersion, MACCS also calculates the health effects of exposure, impacts on the food chain, and the economic impact following an accident.

More specifically, the MACCS code suite models the following:

- Atmospheric transport and dispersion

- Wet and dry deposition
- Probabilistic treatment of meteorology
- Exposure pathways
- Emergency phase, intermediate phase, and long-term phase protective actions
- Dosimetry
- Health effects
- Economic impacts

MACCS2 was first released in April 1997. Since then, it has been routinely updated and modernized by both SNL and the U.S. NRC. In the current version, the 2 has been dropped and it is named MACCS 4.0. The user base, like MELCOR, includes both domestic and international users, including the NRC, DOE and their contractors, several research organizations, nuclear industry licensees/applicants, and academic institutions. Primary uses of MACCS include performing regulatory cost-benefit analysis of Severe Accident Mitigation Alternatives (SAMAs) and Severe Accident Mitigation Design Alternatives (SAMDAs), evaluation of emergency planning, Level 3 PRA studies, consequence studies, documented safety analyses, and other risk-informed activities. Also, of significance, MACCS is one of few existing tools capable of treating, within a probabilistic framework, all of the technical elements of the ASME/ANS RA-S-1.3-2017 Standard for Radiological Accident Offsite Consequence Analysis (Level 3 PRA) to Support Nuclear Installation Applications. As such, MACCS naturally fills the role of a consequence evaluation tool for the non-LWR PRA standard as well.

2.2 HTGR Mechanistic Source Term

MELCOR model development and maturation for several non-LWRs is ongoing work at SNL and includes capability development and demonstration for HTGRs, MSRs, FHRs, SFRs, and HPRs. For this initial analysis, an accident scenario representing an externally initiated event for a pebble bed HTGR (400 MWth Pebble Bed Modular Reactor) is chosen to illustrate the approach. This externally initiated event is represented in Figure 1 below by the star symbol, in which the selected accident scenario is a depressurized loss of forced cooling (DLOFC).

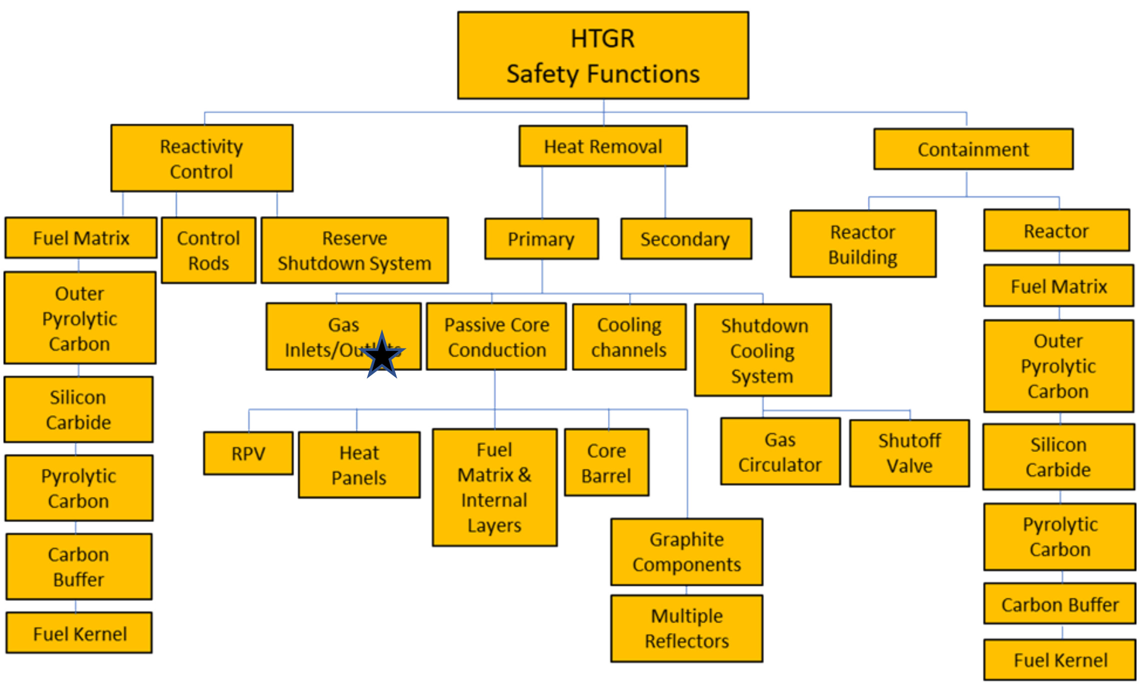

Figure 1: Safety Functions for High Temperature Gas Reactors.

Event progression is impacted by the performance of the primary and secondary heat removal safety functions. The possible scenario evolutions are represented by distinct branches that characterize the accident performance of these safety functions. For the primary system, effective heat removal depends on a) adequate flow of gas coolant over the pebble bed core to prevent fuel overheating to the point of failure, and b) rejection of heat from the core to either the secondary side of the plant or into confinement and ultimately the environment.

Performance of core heat removal relies on a number of SSCs; for example, the recuperative Power Conversion Unit (PCU), reactor pressure vessel (RPV) inlet and outlet lines and associated valves, cooling channels within the reactor core, the shutdown cooling system (which operates the gas circulator and cooling shutoff valve), passive heat transport away from the core via conduction and radiation pathways, heat removal from the reactor cavity/confinement atmosphere by the Reactor Cavity Cooling System (RCCS). A number of scenarios can be postulated in which one or more of the measures supporting the core heat removal function can be challenged. The following discussion outlines one particular scenario.

Under normal operating conditions, the PBMR-400 transfers heat energy directly from the modular pebble bed reactor to the recuperative PCU, which consists of a single-shaft turbine/compressor/generator instead of a steam generator. Several accident scenarios may arise from the potential for structural damage/displacement of multiple elements of the heat removal system. Natural disasters (like earthquakes) could cause damage to the gas coolant lines, channels within the core, and/or displacement of the heat panels on the exterior of the reactor vessel. A commonly postulated scenario is initiated by a seismic event that causes a loss-of-onsite power and a concurrent break in the exit pipe from the reactor to the PCU. The loss of power leads to a loss-of-forced circulation, while the pipe break results in a depressurization of the RPV. The overall event, referred to as a depressurized loss-of-forced-cooling (DLOFC), reduces both the rate of circulation within the RPV and the working fluid pressure (i.e., He). In combination, a reduction in heat removal from the fuel in the pebble bed core occurs, resulting in a fuel temperature excursion.

Under this reduction in heat removal from the core for the DLOFC event, additional heat transport pathways will increasingly become more significant as fuel heat up establishes enhanced thermal gradients from the fuel within the RPV to surrounding structures. This promotes enhanced passive heat transport via conductive and radiative pathways. Passive transport of heat generated in the fuel progresses along the following pathway: conduction and radiation allow heat to move through the graphite core into multiple reflectors surrounding the core, the core barrel and the ultimately the reactor pressure vessel (RPV) structure. Heat conducted through the wall of the RPV is absorbed by heat panels on the exterior of the RPV. This energy is convectively and radiatively transferred to the reactor cavity atmosphere. Should the Reactor Cavity Cooling System (RCCS) be operation, this energy will ultimately be removed from the reactor cavity and rejected to the environment.

As the state-of-knowledge regarding key non-LWR accident processes and phenomena matures, as well as details of non-LWR designs, MELCOR accident progression and source term evaluations will evolve. It is also expected that the scope of evaluations will expand to reflect enhanced understanding in a number of areas as design and siting details mature. Information of relevance include the nature of the reactor site (i.e., the number of units to be located at the same site), site-specific hazards and potential accident scenarios that could occur, specific mitigating systems available in a design along with their performance characteristics, and siting criteria relevant to evaluating off-site consequences.

While it is expected that the source term utilized as demonstration of analysis capability in this paper will evolve considerably, its overall features associated with initiation time for and duration of release are reasonably representative of the nature of many non-LWR source terms. With this source term, the key input to the consequence evaluation is then represented in a manner suitable for a MACCS analysis. Mechanistic source terms from MELCOR are divided into plume segments to best represent varying weather conditions during the release. The source term used for this study was divided into 58 plume segments, each 3-hours long. Each plume segment is characterized by the energy of the release (J/s), mass flow rate (kg/s), gas density (kg/m3), and release fraction for each chemical group. The chemical groups are defined in Table 1:

Table 1: Chemical group definitions.

Chemical Group	Description	Radionuclides
Group 1	Noble Gases	Xe, Kr
Group 2	Alkali Metals	Cs, Rb
Group 3	Alkaline Earths	Ba, Sr
Group 4	Halogens	I
Group 5	Chalcogens	Te
Group 6	Platinoids	Rh, Ru
Group 7	Early Transition	Nb, Co, Mo, Tc,
Group 8	Tetravalents	Ce, Np, Pu, Zr
Group 9	Trivalents	La, Am, Cm, Nd, Pr, Y

The mechanistic source term used in this study is intended to demonstrate overall modeling capability. A key knowledge gap that will progressively be resolved through further fundamental safety research is associated with fission product chemistry and release for the UO2 based TRISO fuel of the PBMR reactors. Initial estimates are based on measured correlations for Xe, Kr, Sr, Cs, I and Ag, with the remainder inferred from LWR methodology. The Alkaline Earth group is inferred from Sr data. In the case of MELCOR, the generalized representation of fission product thermochemistry being incorporated into the code, and the mechanistic modeling of fission product diffusion within TRISO fuel ensure that analyses can be updated as data become available without fundamental modification of code models. However, the assessment in this analysis is intended to identify fundamental areas in which new data will have the most significant impact on source term estimation and associated consequences of important to regulatory decision-making.

2.3 Atmospheric Transport and Dispersion Modeling

To perform the necessary atmospheric transport and dispersion modeling for this analysis, the Gaussian plume segment model in MACCS was utilized. Input specifications included building dimensions, wake effects, radial spatial intervals, and the surface roughness of the area. All additional pertinent information needed for atmospheric transport and dispersion modeling were chosen to align with the MACCS best practices used in the State-of-the-Art Reactor Consequence Analyses (SOARCA) project [1]. An average representation of weather within the United States was also used for this analysis.

To incorporate building wake effects, MACCS utilizes the virtual source approach in which initial plume dimensions are characteristic of the building height dimensions [2]. The building height (H) and width (W) were set as 20 m for all release paths to be conservatively consistent with anticipated small modular reactor dimensions. Initial plume dimensions were then calculated using the following equations [3]:

$$\sigma_{y0} = \frac{W}{4.3} \quad (1)$$

$$\sigma_{z0} = \frac{H}{2.15} \quad (2)$$

Radial Number (NUMRAD)	Distance (mi) (SPAEND)
1	0.10
2	0.35
3	0.65
4	1.00
5	1.35
6	2.00
7	2.50
8	3.00
9	3.50
10	5.00
11	7.00
12	10.00

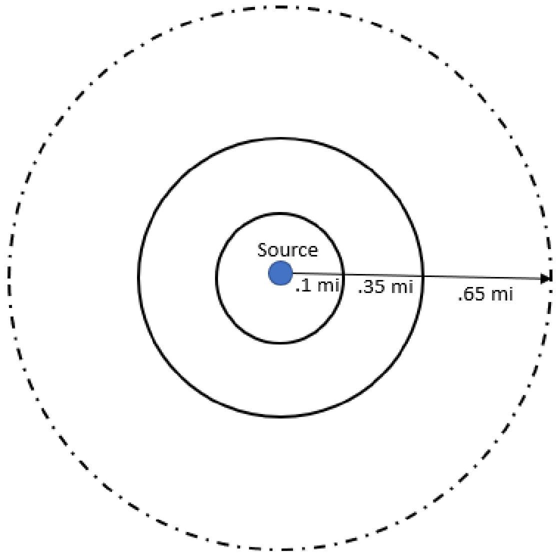

Figure 2: Radial spatial intervals

The specified number of radial spatial intervals from the release point and associated distances are described in Figure 2 below. This information was used to determine the dose at various distances from the source. These distances were also adapted from the MACCS best practices applied in the SOARCA Study [1].

Surface roughness has the potential to affect both the vertical dispersion and dry deposition velocities of aerosol particles. Surface roughness should be accounted for in the model by applying a linear scaling factor to σ_z, which is the vertical standard deviation of the normal concentration distribution. Using the diagram shown in Figure 3 below, a surface roughness value of 40 cm was assigned to represent an average suburban environment that includes both institutional and residential buildings.

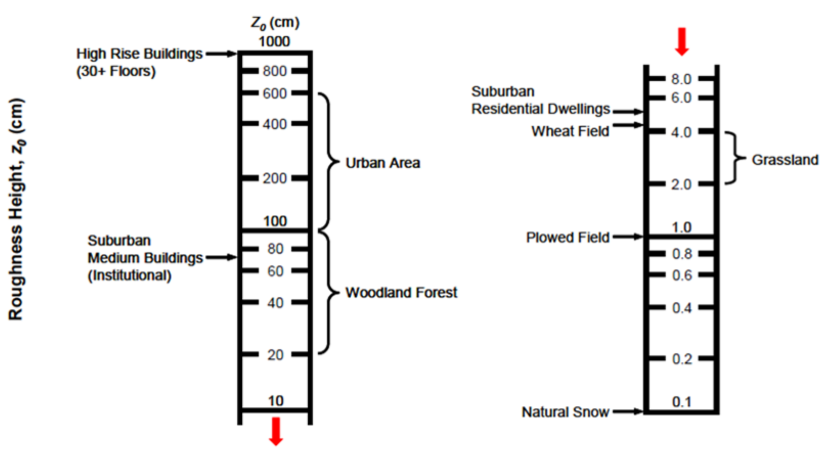

Figure 3: Approximate surface roughness lengths (z) for various surfaces

The assigned roughness values are then used in the empirical equation (3) below [3]. This equation uses $z_{ref} = 3$ cm, which corresponds to the Prairie Grass data from which the dispersion values are derived

[4]. The linear scaling factor (ZSCALE) for the suburban site described by a surface roughness of 40 cm was thus determined to be 1.67

$$ZSCALE = \left(\frac{z_{newo}}{z_{o,ref}}\right)^{0.2} \quad (3)$$

2.4 Population Modeling

Population cohorts may be assigned in MACCS to best represent the actions of particular groups of people, to include time-dependent response to shelter-in-place or evacuation orders from local government officials. Following a similar process laid out by the United States Nuclear Regulatory Commission (NRC) to develop Evacuation Time Estimates (ETEs), the MACCS cohort parameters were determined [5]. The population is divided into cohorts based on the delay time and speed it would take the population to evacuate. Factors such as living situation, and vehicle access are considered. The cohorts are divided into the following cohorts:

- Populations with access to private transportation
- Transit dependent populations
- Special facility (Hospitals, nursing homes, jails, prisons, etc.) residents
- School populations
- Non-evacuating populations

The size of each cohort is determined using demographic survey data from various US government agencies such as the Census Bureau, Centers for Disease Control and Prevention, Department of Justice and Department of Education. Since no specific site is examined in this study, the geographic variance in the cohort sizes are smeared out by using US total populations.

Determining the time to issue evacuation or shelter-in-place orders (OLARM Parameter) is extremely challenging, as there are many unpredictable factors, such as accident progression, risk of release, human factors, who is the decision maker, etc. Furthermore, there is very little applicable historical precedent for two reasons, the events requiring emergency evacuation are rare and the nature of accident response and modeling has changed. Additionally, the reactor designs are not sufficiently mature to have detailed accident procedures. Information was gathered from three emergency evacuations: Fukushima Daiichi, Fukushima Daini, and Oroville Dam. The time to call a general evacuation order since the special situation was declared in the cases of both the Fukushima power stations was 4 hr 5 min and 13 hr 12 min for Daiichi and Daini, respectively (Hatanaka, Yoshida, Ojino, & Ishii, 2014). The Oroville Dam had no formal issuances of a special situation and an evacuation was ordered 1 hr 15 min after a hole had eroded into the hillside (The Associated Press, 2018). With these historical timelines, an initial timeline was set at 9500 s for declaration of a general emergency. This timeline is subject to many factors and is dependent on the specific characteristics of the emergency, and policies yet to be put in place for non-LWR accident scenarios. How a general emergency would be triggered for advanced reactor concepts with significant longer coping times than currently operating reactors is an area that has not yet received extensive attention. However, this represents another area of development for advanced reactors in which MELCOR and MACCS accident progression, source term and consequence evaluations will prove beneficial in developing the appropriate technical bases to support ultimate decision-making.

3. RESULTS

Peak dose on the spatial grid for each cohort individually and for all cohorts combined are modeled in MACCS. In addition to the original mechanistic source term representing HTGR source terms for 400 MWth, 200MWth and 800MWth were also considered for comparison. Figure 4 displays the results of this dose assessment over a distance of 8.5 miles from the source of the release. The data are normalized to the 0.05 mile datapoint for the no scaling, non-evacuating cohort.

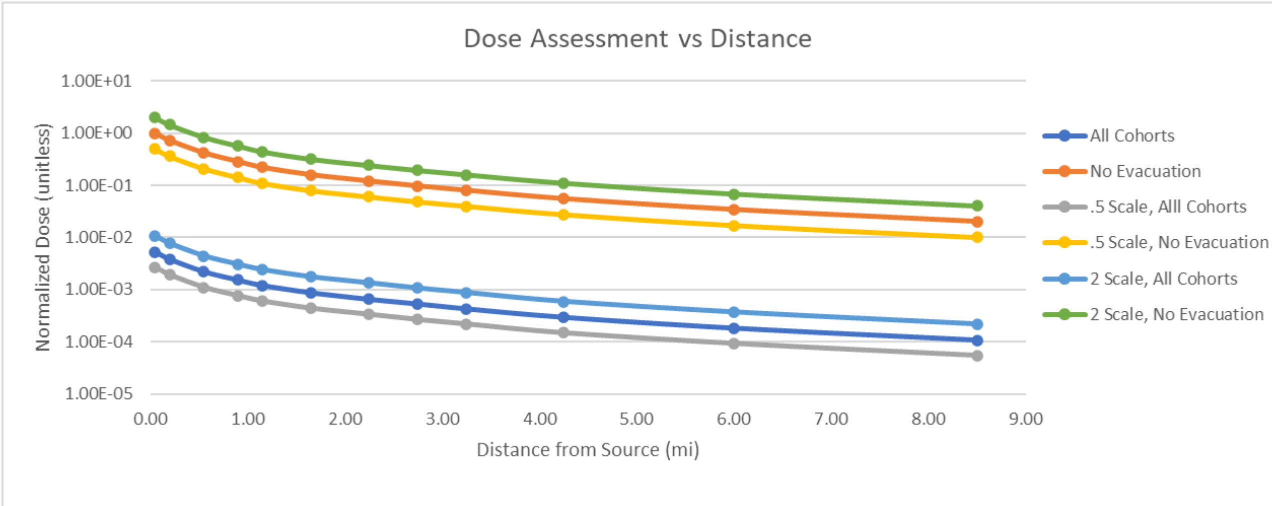

Figure 4: Dose Assessment vs Distance

The results were scaled to the unscaled source term non-evacuating cohort due to the dose assessment results being based on an initial mechanistic source term developed for the purpose of modeling capability demonstration. To best inform this ongoing effort to assess the importance of knowledge gaps to regulatory decisions, a sensitivity analysis to evaluate the contribution of different chemical groups to a dose assessment was performed. Figure 5 displays the contribution of each of the chemical groups, and Figure 6 displays a ratio of the dose assessment when each chemical group's release fraction is increased by a factor of 10.

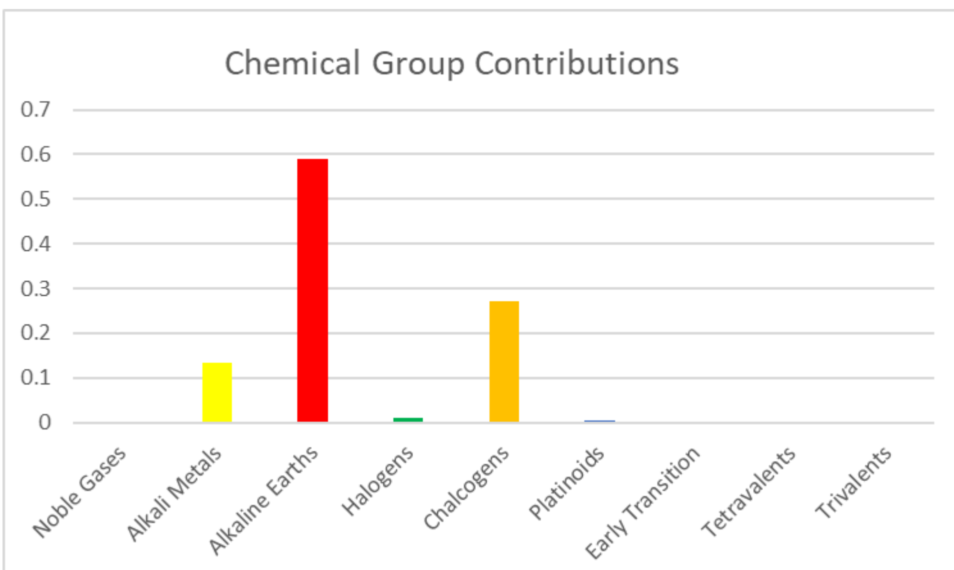

Figure 5: Chemical Group Contributions

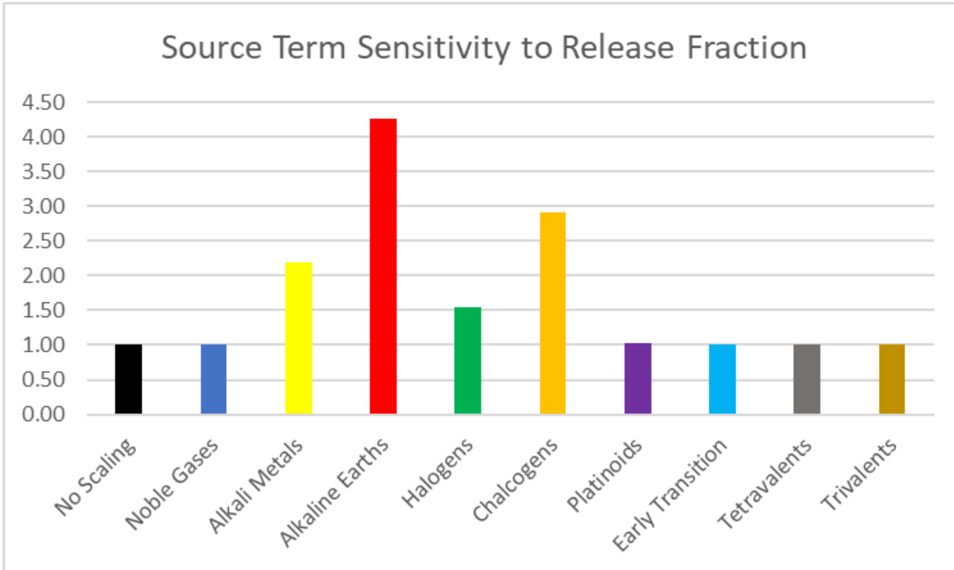

Figure 6: Source Term Sensitivity to Release Fraction

4. CONCLUSIONS

Two primary conclusions can be drawn from this study: (1) evacuation is more important than the core size and potential magnitude of release for this small source term and (2) the primary contributions to dose come from the chemical groups containing Ba, Te, Cs, and I. In refining mechanistic source term models, it is recommended to prioritize improving the fidelity of the models for these elements, as they contribute most to consequences and are also the most sensitive to uncertainties in the release fractions.

5. ACKNOWLEDGEMENTS

This template was adapted from the template for PHYSOR 2002 posted on the Internet.

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