1 Prismatic High Temperature Gas-Cooled Reactor (HTGR) Neutronic Solvers

Nowadays, there are several codes to solve the neutronics of prismatic HTGRs. Most of these codes rely on one of the following methods: stochastic transport (Monte Carlo), deterministic transport, or deterministic diffusion. We focus our interest on the last method.

The history of deterministic diffusion solvers begins in the late 1950s with the Finite Difference Method (FDM) application to the analysis of Light Water Reactors (LWRs). In FDM, mesh spacings are usually of the order of the diffusion length. When solving large multi-dimensional problems, this feature causes the mesh points to reach intractable numbers [38]. The computational expense of these calculations motivated the generation of more computationally efficient techniques [34]. Although there are substantial overlaps, the most common techniques fall into two broad categories: nodal methods and Finite Element Method (FEM).

FLARE [12] is a three-dimensional Boiling Water Reactor (BWR) simulator, and it is representative of the first generation of nodal schemes. Such an approach used adjusted parameters to match actual operating data or the results of more accurate calculations. Most of these methods were implementations of the so-called 1.5 group theory. The second generation of nodal schemes derived spatial coupling relationships by applying the transverse integration procedure (TIP). Such a procedure obtains equivalent one-dimensional equations by integrating the multi-dimensional diffusion equation over directions transverse to each coordinate axis [34]. This approach proved to be highly efficient and accurate in Cartesian geometries.

In 1981, a formulation based on the Nodal Expansion Method (NEM) first demonstrated the feasibility of nodal methods in hexagonal geometries [15]. Nevertheless, this method would introduce non-physical singular terms that required the utilization of discontinuous polynomials. This drawback motivated the development of more effective formulations. The code HEXNOD, introduced in 1988 [66], is an example of such formulations. This algorithm uses the TIP and, in contrast to the NEM, solves the resulting differential equation analytically. The article demonstrated the method's accuracy by comparing the FDM and Monte Carlo calculations for a few benchmark problems.

Another example of more effective methods is the code HEXPEDITE [16]. HEXPEDITE uses the TIP formulation to derive a pseudo-one-dimensional equation. The resulting differential equation is solved analytically. The difference from HEXNOD is that HEXPEDITE uses a different coupling scheme that is simpler and more efficient. Different works [16][17] on the HEXPEDITE methodology tested the approach against the NEM and the FDM. These studies established HEXPEDITE's superiority in terms of accuracy and runtime. HEXPEDITE's use still prevailed until recently in the analysis of HTGRs. In 2010, Idaho National Laboratory (INL) conducted a study [47] in which they compared HEXPEDITE's results against the diffusion codes JAR, CITATION, and CRONOS2, and the Monte Carlo codes MCNP5 and Serpent.

DIF3D [33] and PARCS [13] are examples of other nodal diffusion codes whose use has prevailed until the present. DIF3D has several solution options such as the diffusion FDM, diffusion NEM based on TIP, and the VARIANT nodal transport method. PARCS has several solution options as well, such as a diffusion FDM, diffusion NEM based on TIP, P_N transport methods, and the multigroup transport Simplified P_3 with FDM and NEM discretizations.

Nodal methods solve relatively coarse meshes for approximate solutions. This characteristic makes the process efficient. On the other hand, the method does not provide detailed point-wise accurate solutions [31]. Additionally, the derivation of nodal methods happens in a specific coordinate system for a particular node shape. The application to complex problems is not flexible as different geometries require the integration over other coordinate systems. This lack of flexibility limits the applications of nodal methods to regular geometries only.

The FEM is a well-established method in applied mathematics and engineering. FEM is a numerical technique for finding approximate solutions to Partial Differential Equations (PDEs) by deriving their weak or variational form. Most applications make FEM preferable due to its flexibility in the treatment of curved or irregular geometries. Also, the use of high order elements attains higher rates of convergence [6]. The first engineering application of FEM was in the field of structural engineering and dated back to 1956. In successive years, FEM

became the most extensively used technique in almost every branch of engineering. FEMs have several advantages over the nodal methods. It provides flexibility in the geometry definition, a firm mathematical basis, ease in extension to the multi-group application, and high computational efficiency [36].

In 1973, Kang et al. [31] described the first application of FEM to the neutron diffusion theory. The fundamental motivation for this development was the impractical application of the FDM to three-dimensional problems. In this early work, the author compared different FEM approaches to the FDM in one-dimensional and two-dimensional problems. The studies showed a higher order of convergence achieved by the FEM.

Throughout the last four decades, many codes have used the FEM to solve the diffusion equation. Some of the most recent codes are CRONOS2 [32], CAPP [37], and Rattlesnake [68]. The list of FEM diffusion solvers is more extensive, but we focus on the best-documented codes in the open literature. We also emphasize that most of the FEM diffusion solvers for HTGRs were born as LWR analysis codes.

Commissariat a l'Energie Atomique (CEA) developed CRONOS2 [32] as part of the SAPHYR system. It allows for solving steady-state and transient multi-group calculations taking into account thermal-hydraulic feedback effects. The code solves either the diffusion equation or the transport equation through the SN method. In 2008, Damian et al. [11] conducted a study aimed at understanding the physical aspects of the annular core and the passive safety features of a standard block type HTGR. For such a study, the authors developed the code suit NEPTHIS/CAST3M. NEPHTIS uses a transport-diffusion calculation scheme that relies on CRONOS2.

In 2008, the Korea Atomic Energy Research Institute (KAERI) published an article [36] that presented the code CAPP. The code's purposes are to conduct steady-state core physics analysis, core depletion analysis, and core transient analysis. The article validated the code with two benchmark problems: first, the IAEA PWR benchmark problem; second, Phase I Exercise 1 of the OECD/NEA PBMR-400 Benchmark [48]. The calculations of both problems changed the number of elements and the orders of shape functions.

In 2011, Lee et al. published an article [37] in which they extended the functionalities of the CAPP code to prismatic HTGRs. To take into account the thermal feedback, the authors developed a simplified thermal-hydraulics analysis tool. To validate their model, the authors solved a two-dimensional model of the PMR-200 at the beginning of cycle (BOC). The PMR-200 is a pre-conceptual reactor that KAERI has designed. They validation compared the results against the HELIOS[54] results. The results showed good accuracy. Moreover, the authors implemented a depletion solver based on the one-group flux determined by the neutron flux solver. The authors validated the depletion solver by calculating the multiplication factor as a burnup function of a single fuel block of the PMR-200. They compared the results against the results obtained with HELIOS. The maximum error was less than 200 pcm.

Tak et al. [61] developed a coupling between the CAPP code and the GAMMA+ code [39]. GAMMA+ is a system code for thermal-hydraulics analysis and system transients. In such a study, the authors applied the coupled code to study the steady-state performance of the PMR-200. They conducted several studies, such as a core depletion calculation, a core depletion calculation with a critical control rod position search, and the analysis of the bypass flow effects on the coupled calculations. Their results revealed that neglecting the bypass flow decreases the active core temperatures and, consequently, the multiplication factor increases by approximately 300 pcm.

A recent article by Yuk et al. [69] added to CAPP the capability to conduct transient analyses. This capability solves the time-dependent neutron diffusion equation with the FEM. The primary motivation behind this feature is to enable the code to perform reactivity insertion accidents. Additionally, the article introduces a new method to resolve the control rod cusping effect [29]. To take into account the thermal feedback, the authors developed a simplified thermal-hydraulics analysis tool. The new method integrates over partially rodded computation nodes, and they called it iPRN. To test its accuracy, the authors conducted two exercises with several techniques that reduce the rod cusping effect. The authors used the mesh reconstruction method to obtain the reference results, as such a method eliminates the rod cusping effect by updating the mesh at every time step. The iPRN technique showed higher accuracy than the other methods. To test the new transient capabilities, they analyzed two control rod ejection scenarios and compared the results to those of CAPP/GAMMA+ coupled code. Both codes showed similar results.

RattleSnake [68] is the MOOSE [18] based application for simulating the transport equation. INL has initially developed the Pronghorn code to model Pebble Bed Modular Reactors (PBMRs). The MOOSE neutronics kernel library Yak incorporated the neutron diffusion models initially in Pronghorn [56]. Currently, RattleSnake is the primary tool for solving the linearized Boltzmann neutron transport equation within MOOSE and relies heavily on Yak's use. Various solvers are available under RattleSnake, including low-order multigroup diffusion, spherical harmonics transport, and discrete ordinates transport, all solved with the FEM.

In 2012, INL published a study [28] that coupled Pronghorn and RELAP-7 [1]. Pronghorn solved the coupled equations defining the neutron diffusion, fluid flow, and heat transfer in a three-dimensional model. RELAP-7 is a MOOSE-based system code, and it solves the one-dimensional continuity, momentum, and energy equations for a compressible fluid. It was responsible for modeling the plant system layout, including the hot and cold ducts, the helium circulator, and the steam generator. To test the coupling, INL's team carried out the OECD/NEA MHTGR-350 Benchmark [45]. The original benchmark provides a set of 26 neutron energy group and temperature dependent cross sections. To simplify the debugging, the authors collapsed the 26 groups into two groups. Although using two groups reduces the accuracy of the model, the lower number of groups decreases the calculation time by a factor of ten or more. In this study, a two-dimensional cylindrical model replaced the three-dimensional geometry defined by the benchmark. The integrated system testing included two stages: (1) both stand-alone codes underwent several convergence studies, and (2) the integrated system solved the steady-state problem in an integrated manner. The authors concluded that the coupling between Pronghorn and RELAP-7 was successful.

In 2013, INL conducted the OECD/NEA MHTGR-350 Benchmark [56] without further simplifications. The INL team solved Exercise 1 of Phase I using INSTANT-P1 [67], Pronghorn, and RattleSnake. INSTANT is a transport solver that relies on the spherical harmonics discretization of angles. The results for Pronghorn and RattleSnake are identical. By modifying the cross-sections, INSTANT-P1 returns the diffusion solution. Its results were within 30 pcm from Pronghorn and RattleSnake results. All presented results exhibited good agreement with the benchmark results.

1.1 Energy group structure analysis

The longer neutron mean free path in HTGRs compared to LWR increases the spectral interactions between elements. For this reason, HTGR analyses require more energy groups than conventional LWR analyses. Argonne National Laboratory (ANL) directed a study [35] to compare the accuracy of nodal diffusion calculations employing different energy group structures to generate the homogenized cross-sections. The cross-section homogenization used the code DRAGON, and the diffusion calculations utilized the code DIF3D. For the study, the ANL team implemented a one-dimensional fuel-reflector model in which they used 4, 7, 8, 14, and 23 energy groups. They also used alternative energy group structures for the same number of groups. For simplicity, the authors used the homogenized fuel compact model. They generated all the cross-sections at 300 K. One of their conclusions was that the number of energy groups should be more than 4, and 7 or more would be sufficient for uranium fueled HTGRs. Another finding was that the accuracy of the diffusion calculation is sensitive to the energy group boundaries.

Han's MS thesis [20] focused on selecting energy groups for the reactor analysis of the PBMR. The author used the code COMBINE6 [19] for cross-section generation and the Penn State nodal diffusion code NEM [3] for the reactor analysis. The author compared the results against reference results obtained with the code MCNP5 [9]. To simplify the setup, the model used uniformly distributed isotopes in the fuel. The study performed the calculations at two different temperatures: 300 and 1000 K. To arrive at an optimal group structure, the author compared many combinations of group structures using a trial and error strategy. One conclusion of this work agrees with the previous bibliography [10] [14] that the energy spectrum is critical to yield an accurate description of a nuclear reactor using a few groups.

ANL's study helps set up properly nodal diffusion calculations for an HTGR. Although we can extrapolate those conclusions to FEM diffusion solvers, such a study might be valuable. ANL's team conducted the study

at 300 K, not in the operational range of any HTGRs. On the contrary, Han's thesis included an analysis at 1000 K, and his results showed that the temperature changes have a non-negligible impact. Additionally, ANL's study used the simplified model of the homogenized fuel compact. Han's highlighted that homogenized fuel models of the PBMR underestimate criticality calculations. In 2015, INL presented their results [55] for an International Atomic Energy Agency (IAEA) Coordinated Research Project (CRP) [65] and showed that the homogenization of the compact material underestimates notably the eigenvalue. On the other hand, the open literature has not investigated the impact of such simplification over the homogenized cross-sections.

2 Prismatic HTGR Thermo-Hydraulics

Thermal-hydraulic calculations enable the correct design of HTGRs. The ability to predict the maximum fuel temperature at steady-state is of paramount importance to succeed in such task. We emphasize this statement in the case hydrogen production is desirable. Efficient hydrogen production requires higher coolant temperatures, which in turn increases the temperature of the fuel and the reactor pressure vessel.

The complex geometry of the hexagonal fuel assembly requires elaborate numerical calculations for obtaining accurate evaluations. Thermal-hydraulic studies for early HTGRs consisted mainly of support calculations for Nuclear Regulatory Commission (NRC) safety analysis reports. The analyses employed sets of independent codes that relied on simplistic approximations. Simplified models are helpful to understand some basic aspects of prismatic HTGRs and have the advantage to reduce the computational expense of the calculations.

General Atomics [52] developed the first set of simplistic codes. The following list introduces and summarizes some of these codes and their features:

- FLAC: It determines the coolant flow distribution in the coolant channels and gaps. It solves the onedimensional momentum equation for incompressible flow and the continuity equations for mass and energy.
- POKE: It determines the coolant mass flow, coolant temperature, and fuel temperature distribution. It solves the steady-state mass and momentum conservation equations for parallel channels.
- DEMISE: It determines the steady-state three-dimensional temperature distribution in a standard element. It solves the temperature in a network model.
- TAC-2D: It is a general purpose two-dimensional thermal analysis code. It solves the two-dimensional heat conduction equation.

Several studies have used these codes. For example, INL conducted in 2003 a design study [41] in support to the Next Generation Nuclear Power (NGNP) project. The objective of such study was to investigate options for the NGNP that increased the coolant temperature, with the lowest possible inlet temperature, and the highest overall core power. The authors conducted several parametric studies whose reference reactor was the GT-MHR [2]. Using the code POKE, they evaluated two major design modifications: reducing the bypass flow and better controlling the inlet coolant flow distribution. Reducing the bypass flow fraction from 20 to 10% reduces the peak fuel temperatures by about 50°C. Controlling the inlet flow distribution has a stronger effect. Other studies focused on the dimensions of the reactor and their impact on the maximum fuel temperature. Using the computer codes POKE and TAC2D, the authors investigated taller and higher power reactor cores. The investigation included a 10-block-high 600 MWt, a 12-block-high 720 MWt, and 14-block-high 840 MWt.

Among the simplified approaches we differentiate the flow network model, the equivalent cylindrical model, and the unit cell model. Using the network analysis tool RELAP5-3D/ATHENA [27], Reza et al. [49] conducted a thermal hydraulic study of the GT-MHR. Reza et al. increased the reactor outlet temperature to enable hydrogen production. Additionally, they evaluated alternative coolant inflow paths in an attempt to reduce the reactor vessel temperatures. After finding an optimal configuration, they evaluated the maximum temperatures

in the fuel and the reactor vessel during the low pressure conduction cool-down (LPCC) and the high pressure conduction cool-down (HPCC) events.

An example of codes using the equivalent cylindrical approach is GAMMA [46]. The code's main objective is the modeling of the air ingress event following a LOCA. Following the depressurization of helium in the core, there exists the potential for air to enter the core through the break and oxidize the in-core graphite structure. The oxidation of graphite leads to exothermic chemical reactions and, thus, it is a major concern. The GAMMA code solves heat conduction, fluid flow, chemical reactions, and multi-component molecular diffusion. The code couples the solid and gas equations using the porous media model. Together with the multi-dimensional analysis feature, GAMMA has a one-dimensional analysis capability for modeling a flow network.

Takada et al. [63] carried out another study using the flow network and the equivalent cylindrical model. Focusing on the High Temperature engineering Test Reactor (HTTR), they developed a thermal-hydraulic design code. The code used the flow network analysis code FLOWNET [42] for calculating the coolant flow and temperature distributions. The code TEMDIM [42] solved the fuel temperatures using the equivalent cylindrical model. Finally, the authors validated the calculation scheme by comparing its results with the experimental data from the HTTR.

Nakano et al. [43] studied different fuel assembly configurations using several simplistic approximations. For determining the fuel temperature, they used the TAC-2D code. A previous nuclear analysis calculated the power density. And a previous study calculated the flow distribution using the code FLOWNET. The fuel temperature calculation used the equivalent cylindrical model for a hot channel unit cell. However, the asymmetry of the unit cell configuration makes the temperature distribution asymmetric in the graphite block. The equivalent cylindrical model fails to capture this behavior.

In 2006, In et al. [23] conducted a more detailed analysis using a three-dimensional model of the unit cell in the hot-spot of an HTGR. The objective of the study was to predict the maximum fuel temperature at steady-state. The analysis focused on the GT-MHR 600 at end of cycle (EOC). The CFD code CFX 10 [24] calculated the three-dimensional temperature profile. In such a study, the results showed that the maximum fuel temperature surpassed the design limits and the authors propose a countermeasure accordingly.

Such simplified approaches are helpful to understand some basic aspects of prismatic HTGRs but they may affect the temperature distribution. More detailed thermal-hydraulic evaluations were rare in the open literature until the last 15 years.

Cioni et al. [8] presented an article in 2005 in which they conducted three-dimensional simulations of fuel assemblies of an HTGR. The objective of the study was to investigate an emergency situation due to the blocking of cooling channels in the core. They used the computational fluid dynamics (CFD) code Trio_U [4] to carry out the analysis. The numerical scheme solved the three-dimensional conduction equation in the solid coupled to the one-dimensional thermal-hydraulic equations of the coolant. In the preliminary work, the authors conducted a study of the influence of the bypass flow on the maximum coolant and fuel temperature. Another preliminary study analyzed the consequences of two different blocking in a portion of a fuel assembly. A central blockage exhibits a stronger influence over the maximum temperatures of the assembly compared to a peripheral blockage. At last, they investigated two configurations. First, six fuel elements surrounded the fuel element with the blockage. Second, five fuel elements and one reflector element surrounded it. The results suggested that the blockage increases the temperature on the blocked fuel assembly only and it does not affect the surrounding elements due to the bypass flow. The results also showed that the fuel temperature surpassed the design limits, and that the reactor operators should counteract these effects with active systems.

Simoneau et al. [53] analyzed the transient behavior of an HTGR during the depressurized conduction cool-down (DCC) and HPCC event. The CFD code STAR-CD [40] performed the calculations. The code solved conductive, convective, and radiation heat transfer in a 30° section of the core and reactor vessel. To accommodate the different spatial scales, the code uses the porous media model to represent the coolant flow and the prismatic fuel blocks. The model does not resolve the boundary layer and the use of coefficients prescribe the solid-fluid heat transfer and pressure drop across the core. The authors validated their model against explicit calculations using a single fuel block. One of their results shows that the maximum temperature in the HPCC

event is lower than in the DCC event. However, the extra convective heat transfer causes a thermal stratification in the surrounding air, causing higher temperatures in the upper reactor structures.

In 2008, an article by Tak et al. [60] conducted a three-dimensional CFD analysis on a typical prismatic HTGR fuel column. The commercial code CFX 11 [26] performed the calculations. The fuel column under study was from the PMR-600, a pre-conceptual reactor that KAERI has designed and whose reference design is the GT-MHR. The study considered a one-twelfth section of the fuel due to its symmetry. The model determined the coolant distribution using the one-dimensional thermal-hydraulic equations. Such coolant distribution served as input to the CFD code. Nevertheless, the friction in the channels is dependent on the viscosity which is highly dependent on the temperature. Therefore, obtaining the mass flow rates from a separate solver may introduce errors [51]. As mentioned earlier, the unit cell model may introduce errors in the maximum temperature prediction. In order to asses the accuracy of the unit cell model, the authors compared the CFD results against the unit cell model results. The unit cell model does not consider the bypass flow between assemblies or the radial power distribution within the fuel assembly. Tak et al. conducted a parametric study which analyzed the impact of the bypass gap size on the maximum fuel temperature. By increasing the bypass gap, the maximum fuel temperature grows. The results of this study indicate that the accuracy of the unit cell worsens for larger gaps. Another study imposed different radial peaking factors for the different fuel channels. Such a study showed the effects of considering a non-flat radial power distribution. The authors considered a radial power distribution that did not have a strong impact on the maximum fuel temperature.

Another article [51] carried out CFD calculations of a typical prismatic HTGR with the commercial code FLUENT [25]. Their model considered a one-twelfth section of the fuel column of the GT-MHR. The authors conducted parametric studies changing several factors, such as bypass gap-width, turbulence model, axial heat generation profile, and geometry changes due to irradiation. Their most relevant results show the presence of bypass flow causes a large lateral temperature gradient in the block. Large temperature gradients cause excessive thermal stresses which raise potential structural issues. The authors compared the results from different turbulence models: $k \sim \varepsilon$ and $k \sim \omega$. The $k \sim \omega$ model predicted bulk temperatures that are considerably lower than those from the $k \sim \varepsilon$ model. The differences went up to 49°C. The overall mass flow rate is about 10% greater for the $k \sim \omega$ model. The study suggested that these turbulence models need more verification against prismatic HTGR experiments. Another study analyzed the effect of considering different peak radial factors. Such consideration introduced variations of the maximum fuel temperature of up to 160 °C. Their last study focused on the effects of the graphite dimensional changes on the temperature profile. The shrunk column showed considerably lower temperatures in the fuel.

In spite of the recent developments in CFD tools, a detailed full core explicit analysis for a prismatic HTGR still requires a tremendous computational expense. This requirement is mostly due to the three-dimensional CFD simulation of the coolant flow. Travis et al. [64] developed a method to compute full core thermal-hydraulic analyses of HTGRs. The article presented a simplified method that reduces the computational time and memory requirements while maintaining accurate results. The method solves the three-dimensional heat conduction in the solid and the one-dimensional thermal-hydraulic equations in the channels. The fluid one-dimensional approximation avoids finer meshes near the walls as well as turbulence conservation equations [62]. The validation of the method analyzed a fuel column and compared the results to those of a three-dimensional CFD simulation. The CFD simulation used the commercial software STAR-CCM+ [7]. The new computational scheme reduced the computation time to a 2.5% of the time required by the three-dimensional CFD simulation. The new method provided good predictions of the temperature distribution and the axial variation of the helium bulk temperature. However, it failed to resolve properly the velocity and temperature distribution within the boundary layer. Overall, the method showed good accuracy, and less than a 2% difference to the three-dimensional CFD simulation.

Tak et al. [58] [62] developed CORONA, which uses a practical method for the whole core analysis. The code intends to combine the accuracy from CFD tools and the light computational expense of system analysis codes. The method solves the three-dimensional heat conduction equation in the solid and the one-dimensional thermal-hydraulic equations in the fluid. In order to enhance practicability, the code adopts a basic unit cell

concept, which eliminates an elaborate grid generation process. The basic unit cell concept is an extension of the traditional unit cell method, which uses a single triangular unit cell. This method considers various shapes of unit cells as well as the heat transfer between them. The method provides a way for fast generating computational grids for modeling the solid regions. To validate the new code, the authors compared the results using CORONA against the results using the commercial code CFX and experimental results. The results of the verification and validation studies showed that the CORONA code provides reasonably accurate results.

CFD techniques allow to compute the detailed temperature profile over local models. The fine mesh requirement imposes high computational costs for a whole core CFD analysis, restricting the use of such methods. However, a whole-core thermal analysis has many advantages over local models. In general, the problem set up includes more accurate boundary conditions. Without whole-core modeling, the mass flow distributions in local models are average values of the core flow rate instead of their exact value [21]. This leads to under predicted fuel temperatures for the assemblies with a lower flow rate than the average. Additionally, a coupled analysis with a reactor physics code requires a full core model [58].

3 Coupled Neutronics/Thermal-Hydraulics

Historically, stand-alone simulations have solved the neutronics and thermal-hydraulics of HTGRs. Nonetheless, these physical aspects describe processes that rely heavily on one another. Hence, to consider the interaction between the neutronics and thermal-hydraulics behavior, a coupled analysis is necessary [61].

In 2008, Damian et al. [11] conducted a study aimed at understanding the physical aspects of the annular core and the passive safety features of a prismatic HTGR. They performed analyses on various geometrical scales: unit cell and fuel column located at the core hot-spot, two-dimensional and three-dimensional core configurations including the coupling between neutronics and thermal-hydraulics. The first part of the assessment concerns thermal calculations on steady-state core configurations. Such study used CAST3M [57] code to solve the three-dimensional heat conduction in the solid coupled to the one-dimensional thermal-hydraulic equations in the coolant. The second part of the assessment used the transport code APOLLO2 [50] on a two-dimensional core configuration to minimize the radial power peaking factor. The analysis included the variation of several parameters such as fuel enrichment, fuel loading, and the fuel management scheme. The fuel enrichment variation had the strongest impact. The last part of the study analyzed a three-dimensional core model using the coupled codes NEPTHIS [5] and CAST3M/Arcturus. The codes NEPTHIS and CAST3M/Arcturus calculate the neutronics and the thermal-hydraulics, respectively. NEPHTIS uses a transport-diffusion calculation scheme that relies on APOLLO2 and the diffusion code CRONOS2. The CRONOS2 code solves either the diffusion equation or the even parity transport equation, and it uses a FDM or a FEM discretization. The CAST3M/Arcturus model uses a two-level approach. On the first level, the porous media model solves the homogenized system and the coolant. On the second level, the CAST3M code solves the thermal-hydraulics on the homogenized geometry. The authors conducted several parametric studies and assessed their impact on the power distribution. The studies included the variation of the helium by-pass fraction, average power density, core geometry, reflector materials, and fuel loading strategy. One of their results exhibited that with the reduction of the bypass fraction the average reflector temperature rises. Another result showed that using magnesium oxide as the reflector material yields lower temperatures for both normal operation and transients.

In 2011, Lee et al. published an article [37] in which they extended the functionalities of the CAPP code to prismatic HTGRs. To take into account the thermal feedback, the authors integrated to CAPP a simplified thermal-hydraulics tool. This tool divides a fuel column into six triangular prisms. Each of them hosts a representative coolant channel. Solving the energy equation, the code calculates the axial coolant temperature distribution. After calculating the coolant temperature, a two-dimensional conduction model solves the moderator and fuel compact temperatures. By means of a TRISO particle conduction model, the model obtains the fuel temperature. Finally, a three-dimensional conduction model based on the FDM allows for solving the reflector temperature. To validate their model, the authors solved a two-dimensional model of the PMR-200 at BOC.

They compared the results against the HELIOS code reference results. The results showed good accuracy.

Tak et al. [59] developed a neutronics/thermal-hydraulics coupled code using DeCART [30] and CORONA. DeCART is a whole-core neutron transport code and it was responsible for calculating the power distribution and the fast neutron fluence. CORONA calculated the temperature distribution. To validate the new code, the authors conducted the OECD/NEA MHTGR-350 benchmark. The main objective of the exercise was to validate the code and also identify technical challenges for future development. The authors presented an interesting analysis in which they compared the results from the coupled simulation and the stand-alone simulations. The difference in the multiplication factor was as high as 2597 pcm. The axial offset and maximum fuel temperature exhibited significant differences as well. Such result highlights the importance of the integration of both neutronics and thermal-hydraulic solvers.

Another article [61] introduced a coupling between the CAPP code and the GAMMA+ code. GAMMA+ is a system code for thermo-fluids analysis and system transients. GAMMA+'s development main motivation was the analysis of the air ingress accident and thermo-fluid transients in HTGRs. The code uses the one-dimensional form of the mass, momentum, energy, and species conservation equations to solve the flow and temperature distribution of the fluid. For solids, the code uses three different models: (1) heat conduction model of a TRISO particle, (2) implicit coupling to consider the heat exchange between a fuel compact and TRISO particle, and (3) multi-dimensional heat conduction model of the hexagonal fuel and reflector blocks. In such study, the authors applied the coupled code to study the steady-state performance of the PMR-200. They analyzed the bypass flow effects on the coupled calculations. Some of their most relevant results showed that the maximum fuel temperature reaches a peak near middle of cycle (MOC). Another result revealed that neglecting the bypass flow decreases the active core temperatures and increases the reflector temperatures. Consequently, the multiplication factor increased by approximately 300 pcm. On the other hand, the power density changes were not appreciable.

A recent article by Yuk et al. [69] added the capability to conduct transient analyses to the reactor physics code CAPP. To take into account the thermal feedback, the authors developed a simplified thermal-hydraulics analysis tool. The tool divides a fuel column into six triangular prisms. Each of them hosts a representative coolant channel. After calculating the coolant temperature, a two-dimensional conduction model solves the moderator and fuel compact temperatures. The CAPP code uses predetermined tables of thermal conductivity for each material. For a given fast neutron fluence and temperature, the code obtains the thermal conductivity by interpolation. To test the new transient capabilities, they analyzed two control rod ejection scenarios. They compared the results to those of the CAPP/GAMMA+ coupled code. Both methods showed similar results.

The prismatic HTGR tools available have lagged behind the state of the art compared to LWRs. This delay drives the development of more accurate and efficient tools to analyze the reactor behavior for design and safety evaluations. In addition to the development of new methods, it is essential to define appropriate benchmarks to compare the capabilities of various tools. In 2012, the Organisation for Economic Co-operation and Development (OECD)/Nuclear Energy Agency (NEA) defined a benchmark for the Modular High-Temperature Gas-Cooled Reactor (MHTGR)-350 MW reactor [44]. The purpose of this benchmark exercise is to compare various coupled reactor physics and thermal-hydraulic analysis methods. The MHTGR design serves as a basis for this benchmark. The scope of the benchmark is twofold: (1) to establish a well-defined problem, based on a common given data set, to compare methods and tools in core simulation and thermal-hydraulic analysis, and (2) to test the depletion capabilities of various lattice physics codes available for prismatic HTGRs. The OECD/NEA MHTGR-350 MW benchmark subdivides the coupled system calculation into three phases. Phase I corresponds to the stand-alone neutronics and thermal-hydraulics modeling, and the coupled neutronics/thermal-hydraulics steady-state modeling. Phase II consists of the transient cases. Phase III focuses on lattice depletion calculations.

Sensitivity analysis and uncertainty analysis methods can assess the predictive capabilities of coupled neutronics/thermal-hydraulics simulations. In 2013, the IAEA launched a CRP [65] on the HTGR Uncertainty Analysis in Modeling. The objective of the CRP was to determine the uncertainty in HTGR calculations at all stages of coupled reactor physics/thermal-hydraulics and depletion calculations. This CRP is a natural continuation of the previous

IAEA and OECD/NEA international activities [22][48] on Verification and Validation of available capabilities for HTGR simulations. The technical approach is to establish and utilize a benchmark for uncertainty analysis. The benchmark defines a series of well defined problems with complete sets of input specifications and reference experimental data. The CRP adopted the MHTGR-350 as the reference design and the GT-MHR as a second reference design. The design specification uses the OECD/NEA MHTGR-350 MW benchmark [44] code design specifications. The CRP subdivides the coupled system calculation into three phases. Phase I corresponds to the stand-alone neutronics and thermal-hydraulics modeling. Phase II consists of design calculations, which are the coupled steady-state neutronics/thermal-hydraulics calculations with and without a depletion calculation. Phase III focuses on safety calculations.

References

- [1] D Andrs, R Berry, R Gaston, R Martineau, J Peterson, H Zhang, H Zhao, and L Zou. RELAP-7 level 2 milestone report: Demonstration of a steady state single phase pwr simlulation with relap-7, 2012.
- [2] General Atomics. Gas Turbine-Modular Helium Reactor (GT-MHR) Conceptual Design Description Report, 1996.
- [3] B Bandini. A Three-dimensional Transient Neutronics Routine for the TRAC-PF1 Reactor Thermal Hydraulic Computer Code. Ph.D., The Pennsylvania State University, 1990.
- [4] U Bieder, C Calvin, and P Emonot. PRICELES: an object oriented code for industrial large eddy simulations., June 2000.
- [5] C Cavalier, F Damian, C Trakas, and M Groizard. Presentation of the HTR Neutronic Code System, 2005.
- [6] S Cavdar and H.A Ozgener. A finite element/boundary element hybrid method for 2-D neutron diffusion calculations. *Annals of Nuclear Energy*, 31(14):1555–1582, September 2004.
- [7] CD-Adapco. STAR-CCM+ release 7.04, 2012.
- [8] O. Cioni, M. Marchand, G. Geffraye, and F. Ducros. 3D thermal-hydraulic calculations of a modular block-type HTR core. *Nuclear Engineering and Design*, 236(5-6):565–573, March 2005.
- [9] RSICC Computer Code Collection. MCNP5 Monte Carlo N-Particle Transport Code System, 2003.
- [10] Gulf Oil Company. Nuclear Design Methods and Experimental Data in Use at Gulf General Atomic, 1973.
- [11] Frederic Damian. VHTR Core Preliminary Analysis Using NEPHTIS3 / CAST3M Coupled Modelling. In *Fourth International Topical Meeting on High Temperature Reactor Technology, Volume 1*, pages 419–429, Washington, DC, USA, January 2008. ASMEDC.
- [12] D.L. Delp, D.L. Fischer, J.M. Harriman, and M.J. Stedwell. FLARE, A three-dimensional boiling water reactor simulator, 1964.
- [13] T Downar, D Lee, Y Xu, and T Kozlowski. PARCS v2.6 US NRC Core Neutronics Simulator THEORY MANUAL, June 2004.
- [14] James J. Duderstadt and Louis J. Hamilton. *Nuclear Reactor Analysis*. Wiley, New York, 1 edition edition, January 1976.
- [15] T Duracz. A Nodal Method in Hexagonal Geometry. In *International Meeting on Advances in Mathematical Methods for Solution of Nuclear Engineering Problems*, Munich, Germany, April 1981.
- [16] W. E. Fitzpatrick and A. M. Ougouag. HEXPEDITE: A Net Current Multigroup Nodal Diffusion Method for Hexagonal-z Geometry, 1992.
- [17] William FItzpatrick. *Developments in Nodal Reactor Analysis Tools for Hexagonal Geometry*. PhD thesis, University of Illinois at Urbana-Champaign, Urbana, IL, 1995.
- [18] Derek Gaston, Chris Newman, Glen Hansen, and Damien Lebrun-Grandié. MOOSE: A parallel computational framework for coupled systems of nonlinear equations. *Nuclear Engineering and Design*, 239(10):1768–1778, October 2009.
- [19] R.A. Grimesey. COMBINE/PC-A Portable ENDF/B Version 6 Neutron Spectrum and Cross Section Generation Program, 1994.

- [20] James Sanggene Han. Sensitivity Study on the Energy Group Structure for High Temperature Reactor Analysis, May 2008.
- [21] Alexander Huning. A NOVEL CORE ANALYSIS METHOD FOR PRISMATIC HIGH TEMPERATURE GAS REACTORS, August 2016.
- [22] IAEA. Evaluation of high temperature gas cooled reactor performance: Benchmark analysis related to initial testing of the HTTR and HTR-10, November 2003.
- [23] In, Lee, Lim, and Lee. Three-Dimensional Analysis of the Hot-Spot Fuel Temperature in Pebble Bed and Prismatic Modular Reactors, May 2006.
- [24] ANSYS Inc. CFX 10, 2006.
- [25] FLUENT Inc. FLUENT, 2006.
- [26] ANSYS Incorporated. CFX 11 Manuals, 2006.
- [27] INL. RELAP5-3D/ATHENA Code Manual, 2005.
- [28] J. Ortensi, D. Andrs, A.A. Bingham, R.C. Martineau, and J.W. Peterson. Initial Coupling of the RELAP-7 and PRONGHORN Applications. Technical Report INL/EXT-12-27350, 1060984, INL, October 2012.
- [29] Han-Sem Joo. Resolution of the control rod cusping problem for nodal methods, February 1984.
- [30] KAERI. DeCART v1.2 User's Manual, 2007.
- [31] C. M. Kang and K. F. Hansen. Finite Element Methods for Reactor Analysis. *Nuclear Science and Engineering*, 51(4):456–495, August 1973.
- [32] J.J. Lautard, S. Loubiere, and C Magnaud. CRONOS, A Modular Computational System for Neutronic Core Calculations, September 1990.
- [33] R Lawrence. The DIF3D Nodal Neutronics Option for Two- and Three-Dimensional Diffusion-Theory Calculations in Hexagonal Geometry, March 1983.
- [34] R.D. Lawrence. Progress in nodal methods for the solution of the neutron diffusion and transport equations. *Progress in Nuclear Energy*, 17(3):271–301, January 1986.
- [35] Lee, Zhong, Taiwo, Yang, Smith, and Palmiotti. Status of Reactor Physics Activities on Cross Section Generation and Functionalization for the Prismatic Very High Temperature Reactor, and Development of Spatially-Heterogeneous Codes, August 2006.
- [36] H.C. Lee, C.K. Jo, and J.M. Noh. DEVELOPMENT OF CAPP CODE BASED ON THE FINITE ELE-MENT METHOD FOR THE ANALYSIS OF VHTR CORES. Washington, DC USA, October 2008.
- [37] Hyun Chul Lee, Chag Keun Jo, and Jae Man Noh. Development of the CAPP code for the Analysis of Block Type VHTRs, 2011.
- [38] E.E. Lewis and I. Dilber. Finite element, nodal and response matrix methods: A variational synthesis for neutron transport. *Progress in Nuclear Energy*, 18(1-2):63–74, January 1986.
- [39] Hong Sik Lim and Hee Cheon No. GAMMA Multidimensional Multicomponent Mixture Analysis to Predict Air Ingress Phenomena in an HTGR. *Nuclear Science and Engineering*, 152(1):87–97, January 2006.

- [40] Computational Dynamics Limited. STAR-CD Version 3.24 User Guide, 2004.
- [41] Philip E MacDonald. NGNP Point Design Results of the Initial Neutronics and Thermal-Hydraulic Assessments During Fy-03. Technical Report INEEL/EXT-03-00870 Rev. 1, INL, Idaho Falls, September 2003.
- [42] S Maruyama, T Murakami, Y Kiso, and Y Sudo. Verification of in-vessel thermal and hydraulic analysis code FLOWNET, 1988.
- [43] Nakano, Tsuji, and Tazawa. Conceptual Reactor Design Study of Very High Temperature Reactor (VHTR) with Prismatic-Type Core, 2008.
- [44] OECD NEA. Benchmark of the Modular High-Temperature Gas-Cooled Reactor MHTGR)-350 MW Core Design. Technical Report NEA/NSC/R(2017)4, OECD, 2017.
- [45] OECD NEA. Coupled Neutronic/Thermal- Fluid Benchmark of the MHTGR-350 MW Core Design: Results for Phase I Exercise 1, February 2020.
- [46] Hee Cheon No, Hong S. Lim, Jong Kim, Chang Oh, Larry Siefken, and Cliff Davis. Multi-component diffusion analysis and assessment of GAMMA code and improved RELAP5 code. *Nuclear Engineering and Design*, 237(10):997–1008, May 2007.
- [47] J Ortensi, J.J. Cogliati, M.A. Pope, J.D. Bess, R.M. Ferrer, A. Binghman, and A.M. Ougouag. Deterministic Modeling of the High Temperature Test Reactor with DRAGON-HEXPEDITE. Prague, Czech Republic, October 2010.
- [48] F Reitsma, J Han, K Ivanov, and E Sartori. The OECD-NEA/NSC PBMR400 MW coupled neutronics thermal hydraulics transient benchmark Steady-state results and status, September 2008.
- [49] SM Mohsin Reza, Edwin Harvego, Matt Richards, Arkal Shenoy, and Kenneth Pddicord. Design of an Alternative Coolant Inlet Flow Configuration for the Modular Helium Reactor, June 2006.
- [50] Sanchez, Hebert, Stankovski, Coste, Loubiere, Van der Gucht, and Zmijarevic. APOLLO2 Twelve Years Later, September 1999.
- [51] Hiroyuki Sato, Richard Johnson, and Richard Schultz. Computational fluid dynamic analysis of core bypass flow phenomena in a prismatic VHTR. *Annals of Nuclear Energy*, 37(9):1172–1185, September 2010.
- [52] A.S. Shenoy and D.W. McEachern. HTGR Core Thermal Design Methods and Analysis, December 1974.
- [53] Jan-Patrice Simoneau, Julien Champigny, Brian Mays, and Lewis Lommers. Three-dimensional simulation of the coupled convective, conductive, and radiative heat transfer during decay heat removal in an HTR. *Nuclear Engineering and Design*, 237(15-17):1923–1937, September 2007.
- [54] R.J. Stamml'er. HELIOS Methods, 1998.
- [55] Gerhard Strydom, Friederike Bostelmann, and Su Jong Yoon. Results for Phase I of the IAEA Coordinated Research Program on HTGR Uncertainties. Technical Report INL/EXT–14-32944, 1173079, INL, January 2015.
- [56] Gerhard Strydom, Javier Ortensi, Sonat Sen, and Hans Hammer. INL Results for Phase I and III of the OECD/NEA MHTGR-350 Benchmark, September 2013.

- [57] E. Studer, A. Beccantini, S. Gounand, F. Dabbene, J.P. Magnaud, H. Paillère, I. Limaiem, F. Damian, H. Golfier, C. Bassi, and J.C. Garnier. CAST3M/ARCTURUS: A coupled heat transfer CFD code for thermal–hydraulic analyzes of gas cooled reactors. *Nuclear Engineering and Design*, 237(15-17):1814–1828, September 2007.
- [58] Tak, Kim, Lim, and Noh. A practical method for Whole-Core Thermal Analysis of a Prismatic Gas-Cooled Reactor, March 2012.
- [59] Nam-il Tak, Tae Young Han, and Hyun Chul Lee. Coupled Neutronics and Thermo-Fluid Simulation of Full-Core Prismatic Gas-Cooled Reactor Using DeCART/CORONA Code System. page 4, Gyeongju, Korea, October 2016.
- [60] Nam-il Tak, Min-Hwan Kim, and Won Jae Lee. Numerical investigation of a heat transfer within the prismatic fuel assembly of a very high temperature reactor. *Annals of Nuclear Energy*, 35(10):1892–1899, October 2008.
- [61] Nam-il Tak, Hyun Chul Lee, Hong Sik Lim, and Tae Young Han. CAPP/GAMMA+ code system for coupled neutronics and thermo-fluid simulation of a prismatic VHTR core. *Annals of Nuclear Energy*, 92:228–242, June 2016.
- [62] Nam-Il Tak, Sung Nam Lee, Min-Hwan Kim, Hong Sik Lim, and Jae Man Noh. DEVELOPMENT OF A CORE THERMO-FLUID ANALYSIS CODE FOR PRISMATIC GAS COOLED REACTORS. *NUCLEAR ENGINEERING AND TECHNOLOGY*, page 14, 2014.
- [63] Eiji Takada, Shigeaki Nakagawa, Nozomu Fujimoto, and Daisuke Tochio. Core thermal–hydraulic design. *Nuclear Engineering and Design*, 233(1-3):37–43, October 2004.
- [64] Boyce W. Travis and Mohamed S. El-Genk. Thermal–hydraulics analyses for 1/6 prismatic VHTR core and fuel element with and without bypass flow. *Energy Conversion and Management*, 67:325–341, March 2013.
- [65] Bismark Tyobeka, Frederik Reitsma, and Kostadin Ivanov. HTGR REACTOR PHYSICS, THERMAL-HYDRAULICS AND DEPLETION UNCERTAINTY ANALYSIS: A PROPOSED IAEA COORDI-NATED RESEARCH PROJECT. Rio de Janeiro, Brazil, May 2011. American Nuclear Society.
- [66] M. R. Wagner. Three-Dimensional Nodal Diffusion and Transport Theory Methods for Hexagonal- z Geometry. *Nuclear Science and Engineering*, 103(4):377–391, December 1989.
- [67] Y Wang, C Rabiti, and G Palmiotti. Krylov Solvers Preconditioned with the Low-Order Red-Black Algorithm for The Pn Hybrid FEM for the INSTANT Code. In *International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering*, Rio de Janeiro, Brazil, May 2011.
- [68] Yaqi Wang, Sebastian Schunert, and Vincent Laboure. Rattlesnake Theory Manual, April 2019.
- [69] Yuk, Cho, Jo, Tak, and Lim. Time-dependent neutron diffusion analysis using finite element method for a block-type VHTR core design, January 2020.