Effects of Group Constant Model on Multi-physics Analysis of Fast-spectrum Molten Salt Reactor with Beryllium Oxide Reflector

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1. Introduction

The use of liquid fuel in Molten Salt Reactors (MSRs) introduces unique properties such as direct heat generation within the fuel and a higher thermal expansion coefficient, which necessitate a coupled thermal-hydraulics (TH) and neutronics (N) multi-physics analysis. Concurrently, Beryllium Oxide (BeO) has been suggested as a reflector material for Fast-spectrum Molten Salt Reactors (F-MSRs) to harness the benefits of both fast and thermal spectrum [1,2].

The coexistence of fast and thermal neutrons in the BeO application complicates neutronics and thermal-hydraulics behavior, and consequently, the coupling between them. In particular, a multi-group diffusion analysis is highly dependent on the group constant model (energy-group structure and spatial homogenization method). While our previous study indicated that using a simplified model can simulate the overall behavior of the reactor [3], a high-fidelity analysis necessitates a robust model.

Therefore, this study evaluated the effects of group constant model on multi-physics analysis of a BeO application. Two group constant model were compared: the simplified model (7-group structure with single-region spatial homogenization) and the robust model (30-group structure with three-region spatial homogenization).

2. Methods and results

2.1 Multi-physics code

Multi-group diffusion analysis requires accurate group constant as input, and it was generated by OpenMC in this study [4]. The primary multi-physics analysis was performed using a modified GeN-Foam [5]. The main modification of GeN-Foam V2306 was to: 1) incorporate solid conduction and gamma heating in TH analysis, 2) consider feedback due to temperature change in reflector part, and 3) calculate adjoint neutronics and effective delayed neutron fraction, β_{eff}.

2.2 Reference geometry and conditions

The flow in F-MSRs is a highly multi-dimensional, as the core configuration is cavity with toroidal-shaped reflector (blanket), which can introduce geometric effect in the comparative study. To minimize these effects, a simple vertical cylinder was chosen as the reference geometry, as shown in Fig. 1. Besides the fuel and BeO reflector, internal structure should be presented for fuel cladding, and it is known to highly change the neutronics characteristics. To consider this, 5 mm of SS304 layer was added between fuel and reflector.

The composition of fuel salt is KCl-UCl_3 (46-54 mol%) with 99% enrichment of Cl-37. Relevant physical properties and reference conditions can be found in the previous study [3].

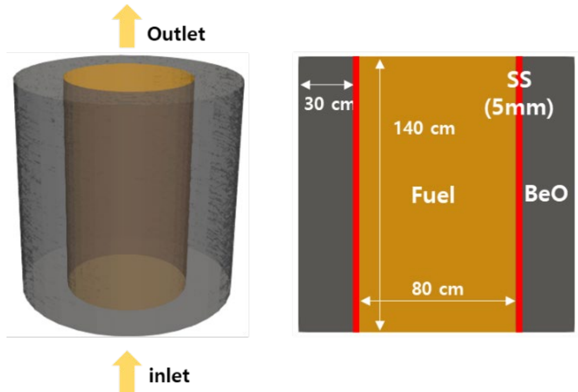

Fig. 1. Reference geometry for the analysis.

2.3 Group constant generation

The group constant is generated in a way to preserve individual reaction rates, as shown in equation (1), where Σ_x is an arbitral cross-section, ϕ is neutron flux, and E_g is discrete energy level. This definition indicates that the generated group constant is highly dependent on energy-group structure and spatial homogenization method.

$$\bar{\Sigma}_{x,k,g} = \frac{\int_{\boldsymbol{r} \in V_k} \int_{4\pi} \int_{E_g}^{E_{g-1}} \Sigma_x(\boldsymbol{r}, E)\phi(\boldsymbol{r}, E, \boldsymbol{\Omega})\, dE d\boldsymbol{\Omega} d\boldsymbol{r}}{\int_{\boldsymbol{r} \in V_k} \int_{4\pi} \int_{E_g}^{E_{g-1}} \phi(\boldsymbol{r}, E, \boldsymbol{\Omega})\, dE d\boldsymbol{\Omega} d\boldsymbol{r}} \tag{1}$$

For the comparative study, we compared two group constant model. The first, a simplified model, is detailed in previous work [3]. The second, a robust model is based on 30-group structure and six-region spatial homogenization.

Regarding the energy-group structure, a pre-defined ECCO-33 structure was used initially for the analysis. However, large discrepancy between OpenMC and GeN-Foam was observed in first three high-energy groups (1 to 3). Accordingly, the three groups were merged into the fourth group, resulting in the 30-group structure used in this study.

The refined spatial homogenization in the robust model is to consider different neutron spectrum and temperature behavior between core center and near-wall region. The spatial homogenization in the two model is illustrated in Fig. 2. For SS304 layer, single-region spatial homogenization was implemented for both models.

Prior to multi-physics analysis, pure multi-group diffusion analysis was conducted and the results indicated that the robust model significantly improves the accuracy; k_{eff} in OpenMC, robust, and simplified models are 1.16008+/-0.00013, 1.16059, 1.17638, respectively. The computing time for each condition is summarized in Table I.

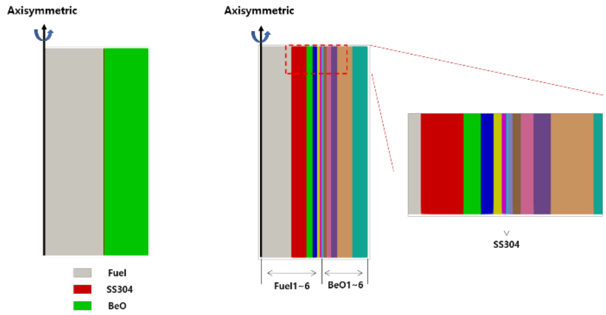

Fig. 2. Single-region (left) and six-region (right) spatial homogenization.

Processor	Condition	Computing time
AMD Ryzen Threadripper PRO 5995WX 2.7 GHz (8 cores were used in this study)	OpenMC	2618.8 s
	Robust model	292.8 s
	Simplified model	5.9 s

2.4 GeN-Foam setup

Fig. 3 illustrates the geometry and domain in GeN-Foam for the multi-physics analysis, in case of the robust model. To construct the axisymmetric geometry, a wedge-style geometry that represents 5° sector out of 360° full geometry was prepared, and the boundary conditions are summarized in Table II. The boundary condition for precursor outlet is to consider precursor decay in ex-core region. The corresponding flow residence time in ex-core region was set to 6.24 s, which is equal to in-core time.

The *solidThermals* (ST) domain was added through this study to account for solid conduction and gamma heating. A separate OpenMC simulation indicated that heat generation rate due to gamma heating was approximately 1.6% of the total power; this was applied as a uniform volumetric heat source in the reflector.

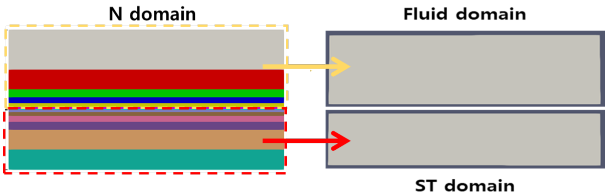

Fig. 3. Geometry and domain in GeN-Foam.

Table II. Boundary conditions for each domain.

Domain	Fields	Inlet	Outlet
Fluid	Velocity	5.8892 kg/s	InletOutlet
	Temperature	620°C	zeroGradient
	Pressure	FixedFlux Pressure	0.1 MPa
N	Neutron	Reflective	Reflective
	Precursor	outletMapped UniformInlet	zeroGradient
ST	Temperature	-	-
Domain	**Fields**	**Interface**	**Outer wall**
Fluid	Velocity	No-slip	-
	Temperature	Turbulent Temperature RadCoupled Mixed	-
	Pressure	FixedFlux Pressure	-
N	Neutron	-	Vacuum
	Precursor	-	fixedValue(0)
ST	Temperature	Turbulent Temperature RadCoupled Mixed	535°C

2.5 Multi-physics analysis results

To investigate the effects of group constant model on multi-physics analysis, three main parameters were examined: k_{eff}, T_{max}, and β_{eff}. Firstly, a base condition was estimated, where a simple mapping of velocity and power density fields were made from independent TH and N analysis. Then, three phenomena were added to the base condition sequentially, including: 1) solid conduction and gamma heating from the ST domain, 2) fuel movement in neutronics, and 3) cross-section feedback due to temperature change.

Table III compares the three main parameters depending on group constant model and calculation condition. Notably, using the simplified model yields a different baseline, particularly in neutronics analysis. In the aspects of thermal-hydraulics, the simplified model predicts a hot spot temperature approximately 9 K lower than that of the robust model, which can be critical to the material integrity.

While the effects of thermal analysis in the ST domain and fuel movement in the N domain do not show significant differences between the two models, the complete multi-physics analysis exhibits considerably different behavior depending on the group constant model. The simplified model overpredict the change in k_{eff}, and further, cannot predict the hot spot mitigation due to cross-section feedback. These results underscore the importance of employing a robust group constant model in multi-physics analysis.

Table III. Individual multi-physics effects.

Group constant model	Calculation condition	T_{max} (K)	k_{eff} (pcm)	β_{eff} (pcm)
Simplified model	Base	1046.75	1.17638	0.00715
	Solid conduction and gamma heating	1012.12	1.17638	0.00715
	Fuel movement in neutronics	1012.56	1.17337	0.00460
	Cross-section feedback	1012.55	1.17777	0.00460
Robust model	Base (nominal value)	1054.15	1.16059	0.00711
	Solid conduction and gamma heating	1016.67	1.16059	0.00711
	Fuel movement in neutronics	1017.07	1.15758	0.00454
	Cross-section feedback	1014.05	1.15962	0.00455

3. Conclusion

In this study, we investigated the effects of group constant model on multi-physics analysis of F-MSR with BeO reflector. Two group constant models were compared: the simplified model (7-group structure with single-region spatial homogenization) and the robust model (30-group structure with six-region spatial homogenization). In particular, effects of multi-physics phenomena on T_{max}, k_{eff}, and β_{eff} were examined.

The comparative study revealed that the simplified model provides less accurate results in the non-coupling case, particularly in neutronics analysis. Moreover, the complete multi-physics analysis shows considerably different behavior depending on the group constant model. Specifically, the simplified model fails to accurately estimate the hot spot mitigation.

As future work, we will examine the effects of group constant model on transient behavior, where multi-physics effects become more pronounced. The discrepancies between the two model under dynamic conditions will also be evaluated.

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