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COUPLED REACTOR KINETICS AND HEAT TRANSFER MODEL FOR NUCLEAR REACTOR TRANSIENT ANALYSIS

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ABSTRACT

Coupled reactor kinetics and heat transfer models have been developed at the University of California, Berkeley (UCB) to study Pebble-Bed, Fluoride-salt-cooled, High-temperature Reactors (PB-FHRs) transient behaviors. This paper discusses a coupled point kinetics model and a two-dimensional diffusion model. The former is based on the point kinetics equations with six groups of delayed neutrons and the lumped capacitance heat transfer equations. To account for the reflector effect on neutron lifetime, additional (fictional) groups of delayed neutrons are added in the point kinetics equations to represent the thermalized neutrons coming back from the reflectors. The latter is based on coupled multi-group neutron diffusion and finite element heat transfer model. Multi-group cross sections and diffusion coefficients are generated using the Monte Carlo code Serpent and defined as input in COMSOL 5.0.

INTRODUCTION

Pebble-Bed, Fluoride-salt-cooled, High-temperature Reactors (PB-FHRs) use TRISO fuel particles in spherical fuel elements and fluoride-lithium-beryllium (flibe) salt coolant. FHR type of reactors receive international consideration because of their intrinsic safety features and economic advantages.

The Mk1 PB-FHR [1] is an initial pre-conceptual design for a 236 MWth PB-FHR at the UCB as a part of an U.S. Department of Energy Integrated Research Project. The MK1 PB-FHR uses 3.0-cm annular fuel pebbles (Figure 1) that are composed of three spherical shell layers: a low-density graphite core, a fuel layer with TRISO particles dispersed in a graphite matrix, and a graphite shell. The TRISO particles contain a fuel kernel, a porous buffer layer, a pyrocarbon layer, a silicon carbide layer and an outer pyrocarbon layer.

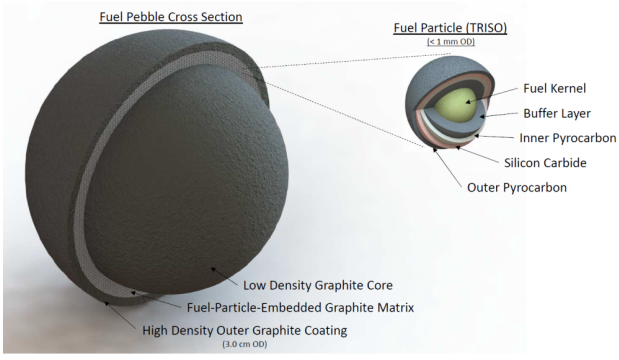

Figure 1: Schematic of the fuel pebble element in FHRs [credit: Grant Buster, UCB]

As shown in Figure 2, the Mk1 PB-FHR has an annular pebble bed core surrounded by the center and outer reflectors. Approximately 30% of the coolant enters from the bottom inlet of the core, while the remaining 70% is

injected from the center reflector and forms mainly cross flow.

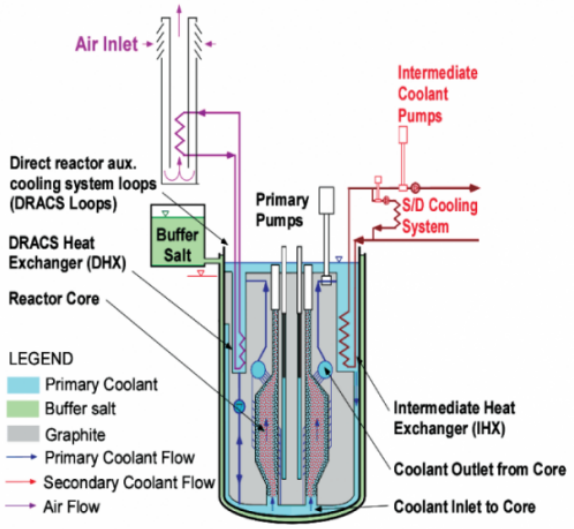

Figure 2: Schematic of Mk1 FHR core design [1]

In China, the Shanghai Institute of Applied Physics (SINAP) plans to construct a 10 MWth Thorium-based Molten Salt Reactor (TMSR-SF1) that uses 6.0 cm diameter spherical fuel elements and flibe salt in the core. The differences in the fuel design between the MK1 PB-FHR and the TMSR-SF1 can be seen in Figure 1 and Figure 4. In the TMSR-SF1 fuel pebbles, TRISO particles are dispersed uniformly in a graphite matrix. The fuel matrix is covered in a 5mm thick graphite shell. As shown in Figure 3, the TMSR-SF1 core doesn't have center reflector as in the Mk1 PB-FHR design, coolant enters at the bottom inlet and flows upward across the pebble region. An outer graphite reflector surrounds the core, providing neutron moderation and reflection. Fuel pebbles are buoyant in the flibe salt and fills the upper region at a packing fraction of 60%, while the lower region of the core is left with flibe salt.

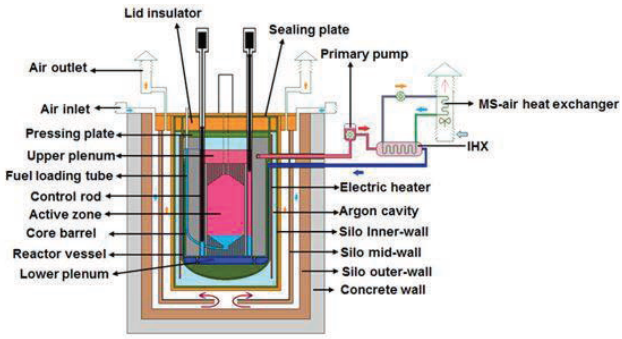

Figure 3: Schematic of TMSR-SF1 core design [2]

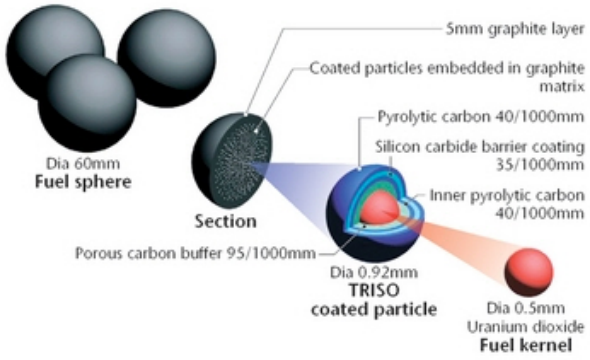

Figure 4: Schematic of the TMSR-SF1 fuel elements

Reactor system response to anticipated transient without scram (ATWS) accidents couples thermal-hydraulics and neutronics. Software used to model such scenarios, as required for licensing nuclear reactors, must therefore couple these physics. This paper discusses two approaches of coupling thermal-hydraulics and neutronics for FHR transient analysis: a model based on the point kinetics equations with six groups of delayed neutrons and the lumped capacitance heat transfer equations and a two-dimensional model that couples multi-group neutron diffusion and finite element heat transfer model.

NOMENCLATURE

A	Surface area
C	Delayed neutron precursor concentration
D	Diffusion coefficient
g	Heat generation density
nd	Number of delayed neutron precursor groups
nr	Number of reflectors
$\dot{m}$	Mass flow rate
k_{eff}	Effective multiplication factor
Re	Reynolds number
Pr	Prandtl number
P	Nuclear power
r	Radius
Ts	Solid temperature
Tf	Fluid temperature
u	superficial velocity $u = \dfrac{\dot{m}}{A\rho}$

Greek symbols

ρ	Density
ρ	Reactivity
λ	Decay constant
Σ_R	Removal cross section
$\Sigma_{sg'g}$	Scattering cross section from group g to g'
ν	Average number of neutrons emitted per fission
Σ_f	Fission cross section
χ_g	Fraction of neutrons born in group g
β	Effective delayed neutron fraction

Λ Effective prompt neutron generation time

Subscripts
i Delayed neutron precursor group number
R Reflector
j Reflector number
g Neutron energy group number

COUPLED HEAT TRANSFER AND POINT KINETICS MODEL

MULTI-POINT KINETIC EQUATIONS

Both the Mk1 PB-FHR and the TMSR-SF1 core contains substantial graphite reflectors that provide moderation and reflection. The reflector thickness is comparable to other neutron free path length scales in the core. Neutrons from the fuel region are transported to the reflectors (where the control rods are located), scatter within the reflectors for some time, and come back to the fuel region to initiate a fission reaction. As shown in Table 1, k_{eff} and prompt neutron lifetime changes dramatically with different reflector configurations. Therefore the effects of reflector neutron moderation must be considered.

Table 1: Effect of reflectors on k_{eff} and prompt neutron lifetime.

Configuration	k_{eff}	Effective prompt neutron lifetime (ms)
Fuel and both reflectors	1.03	0.459
Fuel and outer reflector	0.95	0.384
Fuel and inner reflector	0.88	0.399
Fuel only	0.73	0.227

The (standard) point kinetics equations characterize reactor dynamics by computing time dependent neutron population and delayed neutron precursor concentrations. However it uses averaged neutron lifetime in the reactor core and doesn't take into account the reflector effects on neutron lifetime in a heterogeneous reactor. Multi-point kinetics equations model the slow neutrons coming back from the reflectors into the fuel region in each configuration as additional delayed neutron groups from fictitious neutron [3]. The reflector-induced effects is characterized by the reactivity gain by the reflector ρ_R and the neutron lifetime in the fuel region and in the reflector Λ_R.

The multipoint kinetics model is formulated for FHR cores with additional fictitious delayed neutron groups as follows:

$$\frac{dP(t)}{dt} = \frac{(\rho_{ext}(t) - \beta - \rho_{Ri} - \rho_{Ro})}{\Lambda_c} P(t) + \sum_{i=1}^{nd} \lambda i\, Ci(t) + \lambda_R C_R(t) \quad (1.1)$$

$$\frac{dCi(t)}{dt} = \frac{\beta i}{\Lambda_c} P(t) - \lambda i\, Ci(t),\ i = 1...nd \quad (1.2)$$

$$\frac{dC_{Rj}(t)}{dt} = \frac{\rho_{Rj}}{\Lambda_c} P(t) - \lambda_{Rj} C_{Rj}(t),\ j = 1...nr \quad (1.3)$$

In the multipoint kinetics model, prompt neutron generation time in the fuel region and in the reflectors is distinguished. Λ_c is the prompt neutron generation time in the core, without any reflectors. $\lambda_{Rj} = 1/\Lambda_{Rj}$, where Λ_{Rj} is lifetime of neutrons going in the jth reflector and producing a fission in the core after coming back from the reflector(s). This value can be calculated from Λ_{prt}, the mean prompt neutron lifetime in the reactor with all neutron reflectors, and Λ_{cj}, the prompt neutron generation time in the core with only the jth reflector, by the following relation:

$$\Lambda_{prt} = (1 - \rho_{Ri})\Lambda_{ci} + \rho_{Ri}\Lambda_{Ri} \quad (1.4)$$

where ρ_{Rj} is the reactivity gain by the jth reflector($keff^w$)comparing to the core with only the other reflectors($keff^o$).

$$\rho_{Rj} = \frac{keff^w - keff^o}{keff^o} \quad (1.5)$$

The temperature reactivity feedback coefficients are calculated using a Serpent full core model by varying the temperature and correspondingly density of a material at a time. The coefficients for the three layers in the fuel pebble and the coolant are shown in Table 4. The reactivity is calculated as the sum of external reactivity insertion and linear temperature reactivity feedback:

$$\rho(t) = \rho_{ext}(t) + \alpha_F (T_F(t) - T_{F,0}) + \alpha_M (T_M(t) - T_{M,0}) + \alpha_C (T_C(t) - T_{C,0}) \quad (1.6)$$

HEAT TRANSFER MODEL

Heat diffusion equation

Assuming all the nuclear heat is deposited in the fuel layer in the pebble and transferred to moderator kernel and graphite shell via conduction. 1-D heat diffusion equation in spherical coordinates computes the radial variation of temperature in the pebble as a function of time:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(kr^2 \frac{\partial T}{\partial r}\right) + g \quad (1.7)$$

A Dirichlet boundary condition at r=0 and a mixed boundary condition at r=R are imposed.

$$\frac{\partial T}{\partial r}|_{r=0} = 0$$
$$\left.\frac{\partial T}{\partial r}\right|_{r=R} = \frac{h}{k}(T - T_{\bullet}) \quad (1.8)$$

This equation can be written in a simpler form by introducing a new variable $U(r,t) = rT(r,t)$ as:

$$\frac{\partial U}{\partial t} = a\frac{\partial^2 U}{\partial r^2} + r\frac{g}{rCp} \quad (1.9)$$

And the boundary conditions become

$$U_0 = 0 \quad (1.10)$$
$$\left.\frac{\partial U}{\partial r}\right|_{r=R} = \left(\frac{1}{R} - \frac{h}{k}\right)U + \frac{R}{k}hT_{\infty} \quad (1.11)$$

Convective heat transfer at fuel pebble surface

In this work, a single-phase convective heat transfer model is applied to the coolant as flibe remains in liquid phase between 458°C and 1400°C [4].

$$\frac{dT_c}{dt} = \frac{1}{\left(\rho c_p V\right)_S} * \left[-\dot{m}c_p\left(T_{out} - T_{in}\right) + hA\left(T_s - T_C\right)\right] \quad (1.12)$$

T_{out} and T_{in} are outlet and inlet coolant temperatures. The inlet temperature is assumed fixed at the nominal value 600°C in this study. The bulk coolant temperature is calculated as

$$T_C = \frac{T_{in} + T_{out}}{2} \quad (1.13)$$

Using the Wakao correlation [5] for the pebble bed heat transfer coefficient, the fluid-to-pebble Nusselt number is:

$$Nu = 2 + 1.1Pr^{1/3}Re^{0.6} \quad (1.14)$$

$$Re = \frac{\rho d_p u}{\mu} \quad (1.15)$$

$$Pr = \frac{c_p m}{k} \quad (1.16)$$

The heat transfer coefficient h can then be calculated from

$$h = \frac{Nu.k}{d_p} \quad (1.17)$$

Table 2: Thermal physical properties of the materials in the reactor core.

Component	ρ [kg/m^3]	k [w/K.m]	cp [J/kg.K]
Moderator	1740	15	684
Fuel	2200	15	1818
Shell	1750	15	684
Coolant	2279.92-0.488T	0.7662+0.0005T	2415.78

IMPLEMENTATION IN PYTHON

As shown in Figure 5, the unit cell model represents an average fuel pebble and flibe coolant, with a packing fraction of 40%. The fuel pebble consists of three homogenized annular layers: the central moderator core, the fuel layer, and the graphite shell; TRISO particles are not modeled explicitly. The equivalent thermal physical properties of the fuel layers used in the model are shown in Table 2.

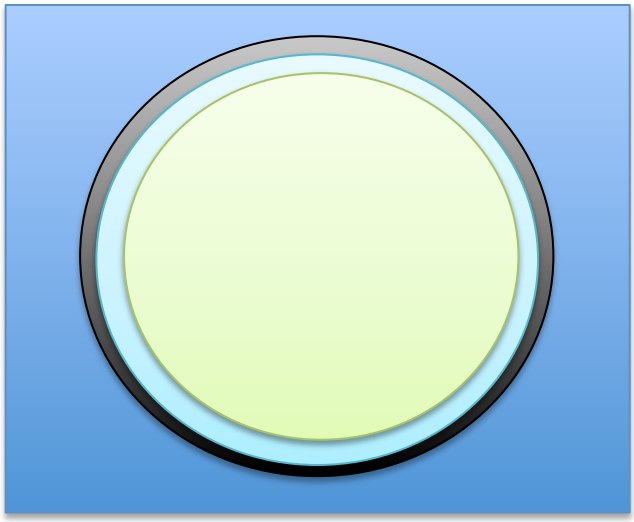

Figure 5: Schematic of the Mk1 PB-FHR unit cell model geometry

A conservative adiabatic condition is imposed on the unit cell boundary. The center and outer reflectors are not modeled explicitly in the unit cell, however their effect on

the average neutron lifetime is included in the multi-point kinetics equations.

The multi-point model parameters (Table 3) and the moderator, fuel and coolant temperature reactivity coefficients (Table 4), as well as the kinetic parameters (Table 5) are computed from a full core model using the Monte Carlo code, Serpent [6].

This model is implemented in the Python for Reactor Kinetics (PyRK [7]) package. This open source Python package is created for design-agnostic nuclear reactor accident analysis. It provides a coupled point-reactor kinetics and thermal hydraulics model and a modular material definition framework. More documentation and examples can be found at pyrk.github.io.

Table 3: Parameters used in the multi-point model for Mk1 PB-FHR core

λ_{Ri}(1/s)	786.31722
λ_{Ro}(1/s)	1209.07947
ρ_{Ri}	0.084349
ρ_{Ro}	0.168983
Λ_c(ms)	0.227

Table 4: Temperature reactivity coefficient of the layers in the Mk1 fuel pebble and the coolant

Component	α(pcm/k)
moderator	-0.70
fuel	-3.19
shell	-0.70
coolant	0.23

Table 5: Kinetic parameters in Mk1 PB-FHR core

group	β_i	λ_i [1/s]
1	2.05E-04	1.25E-02
2	1.16E-03	3.17E-02
3	1.05E-03	1.09E-01
4	2.77E-03	3.17E-01
5	8.40E-04	1.35E+00
6	3.02E-04	8.68E+00

SIMULATION RESULTS

A reactivity insertion (RI) accident occurs when a reactor control element is partially or fully removed from the core, causing a rapid power excursion in the nearby fuel elements. The control rods and blades in the Mk1 PB-FHR can enter the core by buoyancy when their drives fail. Despites the robust design of Mk1 PB-FHR against RI, it's important to understand the time-dependent behavior of the reactor response to intentional or unintentional RIs, because they may cause fast rise in fuel power and temperature and are critical to fuel integrity.

The multi-point model is tested with step reactivity insertion and compared to the standard (single) point kinetics model. Figure 6 shows that the fuel temperature of 1$ RI rises faster with the multi-point kinetics model than with the single-point kinetics model. The reactor experiences rapid change in power and temperature in the fuel and reaches steady state due to negative temperature reactivity feedback. Therefore RI response is dominated by the time scales in the fuel (and coolant) region, where the effective prompt neutron lifetime is 0.000227s compare to the core average value 0.000459s.

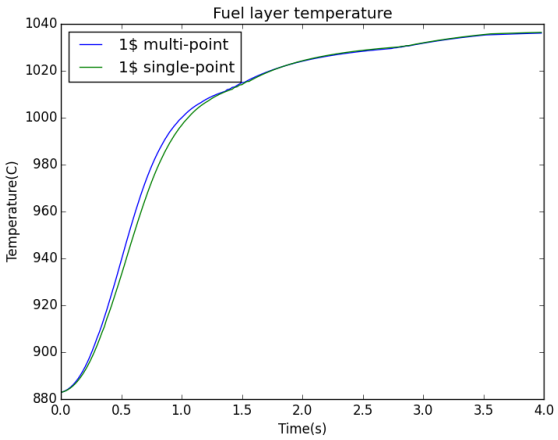

Figure 6: fuel temperature rise following 1$ reactivity insertion

Figure 7 - 10 show the simulated response in fuel and coolant temperature, the power and the reactivity to ramp insertions. Ramp reactivity $\rho = \rho_0(t - t_0)$ is inserted at t_0=10s. Total amounts of 1$, 1.5$ and 2$ insertion are studied. In all three cases, the fuel temperature rises shortly after reactivity insertion, causing a drop in reactivity through the negative reactivity feedback mechanism. The coolant temperature rises following the fuel temperature and causes a small reactivity gain. However, it's neglectable compare to the fuel temperature feedback and does not affect the total reactivity. Maximum average fuel temperature remains under 1220°C in the most severe case, and maximum avarage coolant temperature below 945°C.

Figure 11- 14 show the simulated response in fuel and coolant temperature, the power and the reactivity to a 1$ ramp insertion. External reactivity is inserted in 10s, 5s, 2s and 1s respectively. The power rises rapidly at a similar rage as the reactivity insertion, causing a temperature rise in the fuel and subsequently in the coolant. The reactor stabilizes at the same coolant and

fuel temperatures, as the same temperature feedback is needed to compensate the external reactivity.

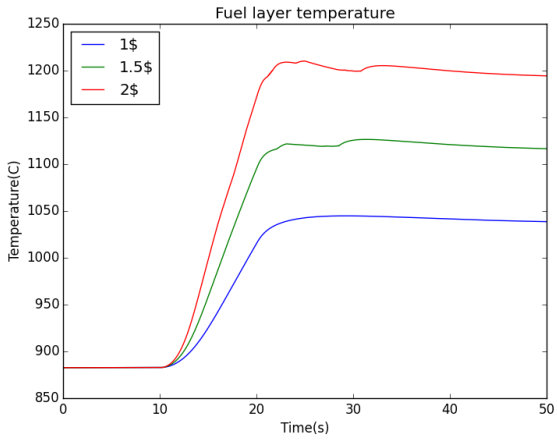

Figure 7: Temporal change in average fuel temperature

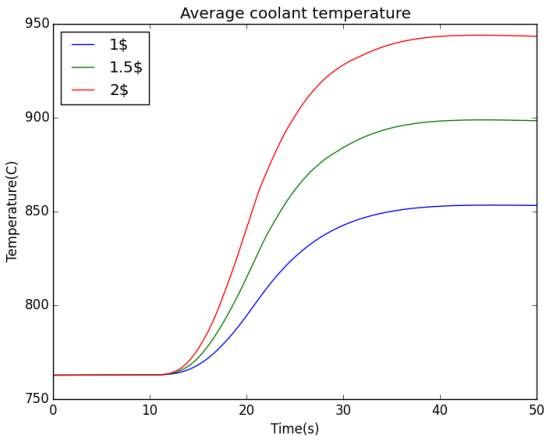

Figure 8: Temporal change in average coolant temperature

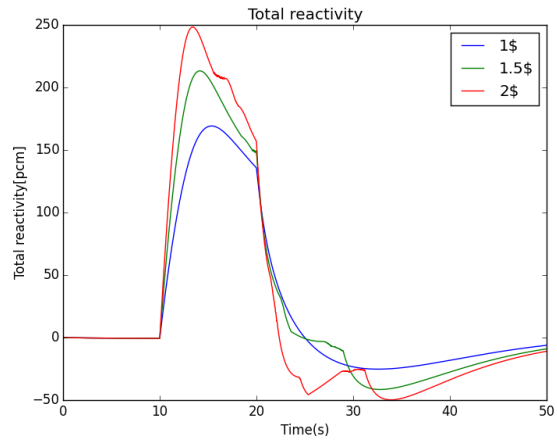

Figure 9: Temporal change in total reactivity

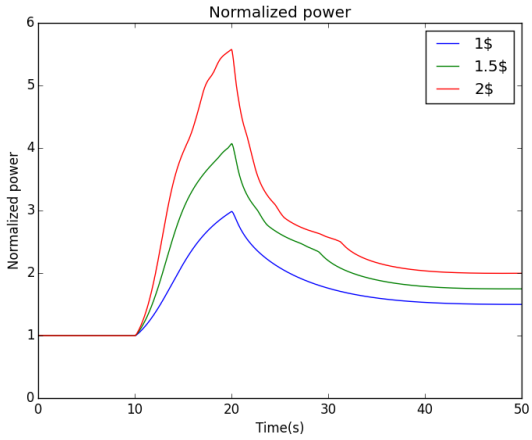

Figure 10: Temporal change in nuclear power

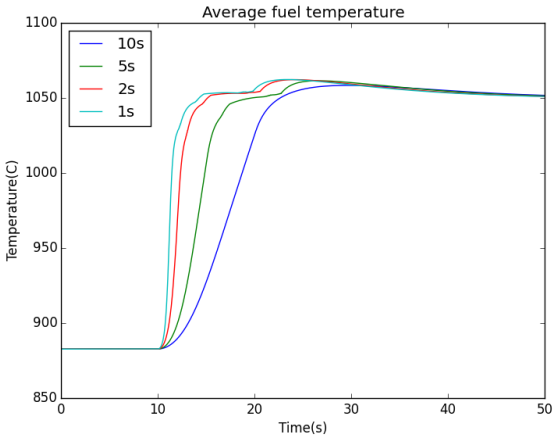

Figure 11: Temporal change in average fuel temperature

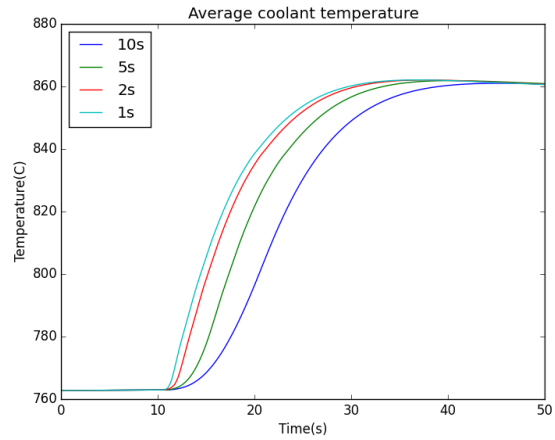

Figure 12: Temporal change in average coolant temperature

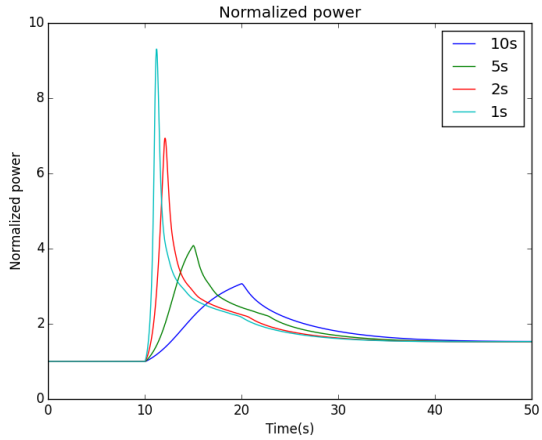

Figure 13: Temporal change in nuclear power

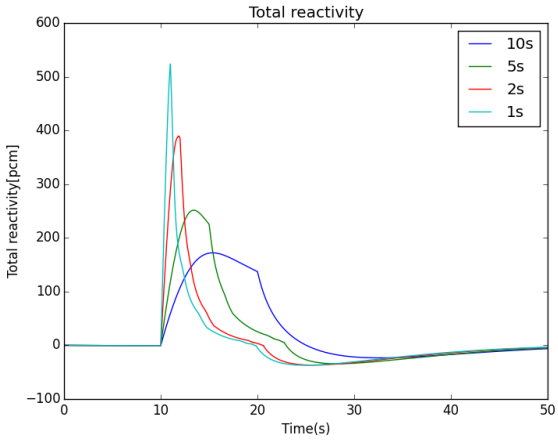

Figure 14: Temporal change in total reactivity

TWO-DIMENSIONAL COUPLED MULTI-GROUP NEUTRON DIFFUSION AND FINITE ELEMENT HEAT TRANSFER MODEL

MULTI-GROUP NEUTRON DIFFUSION MODEL

The multi-group neutron diffusion equation [8] (equation 1.18) is used to determine the neutron distribution in a reactor core. The effective multiplication factor k_{eff} is inserted to the neutron balance equation to represent the variation of neutron population from one generation to another.

$$-\nabla D_g \nabla \Phi_g + \Sigma_{Rg}\Phi_g = \sum_{g'=1}^{g-1} \Sigma_{sg'g}\,\Phi_{g'} + \frac{1}{k_{eff}}\chi_g \sum_{g'=1}^{G} \nu_{g'}\Sigma_{fg'}\,\Phi_{g'} \quad (1.18)$$

Temperature/density dependent scattering and removal cross-sections are modeled as log-linear function of the fuel temperature and as linear function of the flibe density. Fission cross sections in the fuel region are also modeled as a log-linear function of the fuel temperature.

$$\Sigma(T_{fuel}) = c0 + c1 * \log\,(T_{fuel}/T0) \quad (1.19)$$

$$\Sigma(\rho_{flibe}) = c0 + c1 * (\rho_{flibe} - \rho_0) \quad (1.20)$$

c0 and c1 are constant coefficients calculated from linear regression. T0 and ρ_0 are reference fuel temperature and flibe density.

HEAT TRANSFER MODEL

Nuclear power is assumed generated homogeneously inside the solid fraction in the fuel region and transferred to the coolant through heat convection.

$$\rho \mathrm{Cp}\frac{\partial T_s}{\partial t} = \nabla k \nabla T_f + Q \quad (1.21)$$

The heat transfer rate between fuel pebble and coolant is computed as:

$$Q''' = -h\frac{A}{v}(Ts - Tf) \quad (1.22)$$

where h is computed using the Wakao correlation as discussed in the previous section.

Spatial temperature distribution in the fuel region is computed with equivalent thermal properties. A composite material is defined as 40% of fuel pebbles and 60% of flibe salt. Properties such as conductivity, heat capacity is defined as a volume weighted sum of two material properties.

$$\rho \mathrm{Cp}\frac{\partial T_f}{\partial t} + \rho \mathrm{Cpu}\nabla \mathrm{T} = \nabla k \nabla T_f + Q \quad (1.23)$$

IMPLEMENTATION IN COMSOL

A two-dimensional neutron diffusion model is developed for a simplified TMSR core geometry (Figure 15). The reactor core is divided into three regions: fuel, flibe salt and graphite reflector region. The fuel region is composed with a solid fuel material and a liquid flibe salt material. Coupled heat transfer and neutron diffusion equations are solved with different homogenized material properties. Once validated, the methodology can be applied to Mk1 PB-FHR core because of their similarities in design.

The COMSOL Multiphysics is a software package that uses the finite element method for spatial discretization to solve systems of PDEs or ODEs. COMSOL allows user to either use pre-defined multiphysics modules or specify a system of user-defined PDEs. The LiveLink™ for MATLAB® module in COMSOL enables user to define COMSOL models through a MATLAB interface, which further extends its versatility.

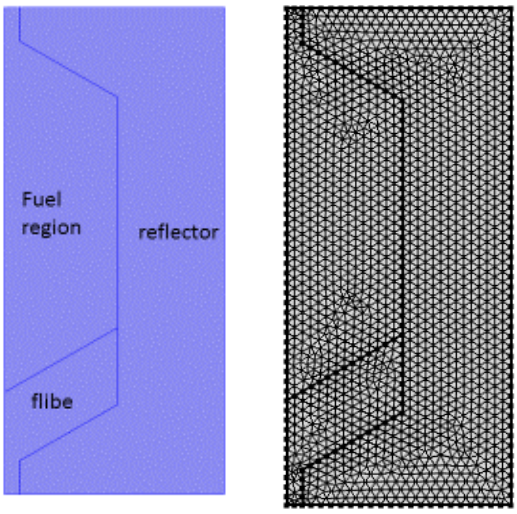

Figure 15: Schematic representation of the COMSOL model and the mesh (49232 degree of freedom)

The group constants used in the diffusion equation are generated with the three-dimensional continuous energy Monte Carlo neutron transport code Serpent. The energy spectrum is divided using an eight-energy group structure in Table 6. The cross sections of Uranium and flibe are plotted in Figure 16. The group boundaries (shown as verticals bars in Figure 16) are chosen to capture the cross section changes in heavy metals and in isotopes in the flibe salt.

Table 6: Energy group structure adopted in the multi-group diffusion model

group	upper bound [MeV]	lower bound [MeV]
1	1.00E+37	1.40E+00
2	1.40E+00	2.50E-02
3	2.50E-02	4.80E-05
4	4.80E-05	4.00E-06
5	4.00E-06	5.00E-07
6	5.00E-07	1.90E-07
7	1.90E-07	5.80E-08
8	5.80E-08	0.00E+00

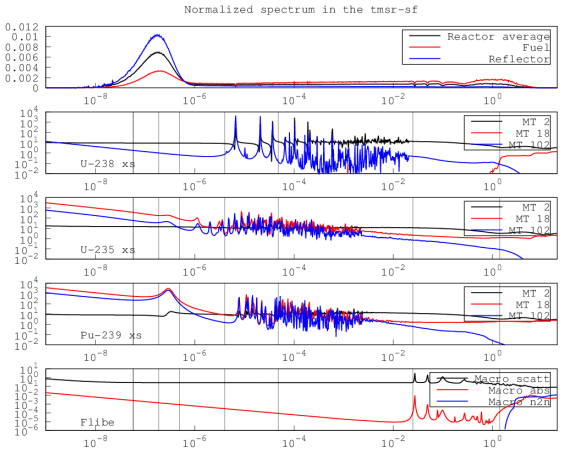

Figure 16: flux and cross section variation with energy

The data are calculated at five different fuel temperatures (300K, 600K, 900K, 1200K, 1500K) and five different flibe densities (17 kg/m^3, 18 kg/m^3, 19 kg/m^3, 20 kg/m^3, 21 kg/m^3). A MATLAB package is developed to automatically read data from Serpent output files and produce temperature/density dependent group constant for as many neutron energy groups as deemed necessary.

The neutron diffusion model is based on the COMSOL built-in 'PDE interfaces' in equation 1.24.

BOUNDARY CONDITIONS (BC)

Neutronics:
A symmetry BC is used at the core centerline(r=0) and a vacuum BC is used at the outer reflector surfaces.

Thermal-hydraulics:
Inlet velocity and temperature are imposed at the bottom boundary. In the TMSR core, coolant enters at the bottom inlet and flows upward at an average velocity of 0.18m/s. Uniform and fixed axial coolant velocity is assumed in the current model. In order to save some computation burden, conservative adiabatic boundary condition is applied at the reflector.

where

$$D\phi + a\phi = 0$$

$$D = \begin{bmatrix} -\nabla D_1 \nabla & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & -\nabla D_G \nabla \end{bmatrix}$$

$$\phi = \begin{bmatrix} \phi_1 \\ \vdots \\ \phi_G \end{bmatrix} \tag{1.24}$$

$$a = \begin{bmatrix} \Sigma_{R1} - \frac{1}{k}\upsilon_1\chi_1\Sigma_{f1} & -\Sigma_{s21} - \frac{1}{k}\upsilon_2\chi_1\Sigma_{f2} \cdots & -\Sigma_{sG1} - \frac{1}{k}\upsilon_G\chi_1\Sigma_{fG} \\ -\Sigma_{s12} - \frac{1}{k}\upsilon_1\chi_2\Sigma_{f1} & \ddots & \vdots \\ \vdots & \cdots & \Sigma_{RG} - \frac{1}{k}\upsilon_G\chi_G\Sigma_{fG} \end{bmatrix}$$

SIMULATION RESULTS

At the nominal fuel temperature (900K) and the nominal flibe density (1900 kg/m3), the neutron flux of eight energy groups are shown in Figure 18, ordered from higher energy to lower energy. Fast neutrons are born in the fuel region and transported into the reflector where they get thermalized. A large portion of thermal neutron population is in the reflector.

MODEL VALIDATION

In order to validate the COMSOL model, results of reactivity are compared to the Serpent full core model. Serpent solves the neutron transport equation in integral form using continuous energy nuclear data with few approximation; therefore it produces valuable reference results for such validation process when experimental data are not available. The reactivity is calculated from k_{eff} as

$$\rho = \frac{k_{eff} - 1}{k_{eff}} \tag{1.25}$$

Figure 17 shows the difference between the reactivity at various fuel temperatures and the reference reactivity at 900K. The results from the COMSOL model match those from the Serpent model closely. The diffusion model captures the neutron balance at a similar accuracy as the Serpent model.

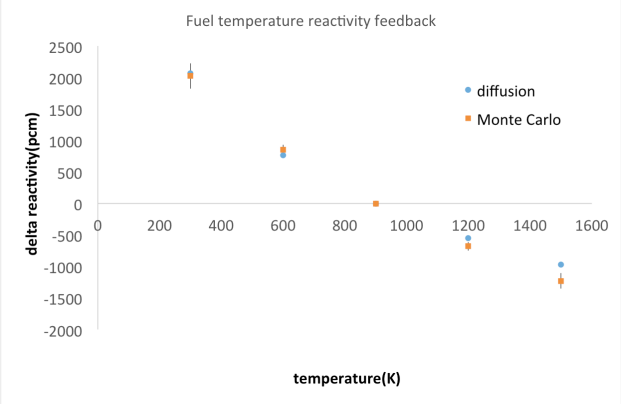

Figure 17: comparison of changes in reactivity with temperature (10% error bar)

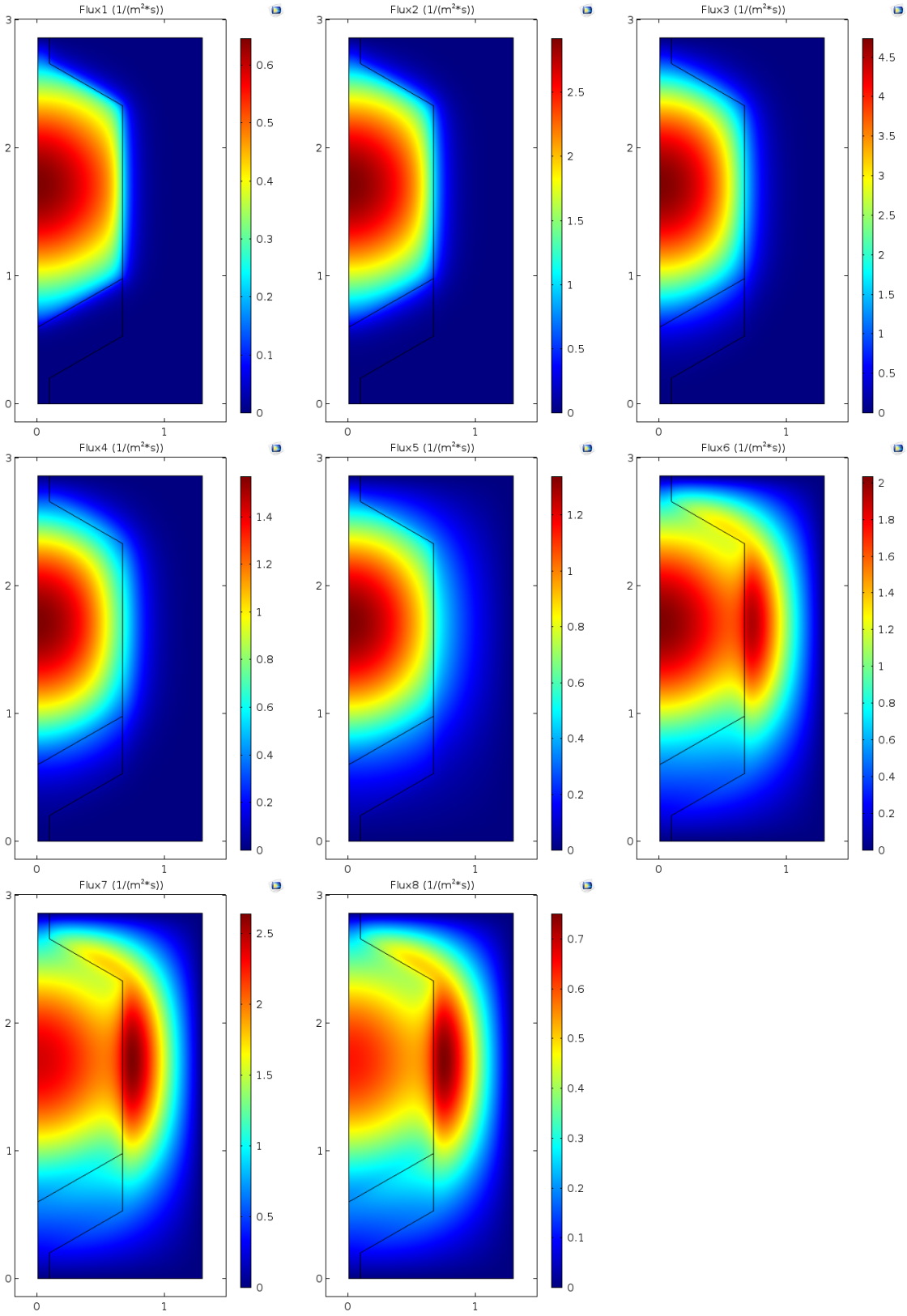

Figure 18: flux of neutrons in eight energy groups, from high energy to low energy

CONCLUSIONS

Coupled neutronics and thermal-hydraulics models are developed for PB-FHR transient analysis. Point kinetics model is used to study reactivity insertion accidents for MK1 PB-FHR. Because the point kinetic model is a simplified model based on an average fuel pebble in the core, this maximum temperature is not necessarily the maximum temperature in a real reactor core, where local hot spots exist, but a good indication of the range that the maximum temperature in a fuel pebble can reach. Study shows that the maximum average fuel temperature in a 2$ reactivity insertion accident is 1220°C, and maximum avarage coolant temperature is below 945°C. Coated particle fuels have the ability to maintain their integrity up to temperatures of 1600°C or higher. Accordingly, the maximum temperature of an average unit cell in the core found by this analysis is well below the safety margin for fuel integrity during the studied reactivity insertion accidents.

A multi-group diffusion model is developed in COMSOL. The reactivity variation with fuel temperature is verified with the Monte Carlo reference results. An eight-energy-group structure is used in the current model. A sensitivity study of the energy group structure is going to be carried out to identify a good tradeoff between computation cost and accuracy.

A coupled Monte Carlo/OpenFOAM model [9] has been developed in parallel of the models discussed in the paper. Results from the discussed models will be validated against the 3-D high fidelity model.

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