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Development and verification of a model for generation of MSFR few-group homogenized cross-sections based on a Monte Carlo code OpenMC

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ABSTRACT

A concept of molten salt fast reactor (MSFR) was proposed in EVOL to burn transuranium element discharged from pressurized water reactors. MSFR is featured by fast spectrum and using liquid fuel salt containing UF_4 or ThF_4. Some issues are presented, for instance, global material arrangement affects the local neutron spectrum due to long neutron free path, and fluoride salt (LiF-BeF_2) has nonnegligible thermal neutron scattering effect. Thus, lattice code prepared for thermal-spectrum reactor is not suitable for MSFR calculation. In this study, "two-step" calculation scheme combining Monte Carlo method and deterministic method was prepared for MSFR calculation. A tool named TRANS was developed to transfer tally data from an open source Monte Carlo code OpenMC into few-group homogenized cross-sections, and one benchmark based on pressurized water reactor and two types of model based on MSFR were used for verification. Besides, the applicability of few-group parameters generated by different model to MSFR whole-core calculation was analyzed. Finally, MSFR neutronics characteristics at steady-state were calculated using MOREL. The results show that the few-group parameters generated by one-dimension (1D) and two-dimension (2D) model are correct, and it is feasible to use OpenMC to generate few-group parameters. In case of 1D homogenization model, few-group parameters by 1D model (b) can give more accurate results both for eigenvalue and flux distribution. In MSFR whole-core calculation, using few-group cross-sections generated by 2D model has better accuracy in flux distribution, however, using few-group cross-sections generated by 1D model has better accuracy in k_{eff} calculation. Moreover, the neutronics parameters of MSFR calculated by MOREL code agree well with that by other institutes.

1. Introduction

Molten salt reactor (MSR) with the fuel dissolved into the liquid salt has been identified as one of the six Generation-IV reactor types in the Generation-IV International Forum (GIF-IV) due to its excellent advantages in terms of sustainability, non-proliferation, safety and waste management (Pioro, 2016). The history of MSR research dates back to 1950s-1980s, when the program of Aircraft Experiment (ARE) (Bettis et al., 1957), Molten Salt Reactor Experiment (MSRE) (Haubenreich, 1969) and the concept of Molten Salt Breeder Reactor (MSBR) (Rosenthal et al., 1972) were developed by Oak Ridge National Laboratory (ORNL). The feature of using liquid fuel in MSR system provides large flexibility in aspect of reactor design and fuel recycling scheme. Historically, thermal-spectrum MSBR with graphite moderator was proposed to breed fissile isotopes based on Th-U fuel cycle. Nowadays, fast-spectrum MSRs as an actinide burning reactor or breeder reactor interest researchers due to the global shortage of uranium resources and the increase of nuclear waste. The energy-dependent effective fission neutron number of fissile nuclide in fast energy region is greater than that in thermal energy region (Yang, 2012), thus, fast-spectrum MSR has more excellent breeding performance. A concept of Molten Salt Fast Reactor (MSFR) was proposed in EVOL (Evaluation and Viability of Liquid Fuel Fast Reactor System) to burn transuranium element (TRU) discharged from pressurized water reactors (PWRs) (Allibert et al., 2016; Fiorina et al., 2014). The primary feature of the MSFR concept versus that of other older MSR designs is the removal of the moderator and other structures from the active core (moderator-free core), which makes it possible to breed U233 based on fast neutron spectrum and thorium fuel cycle. Due to a unique potential (excellent

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safety coefficients, smaller fissile inventory, no need for criticality reserve, simplified fuel cycle etc.), the MSFR has been recognized as a long-term alternative to solid fueled fast neutron systems by the Generation IV International Forum as of 2008 (Serp et al., 2014).

In comparison with traditional solid-fuel reactor and graphite-moderator MSR, MSFR has some special characteristics due to the fact that the liquid fuel salt containing UF_4 or ThF_4 circulates through primary loop and moderator-free core leads to fast-spectrum. Firstly, MSFR has long neutron free path, weak local resonance self-shielding effect and strong global neutron spectrum coupling (Zhou, 2017). Thus, homogenization method considering global material arrangements need to be developed. Secondly, MSFR generally adopts fluoride salt (LiF-BeF_2) as carrier salt, which has nonnegligible thermal neutron scattering effect (Li et al., 2016). However, some lattice codes for PWR lack related thermal scattering data, and it would bring error if those codes are used for MSFR homogenization calculation. Thirdly, the delayed neutron precursors (DNPs) continuously change their position along with fuel circulation and decay in external loop, and the core multiplication factor is dependent on the fuel velocity field. Fourthly, the fact that the fuel is dissolved in the coolant rather than separated from the coolant by the claddings results in a much stronger coupling phenomenon between the neutronics and thermal-hydraulics.

Lot of efforts have been made to study MSR neutronics and thermal-hydraulics characteristics based on different methods and simplifications. Those methods are generally divided into two categories: direct method and "two-step" method.

The direct method refers to a method of directly using the original nuclear data for core calculation, usually with less assumptions. Monte Carlo method is the most common direct method. Heuer et al. and Nuttin et al. employed a Monte Carlo code MCNP (Briesmeister, 1997) and a home-made materials evolution code REM to study MSFR fuel cycle characteristics (Heuer et al., 2014; Nuttin et al., 2005). Aufiero extended the applicability of Monte Carlo code SERPENT (Leppänen et al., 2015) for MSFR effective delayed neutron fraction calculation based on one-group approximation (Aufiero et al., 2014). The MSFR study in The Kurchatov Institute was performed by coupling MCNP-4B and the ORIGEN2.1 code (Brovchenko and Merle-Lucotte, 2013). Aufiero et al. extended SERPENT-2 code for burn-up calculations by taking into account online fuel reprocessing (Aufiero et al., 2013). "Two-step" method is a classical method for core neutronics calculation. Fiorina et al. adopted ECCO cell code to generate few-group cross-sections, then investigated the MSFR core physics and fuel cycle characteristics with ERANOS code (Fiorina et al., 2013). Zhang et al. and Wang and Cao et al. developed MSR code by using DRAGON or HELIOS code for two-group homogenization calculation (Wang and Cao, 2016; Zhang et al., 2009). Linden employed SCALE6 to obtain cross-sections of nine energy groups based on one-dimension (1D) geometry model (Linden, 2012). Frima used 1D transport code XSDRNPM to generate few-group cross-sections based on an equivalent two-dimensional model considering MSFR radial and axial material arrangement (Frima, 2013). In Helmholtz-Zentrum Dresden-Rossendorf, HELIOS 1.10 code system with the internal 47 energy group library was used for MSFR simulations (Rachamin et al., 2013). Fridman et al. generated three-group cross-sections of the core and blanket region using SERPENT code, then performed whole-core deterministic calculations (Fridman and Leppänen, 2011; Tuominen, 2015). Some researchers developed the fuel cycle analysis procedures for MSRs based on SCALE/TRITON (Powers et al., 2013; Sheu et al., 2013; Yu et al., 2017). Zhou et al. and Hu et al. used Monte Carlo code OpenMC (Romano et al., 2015) to generate multi-group cross-sections, but without verification of homogenization geometry model and few-group cross-sections (Hu et al., 2017; Zhou et al., 2018).

Some deficiencies are found in above mentioned MSFR studies. Firstly, even though the Monte Carlo method is flexible for reactor with complex geometry and neutron spectrum, it still spends a lot of computational time in whole-core simulations. And "two-step" calculation scheme shows an advantage in terms of computational time. Secondly, DRAGON and HELIOS codes are usually used for analysis of thermal-spectrum reactors, and a typical thermal spectrum is used for the weighting of their multi-group master libraries. The applicability of those multigroup nuclear data libraries for MSFR has not been demonstrated so far. Thirdly, in MSFR, local neutron spectrum will be affected by global material arrangements due to long neutron free path, and the few-group cross-sections may differ as a function of space, even within the same material. Therefore, it is necessary to develop homogenization model considering global material arrangement for MSFR calculations. Besides, most researchers lack detailed verifications of the accuracy of few-group cross-sections. Fourthly, Monte Carlo code SERPENT is a good choice to generate few-group homogenized cross-sections, however, SERPENT code is only accessed by member institutes.

This study aims to develop a method and model for generating few-group homogenized cross-sections for MSFR whole-core calculation, and to verify comprehensively few-group cross-sections. Considering the advantages of Monte Carlo method and deterministic method, arbitrary energy group structure definition and geometric flexibility for the former and excellent computational efficiency for the latter (Leppänen et al., 2015; Li, 2012; Romano et al., 2015; Wang et al., 2010), "two-step" calculation scheme combining Monte Carlo method and deterministic method was prepared for MSFR calculation. An open source Monte Carlo code OpenMC (Romano et al., 2015) developed by Computational Reactor Physics Group at Massachusetts Institute of Technology (MIT) was used to generate few-group homogenized cross-sections. However, OpenMC can't directly output few-group parameters, thus, a tool named TRANS was developed to transfer tally data of OpenMC into few-group parameters and the method is described in Section 2.1. Furthermore, one benchmark based on PWR, and 1D and two-dimension (2D) models based on the MSFR core configuration were employed to verify the process of generating few-group cross-sections. 1D model only considers radial material arrangement and 2D model represents actual 2D R-Z MSFR system. Then, few-group cross-sections produced by 1D and 2D model were respectively employed in MSFR whole-core calculation, and OpenMC results serve as reference. The neutron flux distribution using few-group parameters generated by 2D model show a better agreement with reference compared with that using few-group parameters generated by 1D model. Finally, a MSR analysis code MOREL (Zhuang et al., 2015) developed in our previous study was performed to calculate the temperature coefficients and effective delayed neutron fraction based on few-group parameters generated by 2D model. To prevent confusion, in the full text, 'steady state' indicates system/core reaches a steady state, however, 'static condition' and 'flow condition' represent fuel salt motion state.

2. Methodology and numerical method

The overview flowchart of generating few-group cross-sections based on OpenMC code is depicted in Fig. 1: 1) temperature-dependent continuous-energy neutron data library in ACE format is produced by NJOY code based on ENDF/B-VII.1 library (MacFarlane and Muir, 1994); 2) Reaction rates of different reaction types and neutron flux are tallied in OpenMC calculation; 3) An in-house development tool TRANS is used to transfer tally data into few-group cross-sections for the following whole-core calculations.