Loosely coupling of thermochemistry code to OpenMC for Chloride-based Molten Salt Reactor

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1. Introduction

Among Generation IV reactors, the Molten Salt Reactor (MSR) stands out due to the complex chemical behavior exhibited by fission products within the fuel salts. This chemical behavior significantly impacts fuel performance, making it essential to integrate neutronic codes with thermochemistry codes for reactor analysis, design and other systems design, such as off-gas management. This integration can be achieved either in a tightly or loosely coupled fashion, with the latter offering greater flexibility and modularity for addressing other complex multiphysics problems [1, 2]. In this study, we applied a loosely coupled approach between neutronic and thermochemistry codes to evaluate the chemical state of off-gas and the reactor core in a chloride-based MSR.

2. Methods and Results

In this section, the chloride-based MSR (Molten Salt Reactor) model is briefly discussed, and the strategy of loosely coupling between the neutronic code and the thermochemistry code is introduced.

2.1 OpenMC Model

The developed model employs a chloride-salt fuel consisting of 42.9 NaCl – 20.3 KCl – 36.8 UCl_3 with 99% ^{37}Cl enrichment. The thermal power of the reactor is 100 MWth, and the volume fraction of InCore is assumed to be 0.45. The recirculation flow rate between InCore and OutCore is assumed to be 641 liter/s. Flux calculations are performed using 250 batches of 50,000 particles, beginning with 100 inactive batches. For the neutronic code, OpenMC v 0.14.0 with the nuclear library of ENDF/B-VII is employed. The overall dimensions of the cylindrical-type of MSR model are schematically shown in Figure 1.

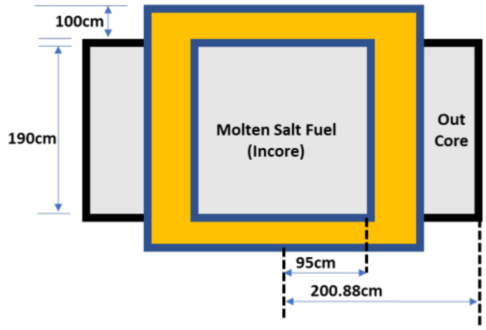

Fig. 1. Schematic diagram of chloride-based MSR

2.2 Dynamic Library of Thermochimica

The thermochemistry code, based on Gibbs free energy minimization, allows for the determination of species mole fraction, moles of phases, and other thermodynamic properties under given input conditions. In this study, Thermochimica [3], designed to integrate with multiphysics codes, was employed. Originally written in Fortran, Thermochimica needed to be adapted for use with OpenMC, which operates under a Python environment. This adaptation was accomplished in three steps: (1) compiling Fortran-based Thermochimica into a shared library, (2) wrapping the source code in C++ by creating wrapper functions and exposing these functions to Python using a binding library, and (3) building a Python-based Thermochimica by linking the shared library and C++ code. For the thermodynamic database, MSTDB-TC v4.0 and FactPS in FactSage were applied. Figure 2 shows a working example of Python based Thermochimica.

Fig. 2. Demonstration of python-based Thermochimica

2.3 Loosely Coupling between OpenMC and Thermochimica

The transformation from Fortran-based Thermochimica to Python-based Thermochimica enables the loosely coupling between OpenMC and Thermochimica more easily. In loosely coupling, the two codes perform calculations alternately. The neutronic code calculates the neutron flux and depletion, leading to the evaluation of the inventory of elements. Then, for input conditions including the inventory mass, the Thermochimica code calculates the phase distribution of chemical compounds by solving Gibbs energy minimization. The inventory for the next neutronic calculation is updated by subtracting the inventory of elements corresponding to the mass of chemical compounds in the gas phase from the inventory determined after performing depletion calculations.

As shown in Figure 3, the main difference between the original loosely coupling[2] and the current coupling is that the system pressure is determined by accounting for the amount of gas compounds released to the off-gas region. Since the release of gaseous chemical compounds contributes to the increase in system pressure, this should be included in the loosely coupling calculations.

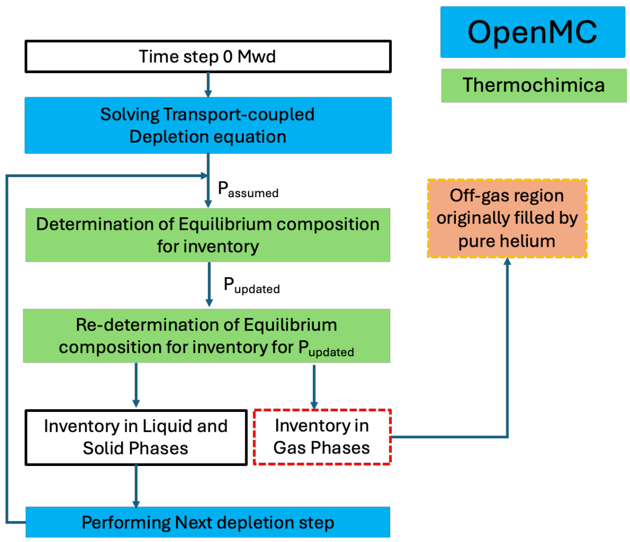

Fig. 3. Schematic diagram of loosely coupling with pressure adjustment.

2.4 Evaluated Chemical compound Inventory

Based on the loosely coupled approach, we have performed depletion calculations at one-year intervals during the 20-year operation of the Molten Salt Reactor (MSR). Figure 4 compares the neutron multiplication factors calculated by the OpenMC-based MSR model with and without loosely coupled Thermochimica. The loosely coupled model shows a slightly higher multiplication factor than the model without coupling because the evolved fission gas products including noble gases, determined from the equilibrium calculation, are not considered in the subsequent transport-coupled depletion calculation. The present approach allows to evaluate pressure buildup in cover gas region during reactor operation. Figure 5 demonstrates that pressure at cover gas region continuously increases if proper off-gas management system such as xenon trapping is not considered.

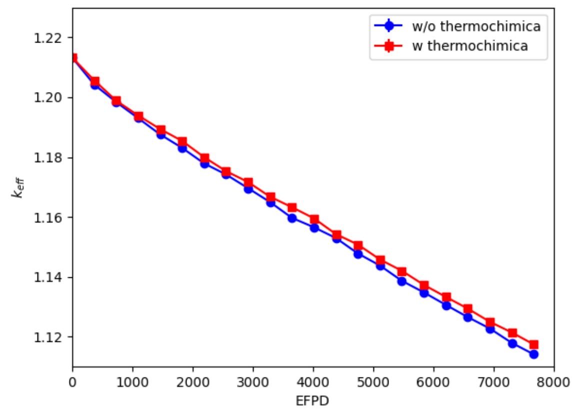

Fig. 4. Effect of the loosely coupling on the neutron multiplication factor

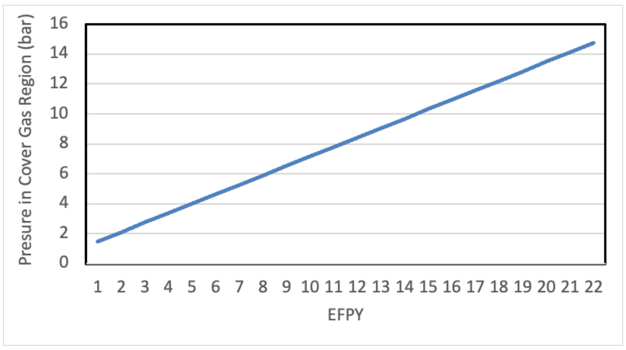

Fig. 5. Pressure buildup during reactor operation

Tables I and II show the evaluated gaseous and liquid chemical compounds, respectively. In the gaseous phase, noble gases are the most dominant, followed by Cd, $ZrCl_4$, and CsCl. In the liquid(or solution) phase, major fission elements were found to form chloride and iodide compounds. Except for ZrI_4, iodine was shown to form iodide compounds with the alkali metals of Group 1. Figure 6 shows the increasing ratio of UCl_4/UCl_3, a representative measure of the redox state in MSR salts, indicating that the fuel salt in the reactor core approaches an oxidizing state as reactor operation continues

Table I: Top 8 Annual release of Gaseous Chemical Compounds During the 20th Year of MSR Operation

Chemical species	Inventory mass(mol)
Xe	37.06
Kr	5.89
Ar	2.29
He	0.89
Cd	0.20
$ZrCl_4$	0.02
CsCl	1.62e-5
NaCl	4.45e-6

Table II: Top 15 Annual release of Liquidus Chemical Compounds During the 20th Year of MSR Operation

Chemical species	Inventory mass(mol)
$PuCl_3$	1152.82
$NdCl_3$	825.10
$CeCl_3$	736.89
CsCl	711.95
$ZrCl_4$	692.35
$BaCl_2$	272.06
$SrCl_2$	255.69
$LaCl_3$	211.88
$MgCl_2$	15.24
ZrI_4	6.12
$CaCl_2$	3.37
NaI	1.31
UCl_4	0.80
KI	0.38
CsI	0.28

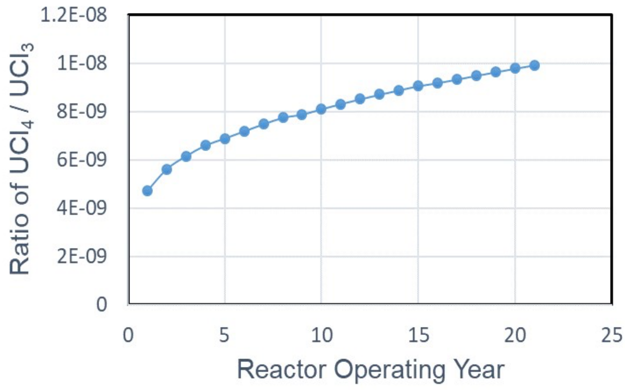

Fig. 6. Estimated ratio of UCl_4 to UCl_3

3. Conclusions

The loosely coupling between OpenMC and pythonbased thermochimica was applied to chloride-based MSR of 20 yr operation and the chemical compounds in gas and liquidus phases were identified. A study is continued that compares with the neutronic calculation without loosely coupling.

Acknowledgement

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