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Coupled neutronics and thermal-hydraulics simulation of molten salt reactors based on OpenMC/TANSY



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ABSTRACT

An OpenMC/TANSY code system has been developed in this paper for the coupled neutronics and thermal-hydraulics simulations of MSRs. The homogenized cross section data library is generated using the continuous-energy Monte-Carlo code OpenMC which provides significant modeling flexibility compared against the traditional deterministic lattice transport codes. The few-group cross sections generated by OpenMC are provided to TANSY which is based on OpenFOAM to perform the full-core coupled neutronics and thermal-hydraulics simulations. In order to verify the OpenMC/TANSY code system, the Molten Salt Fast Reactor benchmark problem was calculated and both the neutronics results and thermal-hydraulics results were compared with those obtained by other researchers. For application of the OpenMC/TANSY codes sequence, the simulation of a representative molten salt reactor core MOSART has been performed. First, to verify the generation of the few-group cross sections, the neutronics results obtained by the "two-step" scheme were compared with those obtained by full-core Monte-Carlo solution. Good agreement can be observed for the multiplication factor as well as the power distributions. Then the full-core coupled neutronics and thermal-hydraulics simulation was performed. The distribution of the important neutronics and thermal-hydraulics parameters are presented and analyzed in detailed in this paper. For the further study of the characteristics of MSRs, several effects like the external-loop transit time, inlet velocity and inlet temperature on the effective delayed neutron fraction and critical fuel concentration have been analyzed. The numerical results indicated that the TANSY code with the cross section library generated by OpenMC has the capability for the steady-state analysis and reactor core design of MSRs.

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1. Introduction

The Molten Salt Reactor (MSR) has been identified as one of the candidates for the generation-IV reactors (Generation IV International Forum, 2002). It presents a promising flexible option in response to the goals and criteria assigned to the future nuclear systems as its fuel-cycle sustainability, safety, environmental impact, proliferation resistance, diversity of applications and economics. Historically, MSRs have been the thermal-neutron reactors in which the neutrons in the reactor core are moderated by unclad graphite. Today both thermal and fast spectrum MSRs are being investigated (Forsberg, 2007). The fast-spectrum MSRs is featured by homogeneous reactor core with no requirement for the moderating media in the core and are structurally simpler than the thermal-spectrum MSRs. Since the fast-spectrum MSRs have the unique advantages for the actinide burning and extending fuel

resources besides the common advantages owned by all MSRs like excellent neutron economy, flexibility of fuel cycle and inherent safety, it is worthy to investigate the core behavior of the fastspectrum MSRs.

The fluid nature of fuel in MSRs gives extra flexibility in reactor design, fuel fabrication and recycling. But because of the application of fluid fuel, MSRs have several special characteristics compared with the traditional solid-fuel reactors. Firstly, the transport of the delayed neutron precursors by the fluid flow reduces the contribution of delayed neutrons to the chain reaction. As a consequence, the multiplication factor (k_{eff}) is not independent of the delayed neutron fraction and the fluid velocity field (Mattioda et al., 2000). Secondly, 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. Thirdly, the shape of the fuel is determined by the container because of the characteristics of fluid, the unstructured meshes are required to model the complex geometry accurately. However most of the conventional



reactor codes were developed for solid-fuel reactor and therefore not capable of taking liquid fuel flow into account. So, we aim to develop a code system which can address all these modeling issues of MSRs in this study.

All these particular characteristics mentioned above must be addressed in the analysis of the MSRs. Although the Monte-Carlo code systems have the advantages in performing the direct whole-core heterogeneous calculation with the geometric modeling flexibility, it is not efficient enough to handle the neutronics calculation with the fluid fuel and difficult to be coupled with the thermal-hydraulics codes. So, the traditional "two-step" scheme is applied for the simulations of the MSRs. In this study, we use the Monte Carlo code OpenMC (Romano and Forget, 2013) to generate the homogenized few-group cross sections and then perform the whole core neutronics/thermal-hydraulics coupling analysis by use of deterministic methods. In the core analysis stage, we solve both neutron diffusion equation and thermo-fluid equation based on the Finite Volume Method (FVM). With this strategy, the important and particular issues of MSRs mentioned above can be solved appropriately.

For the lattice calculations, the homogenization of the fastspectrum molten salt reactor is much more sensitive to both the selection of the multi-group energy bounds and the number of groups (Chin et al., 2013). In the previous researches, some of the homogenization calculations were implemented by DRANGON or HELIOS with the two-group diffusion theory (Zhang et al., 2009a, b; Wang and Cao, 2016), but these codes were originally developed for thermal-spectrum solid-fuel reactors and their applicability for MSRs has not been demonstrated so far. Earlier analysis for the fast-spectrum was also performed by the Monte-Carlo code Serpent but with only one-group neutron (Aufiero et al., 2014a). And all these homogenized cross sections are not well verified. In our work, since the choice of the arbitrary energy group structure is possible, the homogenized 26-group cross sections are selected and generated using OpenMC (Romano and Forget, 2013). In order to verify the generation process of the few-group cross sections. the results obtained by the "two-step" scheme using the fewgroup cross sections provided by OpenMC are compared with the direct full-core heterogeneous calculation results obtained by OpenMC.

For the full-core coupled neutronics and thermal-hydraulics calculation, several codes have been developed with the structured meshes (Yamamoto et al., 2005; Wang et al., 2006; Krepel et al., 2005; Krepel et al., 2007; Zhang et al., 2009a; Zhang et al., 2009b; Nagy et al., 2014) or unstructured meshes (Cammi et al., 2011; Aufiero et al., 2014b). As the unstructured meshes have the capability of characterizing the complex geometry, a full-functional unstructured-mesh based code system has been developed in this work. Besides the coupled simulations, the calculation of the safety-related parameter effective delayed neutron fraction and the critical fuel concentration are also capable in our developed code. With the notable advantages of the thermalhydraulics capability, automatic matrix construction and solution capabilities for the scalar and vector equations, the open source C ++ library OpenFOAM (Weller et al., 1998; Jasak et al., 2007) has been selected as the development base for the full-core coupled neutronics and thermal-hydraulics calculation. In previous OpenFOAM based solvers, the solution region was restricted in the fluid region thus the reflectors have to be represented by albedo boundary condition (Aufiero et al., 2014a, b). With these simplification and approximation, the power distributions near the reflectors were not accurate. In this work, an OpenFOAM based multi-region solver has been developed. It allows the different solution regions for neutronics and thermal-hydraulics calculation to provide more flexibility in modeling and accuracy in simulation results.

The paper is organized as follows. Section 2 describes the theories and methods for the neutronics and thermal-hydraulics, with the coupling scheme also presented. Section 3 contains the numerical results for the verification of the simulation capability of the self-developed code TANSY and numerical results of the molten salt reactor MOSART are also presented. Conclusions and some proposals for future area of investigations are given in section 4.

2. Theories and methods

2.1. Overview of the "two-step" scheme

Since the direct heterogeneous calculation for the whole core is quite complicated and time-consuming, the traditional "two-step" scheme for the neutron-physics calculations is adopted for the simulation of MSRs. The calculation procedure is described in Fig. 1. The simulation of MSRs core is performed with the following steps, i.e. the generation of the few-group cross sections, the functionalization of the group cross sections and the full-core coupled neutronics and thermal-hydraulics simulation. Firstly, the fewgroup cross sections are generated by using OpenMC. Then the in-house developed code NECP-Lilac is adopted for the functionalization of the few-group cross sections. Finally, the full-core coupled neutronics and thermal-hydraulics calculation is performed by TANSY, a self-developed code based on FVM.

2.2. The generation of the few-group cross section

The approach for the generation of the few-group cross sections to be used by the TANSY code is introduced in detailed in this subsection.

In MSRs, the shape of the molten salt is determined by the container. So the geometries of the homogenization regions may be complex, depending upon the specific reactor design. Conventional deterministic lattice transport codes were designed to treat the regular geometry such as square or hexagonal assembly in the traditional solid-fuel reactors. Therefore, the homogenization of MSRs is beyond the capabilities of these codes. However the geometric modeling flexibility of the Monte-Carlo codes makes it appropriate for the generation of few-group cross sections for MSRs. The OpenMC code developed by MIT is capable of handling complex geometry without any major approximations and hence can be used to generate cross section data for MSRs. Besides the accuracy of geometric modeling, it can also calculate the homogenized fewgroup cross sections in an arbitrary energy group structure. However, high computational cost is the major limitation of this method. For this reason, the two-dimension R-Z homogeneous core model is used for the generation of the few-group cross sections in this work.



Fig. 1. "Two-step" scheme.

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