

Multiphysics Modeling and Adjoint-based Sensitivity Analysis of Molten Salt Reactor

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1. Introduction

Molten salt reactor (MSR) is one of the most promising reactor concepts among generation IV reactor design concepts in terms of safety and sustainability. In fact, the concept of liquid fueled MSR was demonstrated successfully by MSRE with aims of Oak Ridge National Laboratory of USA in 1950s. Eutectic mixture of uranium and plutonium or thorium with molten salt takes a role of both fuel and coolant. Liquid state fuel brings lots of advantages from its characteristics in terms of inherent and passive safety, as well as waste management or resource utilization.

In case of MSR, a circulating liquid fuel system, transport of the delayed neutron precursors from fuel salt flow influences neutron flux distribution and overall power distribution due to their decay at different location in the reactor core [1]. In addition, small variation of temperature affects thermophysical properties of salt, for instance, density, which determines a reactivity feedback coefficient as well. From its strongly coupled physics behavior; i.e. neutronics and thermal-hydraulics, Multiphysics approaches is required for design and analysis of the MSR.

This paper introduces the adjoint method for sensitivity analysis applied to a circulating liquid fuel system and investigates with model sensitivity on the Multiphysics approach. Molten salt fast reactor (MSFR), developed by EURATOM EVOL project [2] was chosen as a representative case of the circulating liquid fuel system, shown in Fig. 1.

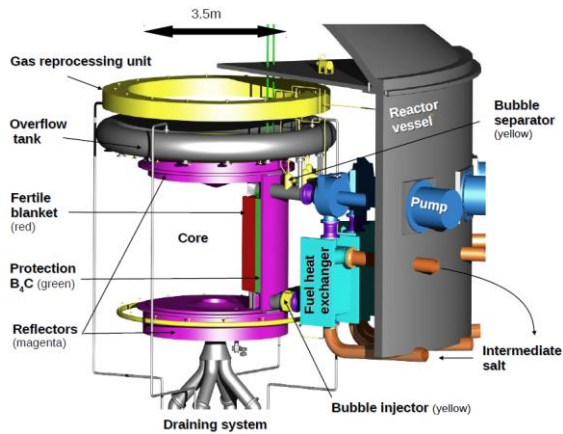


Fig. 1. Configuration of MSFR primary loop [2]

2. Multiphysics Modeling

Multiphysics model of liquid-fueled MSR includes neutronics and thermal-hydraulics; they should be solved at the same time. Considering flow effect of fuel salt, convection term is included in both neutron precursor and decay. This modeling approach was adopted into OpenFOAM Multiphysics solver [3] and verified by benchmarking against previously published simplified models for circulating liquid fuel system [4]. Besides, the need for model sensitivity analysis for this system has been emerged.

In this study, one group neutron diffusion equation and 8 groups of neutron precursor balance equations for neutronic part and energy balance equation and 3 groups of decay heat group balance equation for thermal-hydraulic part from equation (1) to (4) with constant mass flux G . Circulating liquid fuel loop in one dimensional, steady state is modeled by components consisting a reactor core, heat exchanger, hot leg and cold leg without radial blanket or top/bottom reflector, shown in Fig. 2. To distinguish each part, fission generation term, $\nu\Sigma_f$ in (1) and heat transfer coefficient h in (3) are considered only for core and HX, respectively.

$$-\nabla \cdot (D\nabla\phi) + \left(\Sigma_a - \frac{1-\beta_l}{k_{eff}} \nu\Sigma_f \right) \phi = \sum_{i=1}^8 \lambda_i c_i \quad (1)$$

$$-\nabla \left(\frac{G}{\rho} c_i \right) + \nabla \cdot \left(\frac{v_T}{Sc_T} \nabla c_i \right) - \lambda_i c_i + \beta_i \frac{\nu\Sigma_f}{k_{eff}} \phi = 0 \quad (2)$$

$$\nabla(GC_p T) = -\frac{hp}{A_c}(T - T_w) + (1 - \beta_{h,i}) E_f \Sigma_f \phi + \sum_{i=1}^3 \lambda_{n,i} d_i \quad (3)$$

$$-\nabla \left(\frac{G}{\rho} d_i \right) + \nabla \cdot \left(\frac{v_T}{Sc_T} \nabla d_i \right) - \lambda_{n,i} d_i + \beta_{h,i} E_f \Sigma_f \phi = 0 \quad (4)$$

, where ϕ is a neutron flux, c_i is a concentration of i -th group of neutron precursor, d_i is an energy density of i -th group of decay heat precursors, and T is a salt temperature respectively.

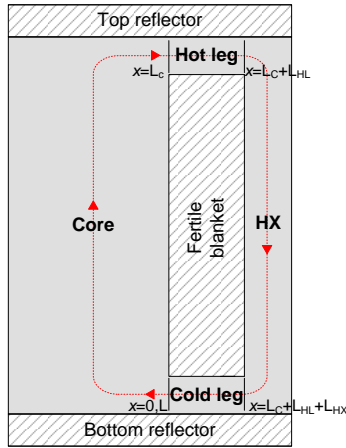


Fig. 2. Schematics of a circulating liquid fuel system

3. Adjoint-based Sensitivity Analysis

For the system equation, $Av=f$ where A is a primal operator, v is a primal function consisting all system variables, adjoint system, $A^*v^*=g$ can be established corresponding adjoint operator A^* and adjoint function v^* showing Lagrange's identity, defined as equation (5). In this case, g can be any function of interests.

$$(Av, v^*) = (v, A^*v^*), \text{ where } (v, w) = \int_{\Omega} vw \, d\Omega \quad (5)$$

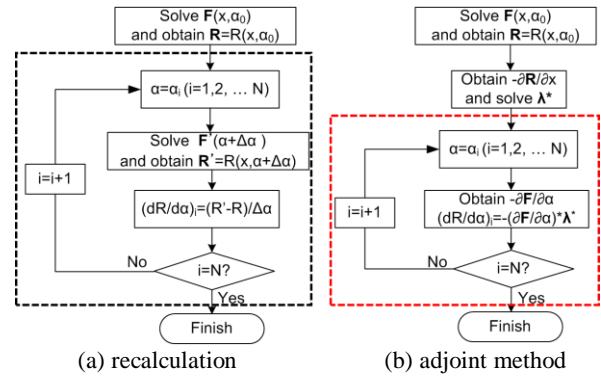
Sensitivity analysis for system response \mathbf{R} , $d\mathbf{R}/d\alpha$ has been conducted by recalculating system response to each model parameter α , traditionally. Or, sensitivity of system response can be evaluated by directly calculating the derivatives of primal functions \mathbf{F} with respect to α , $\lambda=d\mathbf{F}/d\alpha$. Instead, corresponding adjoint functions, λ^* having duality with λ can calculate sensitivity of \mathbf{R} to each parameter efficiently [5]. Fig. 3 shows the comparison of sensitivity analysis procedure in numerical way.

Multiphysics modeling of MSR described in section 2 includes several models; temperature dependencies of nuclear data and thermophysical properties of fuel salt; density and specific heat capacity. For instance, cross section and salt density are updated from temperature as (6) and (7).

$$\Sigma = \frac{\rho}{\rho_o} \left[\Sigma_o + \alpha_{\Sigma} \log \left(\frac{T}{T_{ref}} \right) \right] \quad (6)$$

$$\rho = a_{\rho} T + \beta_{\rho} \quad (7)$$

In addition, kinetic constants for both neutron precursors and decay heat groups are calculated values including fuel salt motion [4]. Extending this to Multiphysics system, Adjoint method is applied to sensitivity analysis for the circulating liquid fuel system for operation condition of MSFR.



(a) recalculation (b) adjoint method
Fig. 3. Comparison of recalculation and adjoint method on the parameter sensitivity analysis

Importance of total 39 model parameters are compared for the various types of system response with sensitivity coefficient S , the magnitude of normalized by the magnitude of parameter and system response, $dR/d\alpha * \alpha / R$ shown in Fig. 4. Two most influencing parameters are reference values of absorption cross section (SA0) and fission generation term (NSF0), since neutron flux governs all field variables for all types of system response in this case. In addition, wall temperature of primary side of heat exchanger (T_w) have high importance on determining fission and decay power. This implies that temperature field as also dominant influence on the overall system behavior from heat exchanger design, which is not yet determined.

Likewise, other model parameters can be interpreted for any type of system response other than fission power or decay power indicated in this paper as of interest using adjoint method. For all parameters and types of system response, adjoint method can predict sensitivity within $\pm 10\%$ compared with recalculated results including coupled system characteristics. Moreover, computational resources required for sensitivity analysis is reduced significantly with adjoint method. Fig. 5 shows the comparison of computation time for sensitivity analysis of MSR in this study using recalculation and adjoint method with respect to number of model parameters.

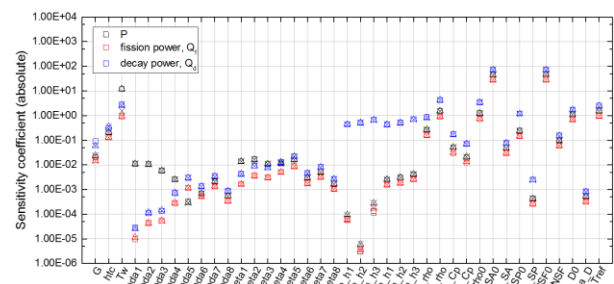


Fig. 4. Importance of model parameter to P, fission power, and decay power (x: recalculation, square: direct, triangle: adjoint)

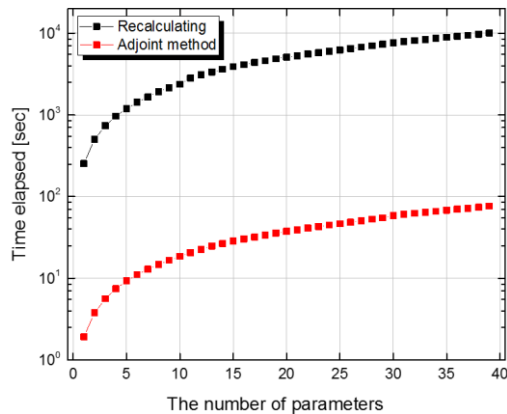


Fig. 5. Comparison of time elapsed for computing sensitivity of system response with recalculation and adjoint method

4. Summary and Future Work

In this paper, Multiphysics modeling and adjoint-based sensitivity analysis method for the molten salt reactor are introduced. With many advantages of the adjoint method, sensitivity of 3 types of system responses to the 39 model parameters are evaluated for MSFR case, including temperature dependencies of nuclear data and salt properties, calculated values of kinetic constants for precursors, and reactor design parameter. Adjoint method can predict within $\pm 10\%$ accuracy for all data with 77.3 times less computational time, compared to method of recalculating system response. Adjoint method has strong advantages for its applicability based on the straightforward mathematical background, such that it can be applied to any system involving multiple and interacting physics: turbulent reacting flows, combustion problems, or thermomechanics are just few examples. In this view, current work is extended to future implementation of adjoint method in 3D simulation tools for nuclear reactor analysis such as Multiphysics toolkit, OpenFOAM [6], as a design and analysis code for molten salt reactor.

ACKNOWLEDGEMENTS

This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Korea government(MSIT) (No. 2017R1A2B2008031).

REFERENCES

- [1] A. Cammi, V. D. Marcello, L. Luzzi, V. Memoli, M. E. Ricotti, A multi-physics modelling approach to the dynamics of Molten Salt Reactors, *Annals of Nuclear Energy*, Vol. 38, p. 1356-1372, 2011.
- [2] M. Brovchenko, D. Heuer, E. Merle-Lucotte, M. Allibert, N. Capellan, V. Ghetta, A. Laureau, Preliminary safety calculations to improve the design of Molten Salt Fast

Reactor, Proceedings of the PHYSOR2012, Knoxville, USA, April 15-20, 2012.

[3] M. Aufiero, A. Cammi, O. Geoffroy, M. Losa, L. Luzzi, M. E. Ricotti, H. Rouch, Development of an OpenFOAM model for the Molten Salt Fast Reactor transient analysis, *Chemical Engineering Science*, Vol. 111, pp. 390-401, 2014.

[4] M. Aufiero, M. Brovchenko, A. Cammi, I. Clifford, O. Geoffroy, D. Heuer, A. Laureau, M. Losa, L. Luzzi, E. Merle-Lucotte, M. E. Ricotti, H. Rouch, Calculating the effective delayed neutron fraction in the molten salt fast reactor: Analytical, deterministic and Monte Carlo approaches, *Annals of Nuclear Energy*, Vol. 65, p. 78-90, 2014.

[5] D. G. Cacuci, *Sensitivity and uncertainty analysis: Theory*, Vol. 1, Chapman & Hall/CRC, Boca Raton, 2003.

[6] "OpenFOAM | The OpenFOAM Foundation." [Online]. Available: <https://openfoam.org/>.