INL/CON-22-67818-Revision-0

COUPLED MULTIPHYSICS PRIMARY LOOP SIMULATIONS OF THE Mk1-FHR IN THE VIRTUAL TEST BED

November 2022

Guillaume Louis Giudicelli, Abdalla Abou Jaoude, Cole Mueller, Jun Fang, Daniel Nunez

Changing the World's Energy Future

Idaho National Laboratory

INL is a U.S. Department of Energy National Laboratory operated by Battelle Energy Alliance, LLC

INL/CON-22-67818-Revision-0

COUPLED MULTIPHYSICS PRIMARY LOOP SIMULATIONS OF THE Mk1-FHR IN THE VIRTUAL TEST BED

Guillaume Louis Giudicelli, Abdalla Abou Jaoude, Cole Mueller, Jun Fang, Daniel Nunez

November 2022

Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

Prepared for the
U.S. Department of Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

COUPLED MULTIPHYSICS PRIMARY LOOP SIMULATIONS OF THE Mk1-FHR IN THE VIRTUAL TEST BED

Guillaume Giudicelli,[0] Cole Mueller,[1] Daniel Nunez,[2] Thanh Hua,[2] Jun Fang,[2] Abdalla Abou-Jaoude[3]

[0]*Computational Frameworks,* [1]*Thermal Fluid Systems Methods & Analysis,* [3]*Advanced Reactor Technology and Design, Idaho National Laboratory, Idaho Falls, ID 83415, USA, guillaume.giudicelli@inl.gov*

[2]*Argonne National Laboratory, 9700 S. Cass Avenue, Lemont, IL 60439-4854, USA*

doi.org/10.13182/T127-39765

To support advanced reactor demonstrations, the Virtual Test Bed (VTB) [1] repository hosts a wide range of challenge problems for showcasing modeling and simulation capabilities in support of advanced reactor demonstrations. This document presents a coupled multiphysics model of the Mark 1 pebble-bed fluoride-salt-cooled high-temperature reactor (PB-FHR). The analysis leverages NEAMS tools (Griffin [2], SAM [3], Pronghorn [4], and the MOOSE [5] heat conduction module) for core neutronics, thermal hydraulics of the core and primary loop, and multiscale fuel performance simulations. The analysis was entirely created by coupling standalone simulations of the reactor that were previously available on the VTB. All input files and documentation developed for this example are available on the VTB website: `mooseframework.inl.gov/virtual_test_bed/`. *This model was featured in the National Reactor Innovation Center Tech Talk presented in December 2021.*

INTRODUCTION

The pebble-bed fluoride-salt-cooled high-temperature reactor (PB-FHR) is a promising advanced reactor design that affords numerous inherent safety features such as a low-pressure coolant, an accident-tolerant and multilayered particulate fuel (TRi-structural ISOtropic), and improved decay heat removal. These features are expected to enable reactors of this design type to achieve "walk-away" safety under a wide range of potential accident conditions. The higher coolant temperature also benefits thermodynamic efficiency, and the pebble design provides an online refueling capability. Both these features are highly desirable for the economic performance of future reactors.

However, these advanced features also pose a significant modeling challenge compared to the existing light-water reactor fleet. The fuel is more heterogeneous, with millimeter-scale particulate fuel mixed inside centimeter-scale pebbles, themselves in a large, several-meters-wide bed. While explicitly modeling all heterogeneity may provide higher fidelity, the computational cost would be excessive for daily analysis. With this prospect in mind, an intermediate-fidelity thermal-hydraulics model leveraging a multiscale approach was developed [6]. This model features a coarse discretization of the reactor, using closure relations to model drag from the pebbles, convective heat transfer, and effective thermal conduction in both the solid and fluid phases. The model was coupled with a homogenized neutronics calculation, and the thermal hydraulics solve was converted to finite volume [7]. Control rod transient simulations were investigated using that model [8], but necessitate improvements in the cross-section generation, which are under development. This model is now supplemented by a primary loop thermal hydraulics simulation using SAM. The model, its documentation and various stages of its evolution are accessible by academic, governmental, and industrial partners via the National Reactor Innovation Center's Virtual Test Bed (VTB) repository.

This paper is organized as follows. Section 2 describes the Pronghorn thermal-hydraulics multiscale model and the finite-volume implementation. Section 3 describes the neutronics model with multigroup cross-section generation using Monte Carlo methods in a diffusion-based model in Griffin. Section 4 describes the SAM model of the primary loop. Section 5 describes the coupling of all the different parts of the simulation. Finally, Section 6 reports the computed steady-state condition of the system.

THERMAL-HYDRAULICS MODEL

The thermal-hydraulics model of the core is based on the porous media incompressible Navier-Stokes equations. This not only includes the mass and momentum equations, but also the energy equations (Eq. 1, 2, 3) for the fluid, as well as the conservation of energy (Eq. 4) for the solid phase. This equation set is derived from that was used in [9], apart from some minor modifications, such as neglecting work and kinetic energy terms and assuming a constant specific heat. The nonlinear variables used are the superficial velocities, pressure, and fluid/solid phase temperatures. No turbulence modeling was included.

$$\nabla \cdot (\mathbf{u_D}) = 0 \tag{1}$$

$$\rho \frac{\partial \mathbf{u}_D}{\partial t} + \nabla \cdot \left(\frac{\rho}{\epsilon} \mathbf{u}_D \otimes \mathbf{u}_D \right) = \nabla \cdot \left(\epsilon \mu \nabla \frac{\mathbf{u}_D}{\epsilon} \right) - \epsilon \nabla p + \epsilon (\mathbf{F}_g + \mathbf{F}_b + \mathbf{F}_f) \tag{2}$$

$$\epsilon \rho c_{pf} \frac{\partial T_f}{\partial t} + \nabla \cdot (\mathbf{u}_D \rho c_{pf} T_f) = \nabla \cdot (\kappa_f \nabla T) - \alpha (T_f - T_s) \tag{3}$$

$$(1 - \epsilon) \rho_s c_{ps} \frac{\partial T_s}{\partial t} = \nabla \cdot (\kappa_s \nabla T) + \alpha (T_f - T_s) + \dot{Q} \tag{4}$$

In the equations above, ρ is the constant density, ϵ the porosity, $\mathbf{u}_D$ the superficial velocity, μ the viscosity, and p the pressure, while F_g, F_b, and F_f are the gravity, Boussinesq, and friction forces, respectively. $T_{f/s}$ is the fluid/solid temperature, $c_{pf/s}$ the fluid/solid heat capacity, κ the effective thermal conductivity, α the volumetric inter-phase heat transfer coefficient, and $\dot{Q}$ the volumetric heat source. For more information on the selected equation set, interested readers should consult the MOOSE Navier-Stokes module documentation. These equations were discretized using the finite-volume method with a cell-centered scheme and Rhie Chow

interpolation for velocities, first order upwind for advected quantities. The model is described in further detail on the VTB website [10].

Numerous closure relations underpin the porous media approximation for the pebble bed. The pebble-bed heat transfer coefficient uses the Wakao correlation, the friction coefficient uses the Ergun drag model, and the effective thermal conductivity in the fluid uses a linear Peclet thermal dispersion model. The effective thermal conductivity in the solid phase is based on contributions from stagnant conduction, contact conduction, and radiation. More information on the closure relations may be found in [11]. The published range of applicability of these closures is automatically checked by Pronghorn during simulations. Additional development may be required to model turbulent heat transfer and near-wall pebble packing effects, and to better account for radiative heat transfer in the bed. Higher fidelity simulations can help fine-tune these models and recover part of the discretization errors introduced by the coarse mesh. Readers are referred to [6] and the VTB website for a detailed explanation of the mesoscale pebble heat-conduction model and microscale particulate model.

NEUTRONICS MODEL

PH-FHR neutronics still holds numerous challenges, and generating group cross sections for these reactors is rather complicated, since they must account for a multiscale double-heterogeneity effect [12]. Direct homogenization of pebble and TRISO particles is highly inaccurate [13], and deterministic methods based on collision probabilities [14] or transport theory for stochastic media [15] were developed to treat these effects.

To avoid such challenges, a Monte Carlo simulation was used for neutron-group cross-section generation. Such application of Monte Carlo simulation is increasingly common in the nuclear reactor physics community. Monte-Carlo-generated group cross sections are now used in studies of both advanced and light-water reactors. The main advantages of this approach are that it uses both a fully heterogeneous exact representation of the reactor—avoiding geometrical or initial homogenization approximations—and a continuous-energy representation of group cross sections. This method avoids complex models regarding the interference between resonances and nuclides, since for group cross-section generation, full-core calculations are preferred over lattice/infinite-medium calculations, as they mitigate the need for leakage-correction models, and more naturally account for environmental effects such as proximity to the reflector and local temperature gradients. (The number of homogenized regions in this work is currently insufficient to account for such effects.)

Serpent 2 [16] was employed for group cross-section generation because its use of delta tracking is efficient when dealing with highly heterogeneous geometries. Serpent 2 has been used for group cross-section generation mostly in the context of nodal diffusion calculations [17]. Serpent 2 input files were generated using the input file generation scripts from [18], with the same eight-group energy structure. The pebbles were packed randomly to a packing fraction of 0.6, using the automatic disperser routine. To cover the entire operating condition range, group cross sections and delayed neutron data were generated for a wide range of operating conditions, as summarized in Table I. For the purpose of group cross-section generation, the fuel and coolant temperatures were assumed uniform throughout the entire core. The group cross sections were tallied on a cylindrical mesh corresponding to the GRIFFIN 2D-RZ model.

TABLE I: Parameter grid for Monte Carlo group cross-section generation.

Parameter	Range	Steps (-)
Fuel temperature (K)	[300, 1500]	5
Salt temperature (K)	[300, 1500]	5
Control rod insertion (%)	[0, 100]	5

The steady-state uncoupled eight-group diffusion equation was solved in Griffin on a 2D-RZ mesh model. The preconditioned Jacobian-free Newton-Krylov nonlinear eigenvalue solver was used to obtain convergence in five nonlinear iterations for a single statepoint. The steady-state (rods out, nominal temperatures) model with no-equivalent was verified against the Monte Carlo simulation, with the results showing less than 6% error on fission rates and 200 pcm on the eigenvalue. Griffin compares favorably, though the low eigenvalue error is partially due to error cancellations, as the 2D-RZ homogenization of the inner reflector coolant channels induces a 200 pcm bias. The maxima of the error are located near mismatches between the unstructured mesh used for the calculation and the structured mesh used for the Monte Carlo tallies and the comparison. This comparison is expected to be improved in future work. The model is described in further detail on the VTB website [10].

PRIMARY LOOP MODEL USING SAM

The SAM [3] input files were built to model the Mark 1 PB-FHR primary loop [19]. A schematic of the reactor can be found in [20]. The primary loop consists of three branches: the core, direct reactor auxiliary cooling system heat exchanger (DRACS), and coiled tube air heater (CTAH). Each branch of the loop is discretized in the SAM model, using SAM components. The model is described in further detail on the VTB website [10]. It exists in the test bed as both a standalone SAM simulation of a steady-state and a loss of flow transient, and as part of the plant coupled model.

PRIMARY LOOP COUPLING

The multiphysics core model, which uses Griffin for neutronics and Pronghorn for coarse mesh porous media CFD, is coupled with the primary loop model, which uses SAM to simulate the 1-D thermal hydraulics of the primary loop. A Picard fixed-point iteration is set up between the reactor physics and the thermal-hydraulics models. It converges in approximately five iterations. Griffin solves the eigenvalue problem, while the simulation of the primary loop relaxes to

a steady state, starting from a pseudo-transient simulation.

The coupling scheme is summarized in Figure 1. The connection between the core model and the BOP simulation is made through the inlet and outlet of the core in the primary loop. Instead of a fixed inlet mass flow rate and a fixed outlet pressure as in the previous model, those quantities will be provided by the simulation of the rest of the primary loop. Flux boundary conditions were initially utilized, as they are naturally conservative in a finite volume method, though support for conservative Dirichlet boundary conditions was also subsequently added. The fluxes for the mass, momentum, and energy equations are all provided, as computed by the boundary conditions based on the mass flow rates, local density, and inlet surface area.

In the other direction of the coupling, the boundary conditions that will be passed to SAM are collected using side integrals and flow rate post-processors. These are executed at the end of each time step and collect the outlet flow conditions as well as the inlet pressure. The inlet temperature is also computed in case of a flow reversal.

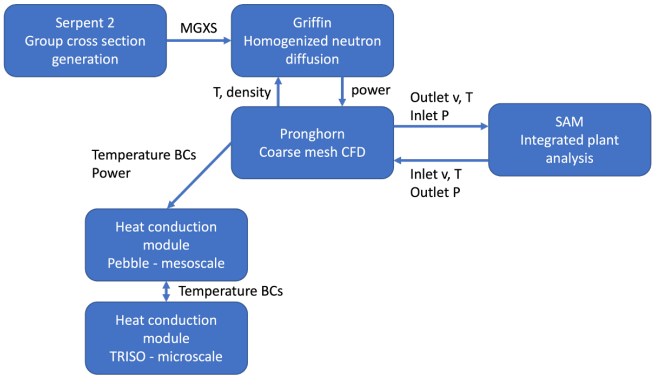

Fig. 1: Primary loop multiphysics coupling scheme

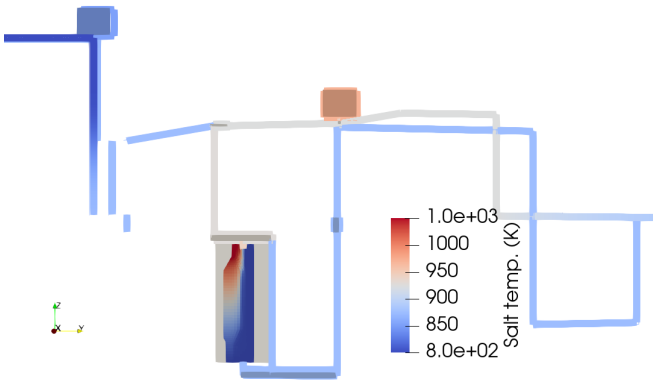

Fig. 2: Steady-state salt temperature in primary loop

STEADY STATE RESULTS

In this section, we present sample results for the coupled plant simulation in a relaxation-to-steady-state transient. Both simulations start out reasonably initialized, and come to

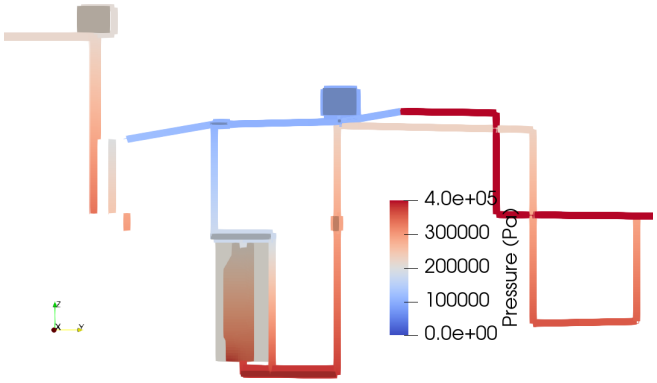

Fig. 3: Steady-state salt pressure in primary loop

an equilibrium as the mass flow rates and the pressure drops in the core and in the various 1-D components adjust for the head output by the pumps in the SAM model.

The 2-D Pronghorn results are overlaid on the 1-D SAM results in Paraview. For legibility, the 1-D component widths are artificially inflated in Paraview. In Figure 2 and 2, both the pressure and salt temperature show continuity at the interface between SAM and Pronghorn, as ensured by the boundary conditions. The spatial profile of the core outlet salt temperature is homogenized in the transition to SAM for the rest of the primary. The salt cools through heat exchangers, and pressure drops can be observed through pumps and other components.

CONCLUSIONS

This study achieved fully coupled multiphysics simulations of the Mark 1 PB-FHR reactor by using the MOOSE-based applications SAM, Griffin, and Pronghorn, and by deploying new finite-volume capabilities [21] in Pronghorn. The complexity of the pebble-bed reactor was treated using homogenized diffusion models, a homogenized porous medium, and a 1-D BOP approach, respectively. All simulations were run on a laptop, with particular emphasis on keeping the computational costs reasonable. Using the upcoming capability in Griffin, the model will be further developed so as to generate its own group cross sections for pebble-bed reactors and to track pebble depletion [22]. The latter feature will be required for further studies of transient simulations involving the plant model.

ACKNOWLEDGEMENTS

This manuscript was authored by Battelle Energy Alliance, LLC under contract no. DE-AC07-05ID14517 with the U.S. Department of Energy (DOE). This work was prepared for DOE through the National Reactor Innovation Center (NRIC). The submitted manuscript was co-authored by UChicago Argonne, LLC, operator of Argonne National Laboratory (ANL). ANL, a U.S. DOE Office of Science laboratory, is operated under contract no. DE-AC02-06CH11357. It also made use of the resources of the High Performance Computing Center at Idaho National Laboratory, which is

supported by the DOE Office of Nuclear Energy and the Nuclear Science User Facilities under contract no. DE-AC07-05ID14517, for convergence studies and the generation of group cross sections. The U.S. Government retains for itself, and others acting on its behalf, a paid-up, nonexclusive, irrevocable worldwide license to said article, enabling it to reproduce the article, prepare derivative works, distribute copies to the public, and publicly perform or display portions thereof, by or on behalf of the Government. DOE will provide public access to these results of federally sponsored research, in accordance with the DOE Public Access Plan: energy.gov/downloads/doe-public-access-plan.

REFERENCES

1. G. L. GIUDICELLI, C. PERMANN, D. GASTON, B. FENG, and A. ABOU-JAOUDE, "The Virtual Test Bed (VTB) Repository:A Library of Multiphysics Reference Reactor Models Using NEAMS Tools," in "Proceedings of PHYSOR," (2022).
2. M. DEHART, F. N. GLEICHER, V. LABOURE, J. ORTENSI, Z. PRINCE, S. SCHUNERT, and Y. WANG, "Griffin User Manual," Tech. Rep. INL/EXT-19-54247, Idaho National Laboratory (2020).
3. R. HU, "An Advanced One-Dimensional Finite Element Model for Incompressible Thermally Expandable Flow," *Nuclear Technology*, pp. 313–322 (2015).
4. A. NOVAK, R. CARLSEN, S. SCHUNERT, P. BALESTRA, D. REGER, R. SLAYBAUGH, and R. MARTINEAU, "Pronghorn: A Multidimensional Coarse-Mesh Application for Advanced Reactor Thermal Hydraulics," *Nuclear Technology* (02 2021).
5. C. J. PERMANN, D. R. GASTON, D. ANDRŠ, R. W. CARLSEN, F. KONG, A. D. LINDSAY, J. M. MILLER, J. W. PETERSON, A. E. SLAUGHTER, R. H. STOGNER, and R. C. MARTINEAU, "MOOSE: Enabling massively parallel multiphysics simulation," *SoftwareX*, **11**, 100430 (2020).
6. A. NOVAK, S. SCHUNERT, R. CARLSEN, P. BALESTRA, R. SLAYBAUGH, and R. MARTINEAU, "Multiscale thermal-hydraulic modeling of the pebble bed fluoride-salt-cooled high-temperature reactor," *Annals of Nuclear Energy*, **154** (01 2021).
7. G. GIUDICELLI, A. J. NOVAK, and A. A. JAOUDE, "Coupled Multiphysics Simulations Of The Mk1-Fhr In The Virtual Testbed," in "Transactions of the American Nuclear Society," (2021).
8. G. GIUDICELLI, A. LINDSAY, P. BALESTRA, R. CARLSEN, J. ORTENSI, D. GASTON, M. DEHART, A. ABOU-JAOUDE, and A. J. NOVAK, "Coupled Multiphysics Multiscale Transient Simulations of the Mk1-FHR using Finite Volume Capabilities of the MOOSE Framework," in "Math. & Comp. for Nuclear Sci. and Eng., Rayleigh NC," (2021).
9. C. FIORINA, I. CLIFFORD, M. AUFIERO, and K. MIKITYUK, "GeN-Foam: a novel OpenFOAM® based multi-physics solver for 2D/3D transient analysis of nuclear reactors," *Nuclear Engineering and Design*, **294**, 24–37 (2015).
10. NATIONAL REACTOR INNOVATION CENTER, "Virtual Test Bed documentation," https://mooseframework.inl.gov/virtual_test_bed/ (2021).
11. A. NOVAK, *Multiscale Thermal-Hydraulic Methods for Pebble Bed Reactors*, Ph.D. thesis, University of California Berkeley (2020).
12. M. NAKAGAWA and H. INOUE, "Double Heterogeneity Effect of Fuel Pin and Subassembly in a Fast Power Reactor," *Nuclear Science and Engineering*, **83**, 214–228 (1983).
13. L. WANG, J. GUO, F. LI, J. HOU, and K. IVANOV, "Effect Of Double Heterogeneity Treatment On Neutronics Modeling of HTGR Unit Cell," in "International Topical Meeting on High Temperature Reactor Technology," (11 2016).
14. A. HEBERT, "A Collision Probability Analysis of the Double-Heterogeneity Problem," *Nuclear Science and Engineering*, **115**, 177 (1993).
15. R. SANCHEZ, "A statistical analysis of the double heterogeneity problem," *Annals of Nuclear Energy*, **18**, 371–395 (12 1991).
16. J. LEPPÄNEN, *Serpent – A Continuous-Energy Monte Carlo Reactor Physics Burnup Calculation Code*, VTT Technical Research Centre of Finland (2013).
17. J. LEPPÄNEN, R. MATTILA, and M. PUSA, "Validation of the Serpent-ARES code sequence using the MIT BEAVRS benchmark – Initial core at HZP conditions," *Annals of Nuclear Energy*, **69**, 212–225 (2014).
18. X. WANG, K. HUFF, M. AUFIERO, P. PETERSON, and M. FRATONI, "Coupled reactor kinetics and heat transfer model for fluoride salt-cooled high-temperature reactor transient analysis," in "International Conference on Nuclear Engineering, Proceedings, ICONE," American Society of Mechanical Engineers (ASME) (Jan. 2016).
19. K. K. AHMED, R. O. SCARLAT, and R. HU, "Benchmark Simulation of Natural Circulation Cooling System with Salt Working Fluid Using SAM," in "17th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-17)," American Nuclear Society, Xi'an, China (2017).
20. C. H. ANDREADES, A. T. CISNEROS, J. K. CHOI, A. Y. CHONG, M. FRATONI, S. HONG, L. R. HUDDAR, K. D. HUFF, D. L. KRUMWIEDE, M. R. LAUFER, M. MUNK, R. O. SCARLAT, N. ZWEIBAUM, E. GREENSPAN, and P. F. PETERSON, "Technical Description of the Mark 1 Pebble-Bed Flouride-Salt-Cooled High Temperature Reactor (PB-FHR) Power plant," Tech. rep., University of California, Berkeley, Berkeley, CA (2014).
21. G. L. GIUDICELLI, A. D. LINDSAY, R. FREILE, and J. LEE, "NEAMS-TH-CRAB," Tech. Rep. INL/EXT-21-62895, Idaho National Laboratory (2021).
22. Y. WANG, J. ORTENSI, S. SCHUNERT, and V. LABOURE, "A Pebble Tracking Transport Algorithm for Pebble Bed Reactor Analysis," *Proceedings of PHYSOR 2018* (4 2018).