

THE FRAMEWORK OF RADIONUCLIDE RELEASE FROM RESEARCH REACTOR FUEL CONDITIONING (4RFC): A SIMULATION TOOL IN DEVELOPMENT

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ABSTRACT

The oxide chemical form of power reactor fuel makes it well suited for storage and disposal. Often, the corrosion-resistant oxide can be an important safety feature in the safety case of Deep Geological Repository design for fuel disposal. Many research reactor fuel designs utilize non-oxide forms such as metals, metallic alloys, carbides, and silicides. These chemical forms are less resistant to corrosion and may pose significant challenges to direct disposal. Stabilization of irradiated research reactor fuel to an oxide form is a waste management option under consideration and technical development. The conditioning method involves the controlled oxidation of non-oxide fuel via exposure to high temperature and an oxygen containing gas in a furnace within a hot cell facility. For irradiated fuel, the release of radionuclides during conditioning is an important consideration for safety and the environment. No publicly available simulation tools exist for predicting radionuclide release from research reactor fuel under these conditions. Therefore, a new simulation tool titled Radionuclide Release from Research Reactor Fuel Conditioning (4RFC) is under development to fill this gap and its framework is presented.

BACKGROUND

Fuel Disposal in Canada

Canada's plan for used fuel disposal is to construct a Deep Geological Repository (DGR) to contain millions of used CANDU fuel bundles approximately 500 m underground as shown in Figure 1. The DGR design is a multi-barrier system comprised of the host rock, bentonite clay, the disposal container, the Zircaloy-4 cladding, and the oxide fuel itself (NWMO 2017). The oxide fuel is an important feature as it immobilizes many radionuclides within it. It has low solubility in groundwater in the event of a disposal container failure, slowing the release of radionuclides from the fuel and out of the DGR to the surrounding environment. The Zircaloy-4 cladding is also highly resistant to corrosion and provides another barrier to water contacting the fuel (NWMO 2017).

Research reactor fuel used in Canada and internationally is often not oxide fuel, but rather metals, metallic alloys, carbides, and silicides. These non-oxide fuel forms may pose significant challenges for direct disposal in a DGR designed for CANDU fuel as its properties may vary significantly from CANDU fuel. Studies indicate that non-oxide research reactor fuels are less resistant to corrosion than oxide fuel (Bahr 2017, Brücher et al 2001, Curtius et al 2011, Deissmann et al 2016). Aluminum alloy cladding often used in research reactor fuel designs is significantly less resistant to corrosion than Zircaloy-4 under DGR conditions (Deissmann et al 2016). Furthermore, enriched research reactor fuel can present criticality safety concerns that do not otherwise need to be considered in a DGR designed for CANDU fuel of natural enrichment.

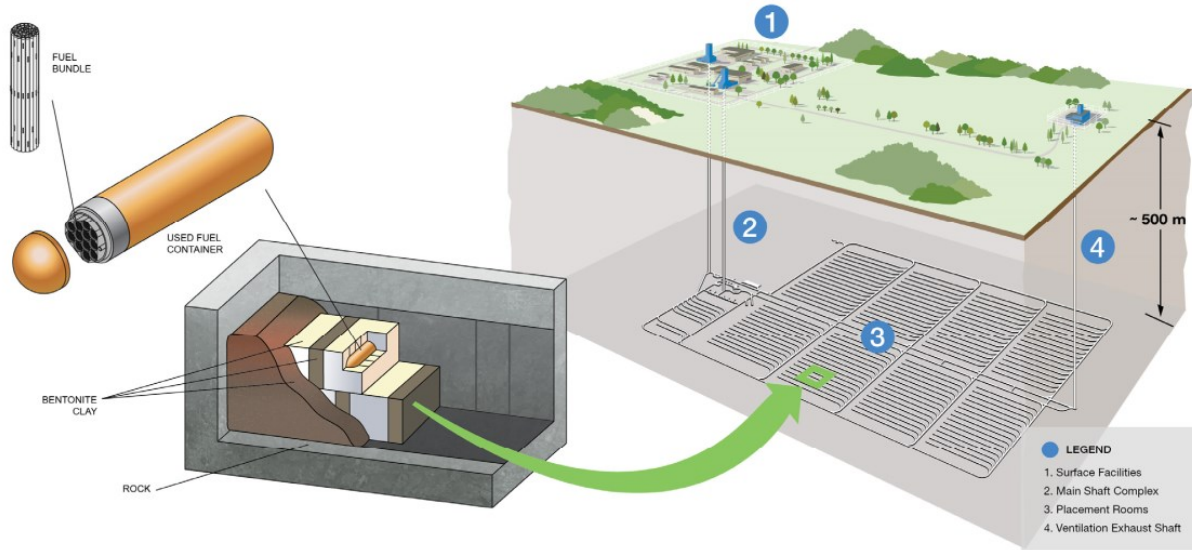


Figure 1. Conceptual Design of the Canadian Deep Geological Repository for Used CANDU Fuel (NWMO 2017)

Fuel Conditioning

Conditioning is an option to convert non-oxide research reactor fuels to a form suitable for disposal in a DGR. Research is ongoing at Canadian Nuclear Laboratories (CNL) to condition research reactor fuel to a form similar to CANDU fuel with respect to properties important to disposal, such as geometry, chemical form, nuclear reactivity, heat load, and dose rate (Prasad et al 2024) (Spencer et al 2023). Such a strategy would leverage most if not all of the existing safety case and national plans for disposal of the used CANDU fuel inventory in Canada. The conditioning steps are expected to include disassembly and sectioning, cladding removal, stabilization, nuclear reactivity reduction, pellet formation, and packaging. All steps require the use of shielded hot cells. Of these steps, stabilization via controlled oxidation and pellet formation via Spark Plasma Sintering (SPS) are expected to result in the highest radionuclide release owing to the high temperatures used in these steps.

Controlled oxidation exposes non-oxide fuel to high temperature and an oxygen containing gas, such as air or steam, in a furnace. The resulting oxide powder is reduced to UO_2 form via reduction in the same furnace under a hydrogen containing gas. Multiple oxidation-reduction cycles are possible. Residual oxides of alloying materials, such as aluminium, silicon, or zirconium, may also be present.

Forming pellets from the oxide powder generated during stabilization significantly reduces the surface area to volume ratio of the powder. A reduced surface area improves the corrosion resistance of the conditioned fuel for disposal. SPS simultaneously applies pressure and heat to sinter powder into a high-density pellet. It offers shorter cycle times and lower temperatures than conventional pellet formation techniques of pressing and sintering, which may translate into lower radionuclide release. An example is shown in Figure 2 of a conditioned UO_2 fuel pellet derived from uranium carbide stabilized via controlled oxidation and formed into a pellet via SPS.

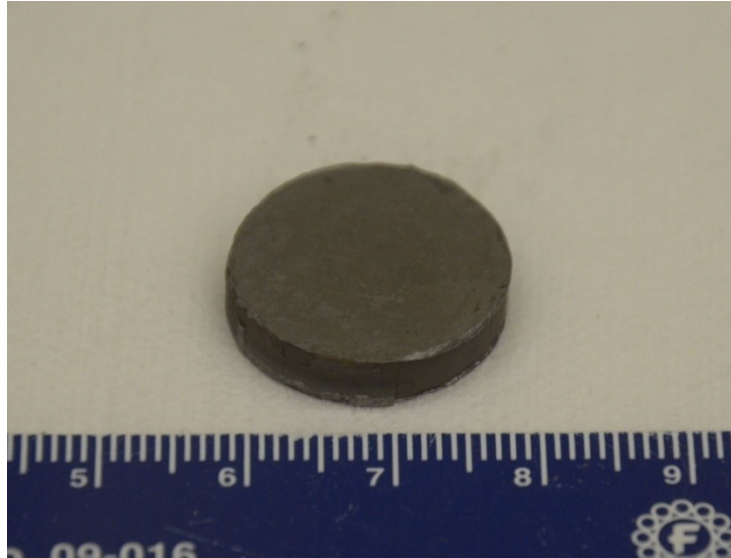


Figure 2. A 20 mm Conditioned UO_2 Fuel Pellet Derived from Initially Uranium Carbide Fuel (Spencer et al 2023)

Radionuclide Release

The release of radionuclides is problematic and must be considered at all stages of the nuclear fuel cycle. During irradiation in-reactor, fuel defects and accidents can result in radionuclides escaping the fuel and coolant, causing increased radiation dose to operations staff. If released from the reactor containment structure, radionuclides can have adverse radiation effects on the public and the environment. Thus, methods have been developed to detect and remove defective fuel and models and assessments used to manage the risk of radionuclide release during accidents (Tayal 2017). For fuel disposal, the overall goal of a DGR is to slow the release of radionuclides such that sufficient decay is achieved prior to reaching the biosphere to limit radiation dose to below acceptable regulatory levels (NWMO 2017).

During research reactor fuel conditioning, radionuclide release will also be important to control. Increased radionuclide release during fuel conditioning will result in higher activity filters and an increase in secondary waste generation. For radionuclides that cannot be easily trapped by filters, such as Kr-85, radionuclide release to the environment will also need to be controlled and shown to be within regulatory limits. Currently, there are no existing tools for predicting radionuclide release under the conditioning parameters for research reactor fuel described above.

4RFC FRAMEWORK

The objective of this research is to create and validate a simulation tool to predict radionuclide release from research reactor fuel during conditioning. This research will make an original contribution to the field by establishing the first simulation tool capable of predicting radionuclide release during conditioning of research reactor fuels via controlled oxidation and SPS. The simulation tool is called Radionuclide Release from Research Reactor Fuel Conditioning (4RFC). It is intended to make 4RFC open source upon the conclusion of the research, which will be accompanied by a thesis report documenting its development and validation.

The goal of 4RFC is to predict the radionuclides released during fuel conditioning when the specific fuel design and conditioning parameters are defined. A preliminary Graphical User Interface (GUI) for 4RFC is shown in Figure 3. The user first defines the properties of the fuel being conditioned, specifically

the fuel design, burnup, time since irradiation, and mass. The user also specifies the conditioning parameters being used, specifically the temperature, time, atmosphere (*e.g.*, air), gas flow rate, and gas pressure. With the click of a single button, the radionuclide release is predicted.

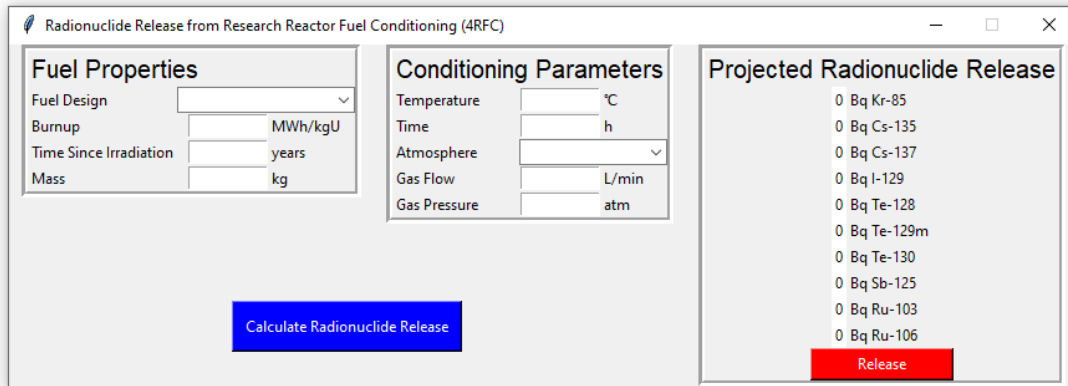


Figure 3. Preliminary Graphical User Interface of 4RFC.

The 4RFC simulation tool will need to be capable of predicting the radionuclide inventory present in the fuel of interest, predicting the chemical form of the radionuclides under the prevailing conditioning parameters, and predicting the release of radionuclides under these conditions over time. It will need to integrate these three prediction capabilities into a single tool with a GUI. Finally, 4RFC will need to be validated against empirical data. These capabilities are illustrated in Figure 4 and described in detail in the following sections.

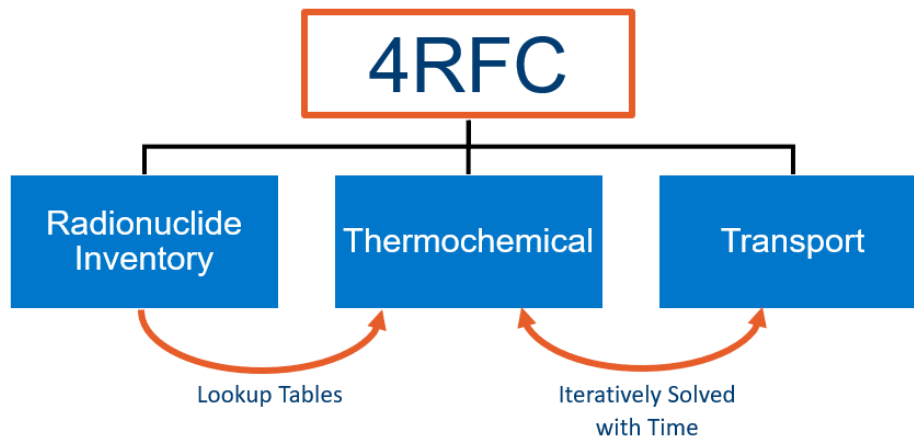


Figure 4. Framework of 4RFC.

Predict Radionuclide Inventory

The radionuclide inventory present in the fuel represents the maximum quantity of radionuclides that could be released during conditioning and therefore is the starting point to predicting radionuclide release. Radionuclide inventory is dependent on fuel mass, fuel design, burnup, and time since irradiation. Fuel designs selected for modelling span a variety of Canadian research reactors, namely the National Research Experimental (NRX) reactor, the National Research Universal (NRU) reactor, and the Whiteshell Reactor

1 (WR-1). The fuel designs also span a variety of chemical forms, including uranium metal, uranium carbide, and uranium silicide dispersed in an aluminium matrix.

The SCALE code system (Rearden et al 2018) is an existing method of calculating radionuclide inventory in irradiated fuel commonly used in industry. The two-dimensional NEWT module of the TRITON code from the SCALE code system is used for predicting the nuclear physics of each fuel design. This is coupled with the ORIGEN module of the SCALE code system, which calculates depletion and the radionuclide inventory at given time steps over the irradiation to account for changes in nuclear physics due to fuel burnup. ORIGEN standalone depletion calculations are conducted to decay the radionuclide inventory at end of irradiation to selected times post irradiation. An overview of this process is shown in Figure 5 (Barry et al 2024).

ENDF/B-VII.1 nuclear data is used for both irradiation and depletion calculations (Chadwick et al 2011). It provides information on fission yields, neutron cross section data, and decay data. This nuclear data is available as part of the SCALE code system package. The TRITON model requires data on the fuel power, burnup, materials, and geometry as well as reactor materials and geometry information. This data has been compiled from publicly available references to the extent possible. Where the required data was not publicly available, internal CNL references were used. Custom TRITON models were created for the specific research reactors of interest.

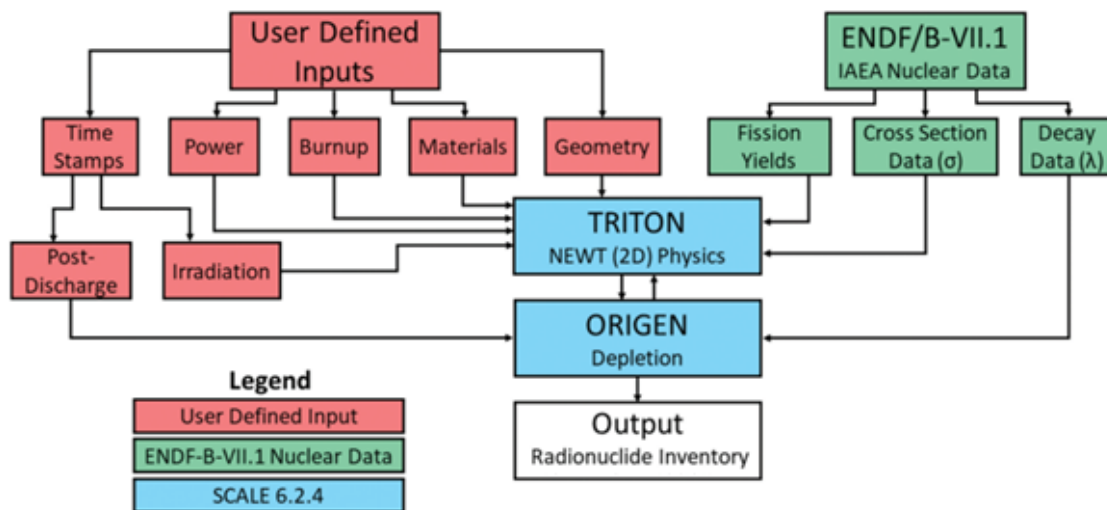


Figure 5. SCALE Modelling Methodology (Barry et al 2024)

The data is stored as a series of lookup tables that provide the radionuclide inventory present for a given fuel design, burnup, and time since irradiation. Interpolation will be used to determine intermediate values. More than a decade of decay post-irradiation has been achieved by all fuel designs selected; therefore, further decay of the radionuclide inventory will be negligible over the several days expected to be needed to complete a conditioning batch.

Predict Radionuclide Chemical Form

The chemical form of the radionuclides present in the fuel dictates its ability to be released. Only gaseous species can be released during fuel conditioning. Fuel conditioning can also change the chemical form of radionuclides in the fuel. Additionally, the chemical phase of the bulk of the uranium fuel may impact the release of the gaseous species from the fuel, as described later when predicting radionuclide transport. Therefore, 4RFC must be capable of predicting the chemical species and phases that will form under the

prevailing conditioning parameters. The conditioning parameters selected for modelling are the temperature range of 25 to 1000 °C, the pressure range 0.1 to 5 atm, and gas atmospheres of air, O₂, Ar, steam, pure H₂, and 4% H₂ in Ar mixture.

Computational thermodynamics can be used to predict the phases and chemical species that are thermodynamically favoured to form when the temperature, pressure, and elemental composition of the system are defined. Such calculations require thermodynamic data and software to execute the calculations. For thermodynamic data, the Thermodynamics of Advanced Fuels - International Database (TAF-ID) (Guéneau et al 2021) provides the state-of-the-art of thermodynamic data for advanced fuels. Uranium metal, uranium carbide, and UO₂ fuel are explicit phases covered by the TAF-ID and uranium silicide is included as a prototype portion of the database. A variety of phases that may also form as intermediaries during fuel conditioning are also included in the TAF-ID, such as uranium nitride (UN), U₄O₉, U₃O₈, and UO₃. Some additional thermodynamic information from the Molten Salt Thermal Properties Database–Thermochemical (MSTDB-TC) (Ard et al 2022) may help to supplement information in the TAF-ID. Thermodynamic data available in the literature may also be needed to fill in information gaps.

For thermodynamic software, FactSage (Bale et al 2016), Thermochemica (Piro et al 2013), ThermoCalc (Sundman et al 1985), and PyCalphad (Otis et al 2017) were considered for use in this research. FactSage and ThermoCalc are proprietary commercial software packages that require licenses at an annual cost. In the interest of having a single simulation tool that does not require any additional cost, licenses, or continual technical maintenance, free and open-source software like PyCalphad or Thermochemica is preferred. Both software suites were investigated and Thermochemica was ultimately selected as the preferred software and was integrated into the 4RFC simulation tool.

The two most common database file types are ThermoCalc format (.tdb) and ChemSage format (.dat). The TAF-ID is formatted in the .tdb file type and the MSTDB-TC is formatted in the .dat file type. A custom-made thermodynamic database was therefore created using database management capabilities present in FactSage. The custom-made database is in .dat file type to correspond to the requirements of Thermochemica and amalgamates select data from both the TAF-ID and MSTDB-TC.

The output of this calculation is a prediction of the fraction of gaseous species present under the prevailing conditioning parameters with the potential to be release from the fuel. Additionally, a prediction of the chemical phases and fractions of the bulk uranium fuel matrix is another output. Both outputs are passed to the transport calculations as shown in Figure 4.

Predict Radionuclide Transport

Studies on chemical composition and microstructure of used UO₂ fuel show that more than 90% of radionuclides remain in the location of the fuel in which they were formed after discharge (Bradley et al 2022). Under irradiation, small amounts of gaseous species diffuse out of the fuel grains and to grain boundaries, cracks, and voids. The relocation of species depends on their chemical form and properties, such as their solubility in the UO₂ matrix (Bradley et al 2022).

Fuel performance codes were reviewed as UO₂ fuel behaviour under irradiation is well researched and the phenomena that drive radionuclide release under irradiation may also apply to conditioning. Additionally, fuel oxidation from cladding defects and during accident conditions are also included in some of these fuel performance codes that may apply to conditioning. The codes SOURCE-IST (Barber et al 2001), BISON (Hales et al 2016), ALCYONE (Noirot 2011), ASTEC – ELSA Module (Brillant et al 2013), MFPR (Veshchunov et al 2006), VICTORIA (Olander et al 1999), MELCOR (Humphries et al 2017), and FEMAXI (Suzuki et al 2013) were reviewed. The radionuclide transport phenomena reviewed in these codes include athermal release, diffusion (including changes in rate from oxidation), grain boundary

sweeping/grain growth, grain boundary coalescence/tunnel interconnection, vapour transport/columnar grains, fuel cracking, gap transport, gap retention, burst release, and amorphous diffusion in U₃Si (*i.e.*, breakaway swelling). For simplicity, only one radionuclide transport model was selected for inclusion in 4RFC tool initially: the Booth diffusion model (Booth 1957). If 4RFC does not provide sufficient results, additional radionuclide transport models will be identified for inclusion in the future.

The Booth diffusion model applies Fick's Law to a fuel grain represented by a sphere. Through this model, Booth derived an equation for the fraction of radionuclides diffused out of the grain (f) shown in (1) (Booth 1957).

$$f = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp(-n^2 \pi^2 D' t) \quad (1)$$

Where t is time in units of s and D' is the effective diffusion coefficient for a specific batch of fuel in units of s⁻¹ (it is defined as $D' = \frac{D}{a^2}$, where D is the diffusion coefficient for all fuels of a particular chemical form in units of cm² s⁻¹ and a is the equivalent radius of the fuel grain in units of cm).

When $\pi^2 D' t \gg 1$, then Booth determined that (1) approximates to (2) as the first term only provides a good approximation (*i.e.*, $n=1$).

$$f = 1 - \frac{6}{\pi^2} \exp(-\pi^2 D' t) \quad (2)$$

When $\pi^2 D' t \ll 1$, then Booth determined that (1) approximates to (3).

$$f = 6 \sqrt{\frac{D' t}{\pi} - 3 D' t} \quad (3)$$

At $\pi^2 D' t \approx 1$, then Booth determined that both approximations are good.

The Booth diffusion model requires empirical diffusion coefficients (D) for the fuel types and radionuclides of interest. These diffusion coefficients have been identified in the literature. The SOURCE-IST code (Barber et al 2001) treats oxidation of UO₂ to UO_{2+x}, U₄O₉, and U₃O₈ by changing the diffusion coefficient to one corresponding to the new oxide form. The same methodology is applied in 4RFC. Therefore, multiple diffusion coefficients are needed based on the fuel chemical form (metal, UC, U₃Si, UO₂, U₃O₈, etc.). The thermochemical model prediction of the chemical phases and fractions of the bulk uranium fuel matrix are used to inform which diffusion coefficient(s) to use for a given time step in the calculations.

The Python programming language is used to implement (2) and (3) for the Booth diffusion model. MatLab, LabVIEW, Wolfram Mathematica, Python, SQL, and Maple were considered as programming languages to implement the radionuclide transport equations. Python was selected as the preferred language owing to being free and open-source software and its ability to easily implement a GUI for the entire simulation tool. It can perform the basic arithmetic shown in (2) and (3).

The output of this calculation is a prediction of the fraction of gaseous species that release from the fuel under the prevailing conditioning parameters over a given time step. Both the chemical species and radionuclide transport may be solved iteratively over several time steps over the conditioning process. This integration is described next.

Integration into a Single Tool

The radionuclide inventory, chemical form calculations, and radionuclide transport calculations are integrated into one single tool such that the data does not need to be passed manually from one model to another. A GUI is used to receive the inputs on the fuel properties and conditioning parameters to use in the calculations and display the calculated radionuclide release. The Python programming language is used, specifically the Tkinter module included in the default Python programming language.

A preliminary GUI for 4RFC has been developed and is shown in Figure 3. This GUI receives the inputs for the fuel properties from the user, namely the fuel design via a drop-down menu and the fuel burnup, time since irradiation, and fuel mass in text input field. It also receives inputs for the conditioning parameters from the user, namely the atmosphere via a drop-down menu and the temperature, conditioning time, gas flow rate, and gas pressure in text input field. Once the inputs are filled in, the user clicks on the blue “Calculate Radionuclide Release” button to execute the calculations. The projected radionuclide release is returned.

The integrated 4RFC simulation tool functions as follows. First, the fuel properties are used to look up the appropriate radionuclide inventory from the look-up tables generated with SCALE-ORIGEN. The radionuclide inventory is used to write an input file for Thermochemica as the elemental composition at time zero. The temperature, pressure, and gas (calculated from the atmosphere, gas flow rate, and pressure) from the conditioning parameters are also used to write the input file. The input file is run through Thermochemica, and the output file is parsed for the predicted chemical composition of the fuel. The fraction of each gaseous species released is calculated using the radionuclide transport prediction capability described above and multiplied by the quantity of that gaseous species predicted to be present. Note that the thermochemical prediction of the bulk uranium chemical form(s) and fractions is also needed in order to select the appropriate diffusion coefficient(s) for (2 and (3). A schematic of this concept is shown in Figure 4.

Validation

4RFC needs to be validated in the future against available data. First, the individual models will need to be verified and benchmarked. The predicted radionuclide inventories will be benchmarked against internal CNL reports. The thermochemical predictions will be benchmarked against other thermochemical software, such as ThermoCalc, which is capable of reading the TAF-ID and performing calculations of large systems, such as irradiated fuel. The implementation of (2 and (3 in the radionuclide transport prediction capability in Python will be verified to function correctly against manual calculations. After the individual components of 4RFC are verified and benchmarked, the integrated tool can be validated. The prediction of radionuclide release will be validated against empirical radionuclide release data from experiments under the same conditions found in literature.

CURRENT STATUS AND FUTURE WORK

To date, a basic functioning simulation tool exists and works as expected. SCALE-ORIGEN modelling for only one fuel design has been completed; thus, future work will require additional modelling of all the additional fuel designs, including some additional research reactor models. The chemical form and transport calculations only function over a single time step. Multiple time steps and iterative solving needs to be implemented by splitting the conditioning time into a pre-defined series of time steps. The released radionuclide inventory will be subtracted from the system, along with any unreacted conditioning gas. The elemental composition will then be passed back to write a new Thermochemica input script, along with additional conditioning gas added for the next time step, and the system solved again for the next time step. This iterative solving between the thermochemical and radionuclide transport models will continue until all

time steps have been completed for the length of time of the conditioning. The sum of all the released radionuclides is then the prediction of radionuclide release.

Robust testing of the code will then be needed over a range of parameters to test for bugs. Verification as described above is required. Finally, the code repository used to manage the development of 4RFC will be made public and the tool released.

CONCLUSION

Non-oxide research reactor fuels may pose significant challenges for direct disposal in a DGR. Conditioning is a mitigation option but may result in radionuclide release during controlled oxidation and SPS. As there are no existing tools for predicting radionuclide release under these conditioning parameters, the 4RFC simulation tool is under development and the framework was presented. 4RFC predicts the radionuclide inventory present in the fuel of interest, predicts the chemical form of the radionuclides under the prevailing conditioning parameters, predicts the transport of radionuclides under these conditions over time, and integrates these three prediction capabilities into a single tool, with a GUI, to predict the radionuclide release during conditioning of research reactor fuel. Further work is required to fully develop the simulation tool and verification and benchmarking is required before the tool can be publicly released.

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