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BY

ROBERTO E. FAIRHURST AGOSTA

THESIS

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Master's Committee:

Assistant Professor Kathryn D. Huff, Advisor  
Professor Segundo Lector

# Abstract

Abstract.

# Acknowledgments

Acks.

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# Chapter 1

## Introduction

### 1.1 The Prismatic High-Temperature Gas-Cooled Reactor

The history of prismatic High-Temperature Gas-Cooled Reactors (HTGRs) or simply Prismatic Modular Reactors (PMRs) begins in the 1960s with the deployment of the Dragon reactor in the United Kingdom (UK). Its initial objective was to demonstrate the feasibility of the HTGR and launch the technology development. The Dragon reactor experiment first operated in July 1965 and reached full-power operation of 20 MWt in April 1966. The reactor operated for long periods at full power, demonstrated the successful operation of many components, and provided information on fuel and material irradiation tests. Simultaneously, interest in the US led to the 40 MWe HTGR at Peach Bottom. The reactor achieved initial criticality in March 1966 and went into commercial operation in June 1967. Peach Bottom provided demonstrated the HTGR concept by confirming the core physics calculations, verifying the design analysis methods, and providing a database for further design activities. Most importantly, the plant demonstrated the ability of HTGRs to function in a load-following manner [4]. After the deployment of these two prototype reactors came the first HTGR demonstration plant, the Fort St. Vrain (FSV) Generating Station. Its electric power generation started in December 1976, reaching full-power operation in November 1981. The FSV plant generated 842 MWt to achieve a net output of 330 MWe. This reactor laid the foundation for future prismatic designs. Beginning with FSV, the US core design included ceramic coated Tristructural Isotropic (TRISO) particles embedded within rods placed in large hexagonal shaped graphite elements [4].

The PMR's most fundamental characteristic is the unique safety philosophy embodied in its design [9]. The control of radionuclides does not rely on active systems or operator actions. TRISO particles, Figure 1.1, play a significant role in this task. They consist of various layers acting in concert to provide a containment structure that limits radioactive product release. A TRISO particle is a microsphere of about 0.8 mm in diameter. It includes a fuel kernel surrounded by a porous carbon layer (or buffer), followed successively by an inner pyrolytic carbon (IPyC) layer, a silicon carbide (SiC) layer, and an outer pyrolytic carbon (OPyC) layer. An additional advantage of the TRISO particles is that they increase the proliferation resistance of HTGRs. They are a very unattractive and the least desirable route for diversion or theft of weapons-usable materials [8].

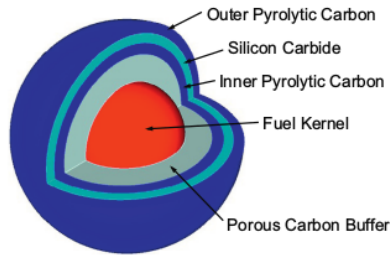


Figure 1.1: Drawing of a TRISO fuel particle. Image reproduced from [6].

Another contributor to the passive safety of the HTGR design is its materials. Combining a graphite core structure, ceramic fuel, and inert helium permits very high operating temperatures [1]. Graphite has a high heat capacity and maintains its strength at temperatures beyond 2760 °C. As a result, temperature changes in the core occur very slowly and without damage to the core structure during transients. Besides, the annular core geometry and a low core power density enable passive heat transfer mechanisms to remove the decay heat following postulated accidents [12]. These passive heat transfer mechanisms rely primarily on the natural processes of conduction, thermal radiation, and convection.

A desirable feature of the HTGR is its higher operating temperature. Higher temperatures offer increased cycle efficiencies. The early HTGR designs converted their heat into electricity using the Rankine steam cycle [7]. In such a system, the helium coolant passes through a heat exchanger generating steam to drive a turbine. This arrangement is around 38% efficient [3]. Some of these designs would superheat the steam to increase their efficiency, but this complicates the plant layout [1]. A practical temperature limit is around 300-400 °C. To take advantage of the high core outlet temperature of the HTGR, the Brayton cycle is a better option, where the helium coolant directly drives a gas turbine in a closed cycle. With such configuration, the system can achieve an energy conversion efficiency of around 48% [3]. Additionally, having helium circulating in a closed cycle removes external sources of contamination of the nuclear circuit. Thus, the need for on-line cleanup systems is vastly reduced [9].

Another advantage of the HTGR over other reactor designs is that higher outlet temperatures and increased cycle efficiencies enable a wide range of process heat applications. Some applications use steam for coal gasification processes, oil refinery processes, and synthesis gas production, methanol, and hydrogen. Several hydrogen production processes benefit from high temperatures. Some examples are high-temperature electrolysis or thermochemical water splitting. Utilizing the HTGR as the energy source of the process eliminates the need to burn fossil fuels to generate the steam those processes require [9].

This thesis focuses primarily on the Modular High-Temperature Gas-Cooled Reactor (MHTGR)-350 [12] [17]. Under the sponsorship of the US Department of Energy (DOE), a team consisting of General Atomics, Combustion Engineering, General Electric, Bechtel National, Stone & Webster Engineering, and Oak Ridge National Laboratory

(ORNL) developed the MHTGR [12]. They designed the basic module to deliver superheated steam at 17.3 MPa and 538 °C. Based on both economic and technological considerations, a 350 MWt modular reactor defines the optimal configuration. The team completed in 1986 the preliminary safety information document for the MHTGR and the complete draft pre-application in 1989 [8].

## 1.2 Motivation

This work's ultimate goal is to support the development of HTGR technology. More specifically, we focus on the development of computational methods for modeling HTGRs. We use *Moltres* as our primary analysis tool.

The Generation IV Roadmap project identified reactor concepts that could meet the future's energy demands in an efficient, economical, and environmentally safe manner [11]. One of these reactor concepts is the Very High Temperature Gas Cooled Reactor (VHTR). VHTR is distinct from HTGR as its coolant outlet temperature reaches higher temperatures. However, the literature often uses these terms interchangeably. In this work, the term HTGR encompasses both terms. The DOE had selected this reactor concept for the Next Generation Nuclear Power (NGNP) Project. This project intended to demonstrate emissions-free nuclear-assisted electricity and hydrogen production by 2015.

Although the DOE has canceled the NGNP Project, HTGRs will become a reality in the near term. Some microreactor designs embody this type of technology and may be operational before 2030. Additionally, as the introduction has already described, the HTGR technology has several favorable characteristics. To recapitulate the most important features, the HTGR relies on passive heat transfer mechanisms, uses TRISO particles as its fuel, has a high proliferation resistance, can achieve high temperatures, and benefits from increased cycle efficiencies. Other beneficial characteristics are that high temperatures enable a wide range of process heat applications, among which we find hydrogen production.

Modeling and prediction of core thermal-hydraulic behavior is necessary for assessing the safety characteristics of a reactor. Determining the temperature inside a reactor, for both normal and transient operation, is of paramount importance as the several materials' integrity depends on it. Most importantly, undesirably high temperatures endanger the TRISO particles' integrity and, consequently, jeopardize a fission product release [18]. Furthermore, the fuel blocks' complex geometry hinders accurate calculations of the fuel temperatures requiring elaborate numerical calculations.

The characteristics of an HTGR are different from those of conventional Light Water Reactors (LWRs). Such differences create a demand for new reactor analysis tools. These new tools should take into account the following peculiarities of HTGRs [16][2]:

- Hexagonal structure: the shape of the fuel blocks does not conform to any orthogonal coordinate system.
- Double heterogeneity: the TRISO particles form the first heterogeneity level, consisting of four layers. The second level arises from the fuel elements, as they encompass the compacts, the coolant, and the moderator.
- Strong dependence of the neutron spectrum and the macroscopic cross-sections on the fuel temperatures.
- The high thermal inertia of the reactor core causes long transients due to large graphite structures.

Historically, linking a stand-alone neutronics solver to a thermal-hydraulics solver allowed for simulating an entire reactor. The coupling of the codes occurred in a black-box fashion, where one code's output served as the other's input, and vice versa. This coupling technique is commonly known as the operator-splitting technique [15]. In such an approach, each individual physics isolates the action of the governing equations upon the variables. Nonetheless, these physical models describe processes that rely heavily on the solution of one another's. The neutron flux determines the power distribution. The power distribution has a strong influence on the temperature field. Due to the HTGR strong temperature feedback, the temperature affects the neutron flux distribution in the core. Because of a large time-scale separation between the different phenomena, multiphysics transient simulations coupled via the operator-splitting approach may introduce significant numerical errors [15] [14].

Multi-physics Object-Oriented Simulation Environment (MOOSE) [5] is a computational framework targeted at solving fully coupled systems. All the software built on the MOOSE framework shares a joint code base. These features facilitate relatively easy coupling between different phenomena and allow for great flexibility, even with a large variance in time scales [13]. Additionally, all codes use MPI for parallel communication and allow for deployment on massively-parallel cluster-computing platforms.

*Moltres* [10] is a Finite Element Method (FEM) simulation code built within the MOOSE framework. *Moltres* solves arbitrary-group neutron diffusion, precursor, and temperature governing equations. Besides, this simulation tool is open source. All these characteristics make *Moltres* suitable for solving the type of physical phenomena described above.

### 1.3 Objectives

As mentioned earlier, the ultimate goal of this work is to support the development of HTGR technology. The following list of main objectives expands on that goal.

**Extend *Moltres* modeling capabilities to HTGRs.** *Moltres* is a multi-physics solver of Molten Salt Reactor (MSR). Enhancing *Moltres* will allow it to model HTGRs as well.

**Couple the different physics phenomena present in an HTGR.** Moltres's current capabilities allow for solving some of the physics in the HTGR design. Nevertheless, the inherent physics in an HTGR needs to be captured by the solver and adequately integrated into the current capabilities.

**Develop safety analysis capabilities in Moltres.** Steady-state simulations help understand the fundamental behavior of an HTGR. They are also necessary for reactor design. Transient simulations are also necessary for reactor design. Transient simulations assess the reactor response in design basis events.

**Understand HTGR contribution to stopping climate change.** HTGRs are capable of attaining high temperatures. Such feature makes them attractive for deployment alongside hydrogen plants. With high temperatures, the efficiency of hydrogen production increases.

The main objectives are somewhat broad. The following list presents secondary objectives that will lead to the fulfillment of the main objectives:

**Predict neutronics appropriately.** Moltres should have the ability to carry out eigenvalue calculations appropriately. Additionally, Moltres should predict the flux shape and magnitude accurately, during steady-state and transient simulations.

**Understand the impact of some simulation parameters.** The underlying physics of HTGRs are different from the physics of other reactors. Consequently, the simulation results will be sensitive to different parameters from other reactor type simulations. This work will focus on the energy group structure and its effects on the diffusion calculations. We will also assess the effect of such parameters on the performance of the simulations.

**Calculate power distribution correctly.** The importance of an accurate neutronics behavior prediction lies in the accurate prediction of the power distribution. The power distribution is the most influential parameter over the thermal-hydraulics as it determines the temperature profile in the reactor.

**Predict temperature profile accurately.** Undesirably high temperatures endanger the integrity of the TRISO particles. Additionally, the temperature influences the neutronics. Hence, an accurate neutronics calculation will not be accurate without an accurate thermal-hydraulics calculation, and vice versa.

**Develop a hydrogen production calculation tool.** There exist several production methods. Most of them have different energy requirements and have different production rates. We will develop a tool to determine such quantities.

# Chapter 2

## Literature Review

### 2.1 Prismatic HTGR Diffusion 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 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 [? ]. The computational expense of these calculations motivated the generation of more computationally efficient techniques [? ]. Although there are substantial overlaps, the most common techniques fall into two broad categories: nodal methods and FEM.

FLARE [? ] 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 [? ]. 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 [? ]. 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 [? ], 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 [? ]. 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 [?] 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 [?] in which they compared HEXPEDITE's results against the diffusion codes JAR, CITATION, and CRONOS2, and the Monte Carlo codes MCNP5 and Serpent.

DIF3D [?] and PARCS [?] 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 [?]. 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 [?]. 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 [?].

In 1973, Kang et al. [?] 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 [?], CAPP [?], and Rattlesnake [?]. 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 à l'Energie Atomique (CEA) developed CRONOS2 [?] 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. [?] 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 NEPTIS/CAST3M. NEPTIS uses a transport-diffusion calculation scheme that relies on CRONOS2.

In 2008, the Korea Atomic Energy Research Institute (KAERI) published an article [?] 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 [?]. The calculations of both problems changed the number of elements and the orders of shape functions.

In 2011, Lee et al. published an article [?] 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 equilibrium cycle (BOC). The PMR-200 is a pre-conceptual reactor that KAERI has designed. They validation compared the results against the HELIOS[?] 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. [?] developed a coupling between the CAPP code and the GAMMA+ code [?]. 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. [?] 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 [?]. 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 [?] is the MOOSE [5] 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 [?]. 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 [?] that coupled Pronghorn and RELAP-7 [?]. 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 [?]. 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 [?] without further simplifications. The INL team solved Exercise 1 of Phase I using INSTANT-P1 [?], 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.

### 2.1.1 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 [?] 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 [?] focused on selecting energy groups for the reactor analysis of the PBMR. The author used the code COMBINE6 [?] for cross-section generation and the Penn State nodal diffusion code NEM [?] for the reactor analysis. The author compared the results against reference results obtained with the code MCNP5 [?]. 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 [?] [?] 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 [?] for an International Atomic Energy Agency (IAEA) Coordinated Research Project (CRP) [?] 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.

## 2.2 Prismatic HTGR Thermal-hydraulics

Thermal-hydraulic calculations enable the correct design of HTGRs. Predicting the maximum fuel temperature at a steady-state is of paramount importance to succeed in such a task. We emphasize this statement in the case that hydrogen production is desirable. Efficient hydrogen production requires higher coolant temperatures, which 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 help understand some fundamental aspects of prismatic HTGRs and have the advantage of reducing the computational expense of the calculations.

General Atomics [?] 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 one-dimensional 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 [11] in support of the NGNP project. Such a study aimed 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 [?]. 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 [? ], Reza et al. [?] 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 fuel and the reactor vessel's maximum temperatures 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 [? ]. 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 significant 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. [?] carried out another study using the flow network and the equivalent cylindrical model. Focusing on the High Temperature Test Reactor (HTTR), they developed a thermal-hydraulic design code. The code used the flow network analysis code FLOWNET [?] for calculating the coolant flow and temperature distributions. The code TEMDIM [?] 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. [?] 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. Moreover, 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. [?] 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 a steady-state. The analysis focused on the GT-MHR 600 at the end of equilibrium cycle (EOEC). The CFD code CFX 10 [?] 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 essential 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. [?] presented an article in 2005 in which they conducted three-dimensional simulations of fuel assemblies of an HTGR. The study's objective 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 [?] to carry out the analysis. The numerical scheme solved the three-dimensional conduction equation in the solid coupled to the coolant's one-dimensional thermal-hydraulic equations. In the preliminary work, the authors conducted a study of the bypass flow's influence 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 assembly's maximum temperatures 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. [?] analyzed the transient behavior of an HTGR during the depressurized conduction cool-down (DCC) and HPCC event. The CFD code STAR-CD [?] performed the calculations. The code solved conductive, convective, and radiation heat transfer in a 30° section of the core and reactor vessel. The code uses the porous media model to accommodate the different spatial scales. 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. [18] conducted a three-dimensional CFD analysis on a typical prismatic HTGR fuel column. The commercial code CFX 11 [?] 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 [?]. As mentioned earlier, the unit cell model may introduce errors in the maximum temperature prediction. To assess 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 that analyzed the bypass gap size's impact 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 strongly impact on the maximum fuel temperature.

Another article [?] carried out CFD calculations of a typical prismatic HTGR with the commercial code FLUENT [?]. 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 that the 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.

Despite the recent developments in CFD tools, a detailed full-core 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. [?] 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 [?]. The method's validation 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+ [?]. The new computational scheme reduced the computation time to 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 the velocity and temperature distribution within the boundary layer properly. Overall, the method showed good accuracy and less than a 2% difference to the three-dimensional CFD simulation.

Tak et al. [?] [?] 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. 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 computing the detailed temperature profile over local models. The fine mesh requirement imposes high computational costs for a whole-core CFD analysis, restricting 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 local models' mass flow distributions are average values of the core flow rate instead of their exact value [? ]. This simplification 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 [? ].

## 2.3 Prismatic HTGR Multi-physics

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, a coupled analysis is necessary to consider the interaction between the neutronics and thermal-hydraulics behavior [? ].

In 2008, Damian et al. [? ] conducted a study aimed to understand 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 a study used CAST3M [? ] code to solve the three-dimensional heat conduction in the solid coupled with the one-dimensional thermal-hydraulic equations in the coolant. The second part of the assessment used the transport code APOLLO2 [? ] 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 most substantial impact. The last part of the study analyzed a three-dimensional core model using the coupled codes NEPTHEIS [? ] and CAST3M/Arcturus. The codes NEPTHEIS 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 an 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 bypass 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 normal operation and transients.

In 2011, Lee et al. published an article [?] 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. The code calculates the axial coolant temperature distribution solving the energy equation. After calculating the coolant temperature, a two-dimensional conduction model solves the moderator and fuel compact temperatures. Through 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. [?] developed a neutronics/thermal-hydraulics coupled code using DeCART [?] 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 exercise's main objective was to validate the code and identify technical challenges for future development. The authors presented an interesting analysis in which they compared the coupled simulation results 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 a result highlights the importance of the integration of both neutronics and thermal-hydraulic solvers.

Another article [?] 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 primary motivation was to analyze 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 fluid's flow and temperature distribution. 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 a 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 the middle of equilibrium 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. [?] 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 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 various tools' capabilities. In 2012, the Organisation for Economic Co-operation and Development (OECD)/Nuclear Energy Agency (NEA) defined a benchmark for the MHTGR-350 MW reactor [?]. The purpose of this benchmarking 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 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 [?] on the HTGR Uncertainty Analysis in Modeling. The CRP objective 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 [?][?] on Verification and Validation of available HTGR simulations capa-

bilities. 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 [?] 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, coupled with steady-state neutronics/thermal-hydraulics calculations with and without a depletion calculation. Phase III focuses on safety calculations.

# Chapter 3

## Methodology

### 3.1 Computational tools

#### 3.1.1 MOOSE

MOOSE[5] is a computational framework whose purpose is to support engineering analysis applications. In a nuclear reactor, several PDEs describe its physical behavior. These equations are typically nonlinear, and they are often strongly coupled to each other. MOOSE targets such systems and solves them in a fully coupled manner.

MOOSE is an open-source code under a Lesser GNU Public License (LGPL). The code itself relies on LibMesh [? ], an LGPL finite element library, and Petsc, a Berkeley Software Distribution (BSD)-licensed toolkit for solving nonlinear equations [? ]. MOOSE applications define weak forms of the governing equations. They modularize the physics expressions into "Kernels." Kernels are C++ classes containing methods for computing the residual and Jacobian contributions of individual pieces of the governing equations. MOOSE and LibMesh translate them into residual and Jacobian functions. These functions become inputs into Petsc solution routines.

MOOSE utilizes the mathematical structure present in Jacobian-Free Newton-Krylov (JFNK) methods [? ]. JFNK methods are synergistic combinations of Newton-type methods for superlinearly convergence of nonlinear equations and Krylov subspace methods for solving the Newton correction equations. The link between the two methods is the Jacobian-vector product. JFNK methods compute such products approximately without forming and storing the elements of the true Jacobian. The ability to perform a Newton iteration without forming the Jacobian gives JFNK methods potential for application throughout problems governed by nonlinear partial differential equations.

All the software built on the MOOSE framework shares a joint code base. The applications, by default, use monolithic and implicit methods. This feature facilitates relatively easy coupling between different phenomena and allows for great flexibility, even with a large variance in time scales [13]. Additionally, all codes use MPI for parallel communication and allow for deployment on massively-parallel cluster-computing platforms.

### 3.1.2 Moltres

*Moltres* [10] is a MOOSE based application initially designed for modeling fluid-fuelled MSRs. This simulation tool is open source and counts with an LGPL license. It uses `git` for version control, emphasizing its openness and promoting quality through peer review.

Moltres solves arbitrary-group neutron diffusion, precursors, and temperature governing equations. It can solve the equations in a fully-coupled way or solve each system independently, allowing for great flexibility and making it applicable to a wide range of nuclear engineering problems.

### 3.1.3 Serpent

The Serpent Monte Carlo code [?] [?] is a three-dimensional continuous-energy neutron transport code. VTT Technical Research Centre of Finland developed it, and it has been in public distribution since 2009. Monte Carlo neutron transport codes have several reactor physics applications related to criticality safety analyses, radiation shielding problems, detector modeling, and validation of deterministic transport codes. The Monte Carlo method's main advantage is its capability to model geometry and interaction physics without significant approximations. The main disadvantage is that modeling complex systems are very computing-intensive, restricting the applications to some extent.

Serpent serves two primary purposes: (1) reactor modeling, and (2) group constant generation. In reactor modeling, the Monte Carlo simulation itself represents the solution to the full-scale problem. In group constant generation, the transport simulation produces input parameters for a deterministic code. Based on a few groups, deterministic codes allow for carrying out coupled full-core analyses.

In this work, Serpent produces group constants that serve as an input for Moltres and solves the heterogeneous system. This last step provides the reference solutions for the validation of the Moltres calculation scheme. For the calculations, we used Serpent 2.1.31 and the cross-section library JEFF3.1.2. The choice of Serpent as the cross-section generation tool comes from one of its capabilities. Serpent allows for the explicit modeling of randomly located TRISO particles. Applying a simple volume homogenization has proven inaccurate due to the resonant self-shielding effect of the kernel and coated layers. Although the particles' explicit modeling is time-consuming, costly, and impractical for most applications, it results necessary.

## 3.2 Mathematical basis

### 3.2.1 Diffusion and precursors equations

Equations 3.1 and 3.2 describe the time dependent behavior of the neutronics.

$$\frac{1}{v_g} \frac{\partial}{\partial t} \phi_g = \nabla \cdot D_g \nabla \phi_g - \Sigma_g^r \phi_g + \sum_{g' \neq g}^G \Sigma_{g' \rightarrow g}^s \phi_{g'} + \chi_g^p \sum_{g'=1}^G (1 - \beta) v \Sigma_{g'}^f \phi_{g'} + \chi_g^d \sum_i^I \lambda_i C_i \quad (3.1)$$

$$\frac{\partial}{\partial t} C_i = \sum_{g'=1}^G \beta_{g'} v \Sigma_{g'}^f \phi_{g'} - \lambda_i C_i \quad (3.2)$$

where

$v_g$  = group  $g$  neutron speed

$\phi_g$  = group  $g$  neutron flux

$t$  = time

$D_g$  = group  $g$  diffusion coefficient

$\Sigma_g^r$  = group  $g$  macroscopic removal cross-section

$\Sigma_{g' \rightarrow g}^s$  = group  $g'$  to group  $g$  macroscopic scattering cross-section

$\chi_g^p$  = group  $g$  prompt fission spectrum

$G$  = number of discrete energy groups

$v$  = number of neutrons produced per fission

$\Sigma_g^f$  = group  $g$  macroscopic fission cross-section

$\chi_g^d$  = group  $g$  delayed fission spectrum

$I$  = number of delayed neutron precursor groups

$\beta$  = delayed neutron fraction

$\lambda_i$  = average decay constant of delayed neutron precursors in precursor group  $i$

$C_i$  = concentration of delayed neutron precursors in precursor group  $i$ .

(3.3)

We apply the vacuum boundary condition to the diffusion equation. The vacuum boundary condition states that no neutrons penetrate the boundary in the inward direction. In other words, the incoming current density

$(J^-(r_s, t))$  is equal to zero, equation 3.4 [? ].

$$J^-(r_s, t) = \frac{1}{4}\phi(r_s, t) + \frac{D}{2}\hat{n}_s \cdot \nabla\phi(r_s, t) = 0 \quad (3.4)$$

### 3.2.2 Thermal-hydraulics

The governing equation for the temperature of the solids is the three-dimensional heat conduction equation [? ].

Equations 3.5 to 3.7 allow for solving the temperature in the fuel, moderator, and reflector.

$$\rho_i c_{p,i} \frac{\partial}{\partial t} T_i = k_i \nabla^2 T_i + Q_i \quad (3.5)$$

$$Q_f = \sum_{g=1}^G \epsilon_g^f \Sigma_g^f \phi_g \quad (3.6)$$

$$Q_m = Q_r = 0 \quad (3.7)$$

where

$i = f$  (fuel),  $m$  (moderator),  $r$  (reflector)

$\rho_i$  = material  $i$  density

$c_{p,i}$  = material  $i$  heat capacity

$k_i$  = material  $i$  thermal conductivity

$T_i$  = material  $i$  temperature

$Q_i$  = material  $i$  volumetric heat source

$\epsilon_g^f$  = energy released per fission

$\Sigma_g^f$  = group  $g$  macroscopic fission cross-section

$\phi_g$  = group  $g$  neutron flux.

The governing equation of the coolant is the one-dimensional form of the continuity, momentum, and energy conservation equations, equations 3.8 to 3.12 [? ][? ].

$$\frac{\partial}{\partial t} \rho_c + \nabla \cdot (\rho_c u) = 0 \quad (3.8)$$

$$\rho_c \left( \frac{\partial}{\partial t} u + u \frac{\partial}{\partial z} u \right) = - \frac{\partial}{\partial z} p - \tau \frac{\varepsilon}{A} - \rho_c g \quad (3.9)$$

$$\rho_c \left( \frac{\partial}{\partial t} (c_{p,c} T_c) + u \frac{\partial}{\partial z} (c_{p,c} T_c) \right) = \frac{\partial}{\partial t} p + u \frac{\partial}{\partial z} p + q'''_{conv} \quad (3.10)$$

$$\tau = \frac{f}{2} \rho_c u^2 \quad (3.11)$$

$$q'''_{conv} = h \frac{\varepsilon}{A} (T_i - T_c) \quad (3.12)$$

where

$\rho_c$  = coolant density

$u$  = coolant velocity

$p$  = coolant pressure

$\tau$  = shear stress

$\varepsilon$  = wetted perimeter

$A$  = cross-sectional area

$g$  = gravity

$c_{p,c}$  = coolant specific heat capacity

$T_c$  = coolant temperature

$k_c$  = coolant thermal conductivity

$q'''_{conv}$  = convective heat transfer

$f$  = friction factor

$h$  = heat transfer coefficient

$T_i$  = solid temperature.

### 3.3 OECD/NEA MHTGR-350 MW Benchmark

The deterministic neutronic thermal-fluids and transient analysis methods available for prismatic HTGRs have lagged behind the state of the art of other reactor technologies. This delay has motivated the development of more

accurate tools for the design and safety evaluations of HTGRs. In addition to the development of new methods, it is essential to define appropriate benchmarks to compare these new methods' capabilities. The OECD/NEA defined such a benchmark [?] using the MHTGR-350 MW reactor [17] as the reference design. 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 fluids analysis, and (2) to test the depletion capabilities of various lattice physics codes available for prismatic HTGRs.

The benchmark defines several Phases and Exercises:

- Phase I: Steady State
  1. Neutronics solution with fixed cross-sections.
  2. Thermal fluids solution with given heat sources.
  3. Coupled neutronics-thermal fluids steady state solution.
- Phase II: Transient Cases
  1. Depressurized Conduction Cooldown without reactor trip.
  2. Pressurized Conduction Cooldown with reactor trip.
  3. Water ingress with reactor trip.
  4. Power 100-80-100 load follow.
- Phase III: Lattice Depletion Case

### **3.4 MHTGR-350 Reactor Description**

This section describes the MHTGR-350 reactor. Table 3.1 lists its main characteristics. The core consists of an array of hexagonal fuel elements in a cylindrical arrangement, Figure 3.1. Nineteen graphite replaceable reflector elements compose the inner reflector region. A ring of identically sized graphite replaceable reflector elements surrounds the fuel elements. Then, a region of permanent reflector elements follows the replaceable reflectors. The reactor vessel encases all the elements.

Ten layers of fuel elements stacked on top of each other compose the 66 fuel columns that integrate the active core. Figure 3.1b shows an axial view of the reactor. The core has two types of fuel elements: a standard element and a reserve shutdown element that contains a channel for Reserve Shutdown Control (RSC). Table 3.2 specifies the details of the MHTGR-350 fuel elements. Twelve columns in the core contain RSC channels for reserve shutdown



Table 3.1: MHTGR350 Characteristics [? ].

Characteristics	Value
Installed Thermal Capacity	350 MWt
Installed Electric Capacity	165 MWe
Core inlet/outlet Temperature	259/687°C
Power Density	5.9 MW/m <sup>3</sup>
Reactor Vessel Outside diam.	6.8 m
Reactor Vessel Height	22 m
Active core radius	2.97 m
Active core height	7.93 m
Top reflector height	1.18 m
Bottom reflector height	1.98 m
Number of fuel columns	66
Number of inner reflector columns	19
Number of outer reflector columns	78

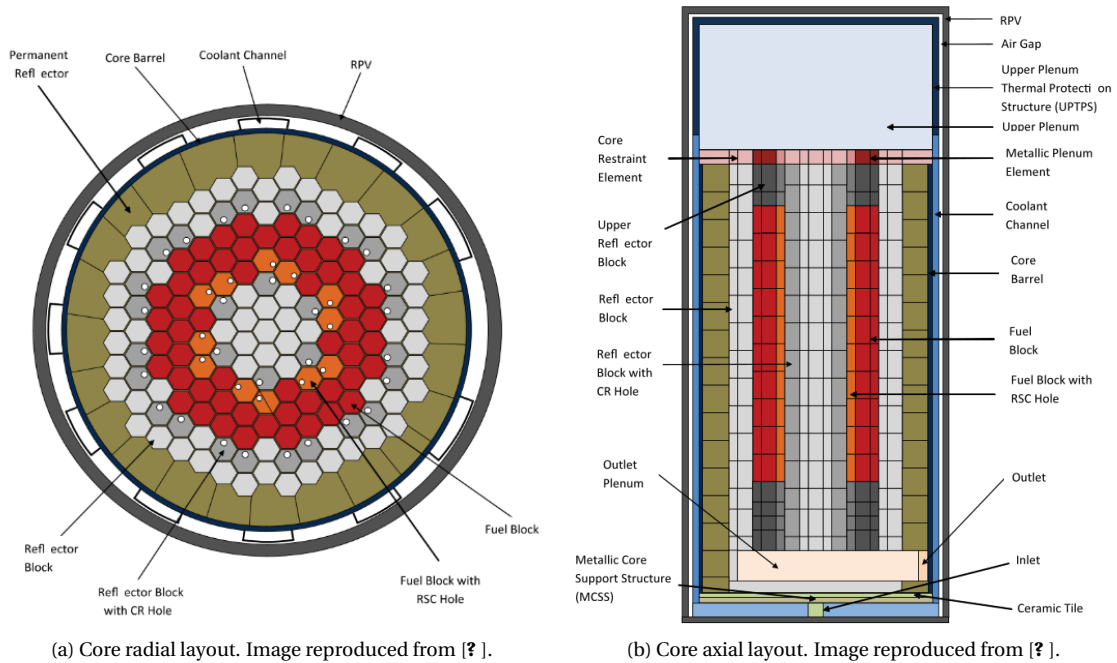


Figure 3.1: MHTGR reactor layout.

borated graphite pellets. Hoppers above the core house the pellets, and if the control rods (CRs) become inoperable, the pellets drop into the channels [? ].

Table 3.2: MHTGR350 fuel element characteristics [? ].

Shared characteristics	Value	Units
Block pitch (flat-to-flat)	36	cm
Fuel length	79.3	cm
Fuel handling diameter	3.5	cm
Fuel handling length	26.4	cm
RSC hole diameter	9.525	cm
RSC center to assembly center	9.756	cm
Fuel/coolant pitch	1.879	cm
Fuel hole radius	0.635	cm
Compacts per fuel hole	15	-
Large coolant hole radius	0.794	cm
Small coolant hole radius	0.635	cm
LBP hole radius	0.635	cm
Block graphite density	1.85	g/cm <sup>3</sup>
Standard element		
Number of large coolant holes	120	-
Number of small coolant holes	6	-
Number of fuel holes	210	-
RSC element		
Number of large coolant holes	88	-
Number of small coolant holes	7	-
Number of fuel holes	186	-

The fuel elements contain blind holes for fuel compacts and full-length channels for helium coolant flow. Table 3.3 specifies the details of the TRISO particle and fuel compact designs of the MHTGR-350.

A combination of LBP and CRs controls the core reactivity. The LBP consists of boron carbide (B<sub>4</sub>C) granules dispersed in graphite compacts. The current design uses six LBP rods per element. Table 3.4 displays the characteristics of the LBP compacts. The reactor counts with 30 CRs. Six of them are start-up CRs, and their location is the inner reflector. The remaining 24 are operating CRs and control the reactivity during power operation and a reactor trip.

Table 3.3: TRISO and fuel compact characteristics [? ].

Characteristic	Value	Units
Fuel	UC <sub>0.5</sub> O <sub>1.5</sub>	-
Enrichment (average)	15.5	wt%
Packing fraction (average)	0.35	-
Kernel radius	0.021,25	cm
Buffer radius	0.031,25	cm
IPyC radius	0.034,75	cm
SiC radius	0.038,25	cm
OPyC radius	0.042,25	cm
Compact radius	0.622,5	cm
Compact gap radius	0.635,0	cm
Compact length	4.928,0	cm
Kernel density	10.50	g/cm <sup>3</sup>
Buffer density	1.00	g/cm <sup>3</sup>
IPyC density	1.90	g/cm <sup>3</sup>
SiC density	3.20	g/cm <sup>3</sup>
OPyC density	1.90	g/cm <sup>3</sup>
Compact matrix density	1.74	g/cm <sup>3</sup>

Table 3.4: LBP compact characteristics [? ].

Characteristic	Value	Units
Absorber	B <sub>4</sub> C	-
Packing fraction	0.109	-
Kernel radius	0.010,0	cm
Buffer radius	0.011,8	cm
PyC radius	0.014,1	cm
Compact radius	0.571,5	cm
Compact gap radius	0.635,0	cm
Rod length	72.187	cm
Kernel density	2.47	g/cm <sup>3</sup>
Buffer density	1.00	g/cm <sup>3</sup>
PyC density	1.87	g/cm <sup>3</sup>
Compact matrix density	0.94	g/cm <sup>3</sup>

## **Chapter 4**

# **Neutronics**

### **4.1 Preliminary studies**

This section will discuss the current capabilities in Moltres and discuss its applicability to PMRs.

### **4.2 OECD/NEA Benchmark**

This section solves the Exercise 1 of Phase I of the OECD/NEA MHTGR-350 benchmark with the current Moltres capabilities.

### **4.3 Serpent-Moltres validation**

This section compares the results from Moltres and Serpent. Serpent generates the homogenized group constants and also solves the heterogeneous system, which provides the reference solutions for the validation of the calculation scheme.

## **Chapter 5**

# **Thermal-hydraulics**

### **5.1 Preliminary studies**

This section carries out some preliminar studies using Moltres and MOOSE heat conduction module.

### **5.2 Unit cell problem**

This section will solve the unit cell problem in the hot spot of an HTGR.

### **5.3 Fuel assembly**

This section will calculate the heat profile of a fuel assembly of a HTGR.

### **5.4 Full core**

This section will extend the methodology to a fullcore problem and it will inted to solve Exercise 2 of Phase I of the OECD/NEA MHTGR-350 Benchmark.

## Chapter 6

# Hydrogen Production

### 6.1 Introduction

Energy is one of the most vital contributors to economic growth. In the future, economies will continue to expand, populations will do so too, and their energy demand will accompany such change [?] [?]. Meeting these future needs requires the development of clean energy sources as environmental concerns continue to rise.

As seen in Figure 6.1, electricity generation was one of the economic sectors that released the most GHGs in the US in 2017. As CO<sub>2</sub> is the main component in GHGs, decarbonizing electricity generation will allow us to meet the increases in energy demand and address the environmental concerns simultaneously.

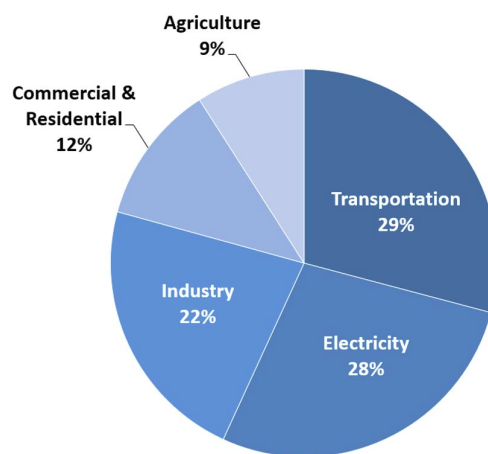


Figure 6.1: Total US GHG emissions by economic sector in 2017. Image reproduced from [?].

To address these concerns, utility companies are relying more and more on renewable energy resources, such as wind and solar [?]. However, high solar adoption creates a challenge. The need for electricity generators to quickly ramp up increases when the sun sets and the contribution from the photovoltaics (PV) falls [?]. The "duck curve" (or duct chart) depicts this phenomenon, Figure 6.2. The California ISO (CAISO) developed the duck curve to illustrate the grid's net load [?]. We define the net load as the difference between forecasted load and expected electricity production from solar.

Moreover, the duck curve reveals another issue. Over-generation may occur during the middle of the day, and high-levels of non-dispatchable generation may exacerbate the situation. As a consequence, the market would experience sustained zero or negative prices during the middle of the operating day [? ].

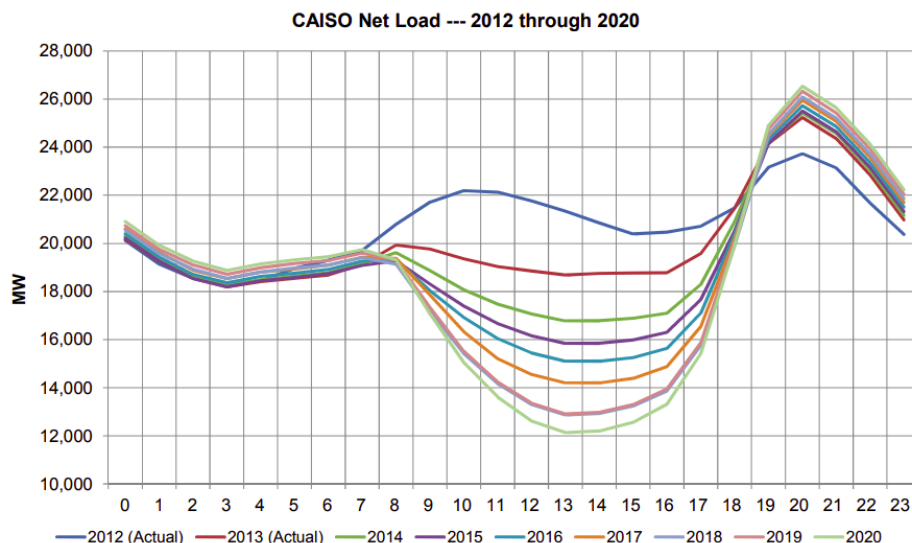


Figure 6.2: The duck curve. Image reproduced from [? ].

The simplest solution to a demand ramp-up is to increase dispatchable generation, resources with fast ramping and fast starting capabilities such as natural gas and coal [? ], and, consequently, decrease non-dispatchable generation, such as geothermal, nuclear, and hydro. Nonetheless, an approach like this is not consistent with the goal of reducing carbon emissions. Hence, our focus drifts to other potential low-carbon solutions, like nuclear generation and electricity storage through H<sub>2</sub> production.

Unfortunately, a carbon-neutral electric grid will be insufficient to halt climate change because transportation is a significant contributor to GHG emissions. As seen in Figure 6.1, transportation released the most GHGs in the US in 2017. Thus, decarbonizing transportation underpins global carbon reduction. One possible strategy is to develop a hydrogen economy, as Japan is currently doing. Japan's strategy rests on the firm belief that H<sub>2</sub> can be a decisive response to its energy and climate challenges. It could foster deep decarbonization of the transport, power, industry, and residential sectors while strengthening energy security [? ]. In the transportation sector, Japan plans to deploy fuel cell vehicles, trucks, buses, trains, and ships.

Although H<sub>2</sub> technologies do not release CO<sub>2</sub>, any H<sub>2</sub> production method is only as carbon-free as the energy source it relies on (electric, heat, or both). Nuclear reactors introduce a clean energy option to manufacture H<sub>2</sub>.

The UIUC is leading by example and actively working to reduce GHG emissions from electricity generation and transportation (among other sectors) on its campus. In pursuance of those efforts, the university has developed the iCAP.

## 6.2 iCAP

In 2008, UIUC signed the American College and University Presidents' Climate Commitment, formally committing to becoming carbon neutral as soon as possible, no later than 2050. The university developed the first iCAP in 2010 as a comprehensive roadmap toward a sustainable campus environment [? ]. The iCAP defines a list of goals, objectives, and potential strategies for six topical areas.

- Energy Conservation and Building Standards:

Focuses on maintaining or reducing campus gross square footage, strengthen conservation efforts, and engage the campus community in energy conservation.

- Energy Generation, Purchasing, and Distribution:

Efforts towards the exploration of 100% clean campus energy options. This includes expanding on-campus solar energy production, the extension of the purchase of clean energy from low-carbon energy sources, and the offset of all emissions from the National Petascale Computing Facility.

- Transportation:

This area comprises the efforts to reduce air travel emissions, reduce Urbana-Champaign campus fleet emissions, and study scenarios for complete conversion of the campus fleet to renewable fuels.

- Water and Stormwater:

This area focuses on improving the water efficiency of cooling towers, perform a water audit to establish water conservation targets, determine upper limits for water demand by end-use, and implement projects to showcase the potential of water and stormwater reuse.

- Purchasing, Waste, and Recycling:

Attempt to standardize office paper purchases, cleaning products, computers, other electronics, and freight delivery services. It also attempts to foment recycling by reducing non-durable goods purchases and reducing municipal solid waste going to landfills.

- Agriculture, Land Use, Food, and Sequestration:

This area will perform a comprehensive assessment of GHG emissions from agricultural operations, and develop a plan to reduce them, implement a project that examines the foodservice carbon footprint for Dining, and increase carbon sequestration in campus soils.



## 6.3 Objectives

As mentioned earlier, we place our attention on two areas: electricity generation and transportation. We will turn our attention to electricity generation and transportation on the UIUC campus. Consequently, this work's objective aligns with the efforts in two of the six target areas defined on the iCAP.

Regarding electricity generation, our analysis focuses on the UIUC grid. The present work quantifies the magnitude of the duck curve in such a grid. To mitigate the risk of over-generation, we propose to use the over-generated energy to manufacture  $H_2$ . We chose a nuclear reactor to be the primary source of energy. The next step is to quantify how much  $H_2$  different production methods can produce. Section 6.4 discusses a few hydrogen production methods considered for our analysis. Finally, we will calculate how much electricity we would generate using the  $H_2$  produced.

Regarding transportation, we study the conversion of the UIUC fleet on campus to Fuel Cell Electric Vehicles (FCEVs). Additionally, the analysis includes the conversion of the Champaign-Urbana Mass Transit District (MTD) fleet as well. The first step is to determine the fuel consumed by both fleets and how much  $H_2$  enables the fleets' complete conversion. Finally, we consider a few reactor designs and analyze which of them could produce enough  $H_2$  to fulfill both fleet requirements.

Both studies propose the same solution, a nuclear reactor coupled to a hydrogen plant. In terms of electricity generation, this solution will decrease the need for dispatchable sources and, consequently, reduce carbon emissions. In terms of transportation, it will eliminate carbon emissions.

In both analyses, many reactor choices can satisfy our needs. The typical UIUC's grid demand is smaller than 80 MW [? ]. Accordingly, we consider reactors of small capacities, such as microreactors and SMRs. Section 6.5 discusses their characteristics.

## 6.4 Hydrogen production methods

This section introduces several hydrogen production processes and their energy requirements.

### 6.4.1 Electrolysis

The electrolysis of water is a well-known method whose commercial use began in 1890. This process produces approximately 4% of  $H_2$  worldwide. The process is ecologically clean because it does not emit GHGs. However, in comparison with other methods, electrolysis is a highly energy-demanding technology [? ].

Three electrolysis technologies exist. Alkaline-based is the most common, the most developed, and the lowest in capital cost. It has the lowest efficiency and, therefore, the highest electrical energy cost. Proton exchange

membrane electrolyzers are more efficient but more expensive than Alkaline electrolyzers. Solid Oxide Electrolysis Cells (SOEC) electrolyzers are the most electrically efficient but the least developed. SOEC technology has challenges with corrosion, seals, thermal cycling, and chrome migration [? ]. As the first two technologies work with liquid water and the latter requires high-temperature steam, we will refer to the first two as Low-Temperature Electrolysis (LTE) and the latter as HTE.

Water electrolysis converts electric and thermal energy into chemical energy stored in hydrogen. The process enthalpy change  $\Delta H$  determines the required energy for the electrolysis reaction to take place. Part of the energy corresponds to electric energy  $\Delta G$  and its rest to thermal energy  $T \cdot \Delta S$ , Equation 6.1.

$$\Delta H = \Delta G + T\Delta S \quad (6.1)$$

where

$$\Delta H = \text{Total specific energy [kWh/kg-H}_2\text{]} \quad (6.2)$$

$$\Delta G = \text{Specific electrical energy [kWh/kg-H}_2\text{]} \quad (6.3)$$

$$T\Delta S = \text{Specific thermal energy [kWh/kg-H}_2\text{]}. \quad (6.4)$$

In LTE, electricity generates thermal energy. Hence,  $\Delta H$  alone determines the process required energy.  $\Delta H$  is equal to 60 kWh/kg-H<sub>2</sub> considering a 67% efficiency [? ].

In HTE, a high-temperature heat source is necessary to provide thermal energy.  $\Delta G$  decreases with increasing temperature, Figure 6.3. Decreasing the electricity requirement results in higher overall production efficiencies since heat-engine-based electrical work has a thermal efficiency of 50% or less [? ]. Figure 6.3 shows  $\Delta G$  and  $T\Delta S$ .  $\Delta G$  considers the SOEC to have an electrical efficiency of 88% [? ].  $T\Delta S$  accounts for the latent heat of water vaporization. Note that the process is at 3.5 MPa.  $\Delta G$  increases with pressure. However, we chose a high pressure to save energy, as compressing liquid water is cheaper than compressing the hydrogen [? ].

Finally, equations 6.5 and 6.6 determine the electrical  $P_{EH2}$  and thermal power  $P_{TH2}$  required by the hydrogen plant.

$$P_{EH2} = \dot{m}_{H2}\Delta G \quad (6.5)$$

$$P_{TH2} = \dot{m}_{H2}T\Delta S \quad (6.6)$$

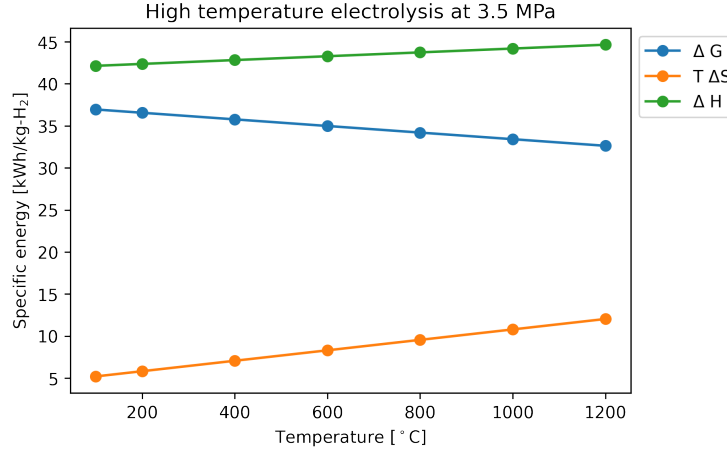


Figure 6.3: Energy required by HTE at 3.5 MPa.

where

$$P_{EH2} = \text{Total electrical power [kW]} \quad (6.7)$$

$$P_{TH2} = \text{Total thermal power [kW]} \quad (6.8)$$

$$\dot{m}_{H2} = \text{H}_2 \text{ production rate [kg/h]}. \quad (6.9)$$

## 6.4.2 Sulfur-Iodine Thermochemical Cycle

Thermochemical water-splitting is converting water into hydrogen and oxygen by a series of thermally driven chemical reactions. The direct thermolysis of water requires temperatures above 2500 °C for significant hydrogen generation. At this temperature, the process can decompose a 10% of the water. A thermochemical water-splitting cycle accomplishes the same overall result using much lower temperatures.

General Atomics, Sandia National Laboratories, and the University of Kentucky compared 115 cycles that would use high-temperature heat from an advanced nuclear reactor [? ]. The report specifies a set of screening criteria used to rate each cycle. The highest scoring method was the Sulfur-Iodine (SI) Cycle.

The SI cycle consists of the three chemical reactions represented in Figure 6.4. The whole process takes in water and high-temperature heat and releases hydrogen and oxygen. The process does not use any electricity. The process recycles all reagents and does not have any effluents [? ]. The chemical reactions are:

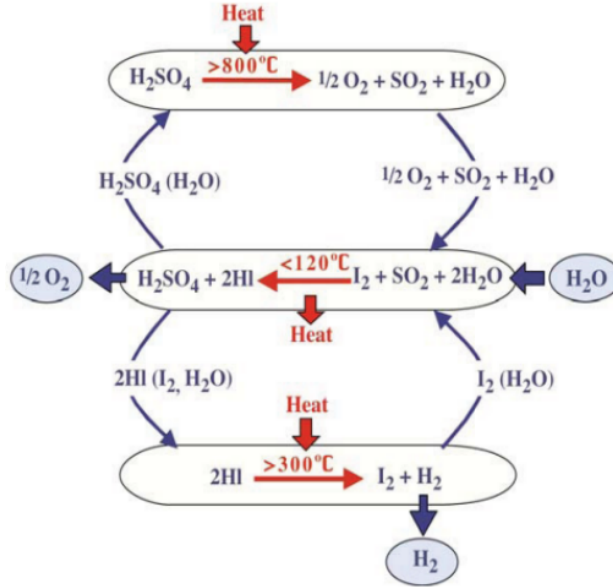


Figure 6.4: Diagram of the Sulfur-Iodine Thermochemical process. Image reproduced from [? ].

Figure 6.5 presents the specific energy requirements of the cycle  $\Delta H$ . Several sources disagree on the minimum temperature for the process to be viable. Our analysis considers the process feasible only for temperatures above 800 °C. Finally, equation 6.13 determines the thermal power  $P_{TH2}$  required by the hydrogen plant.

$$P_{TH2} = \dot{m}_{H2} \Delta H \quad (6.13)$$

where

$$P_{TH2} = \text{Total thermal power [kW]} \quad (6.14)$$

$$\dot{m}_{H2} = \text{H}_2 \text{ production rate [kg/h]} \quad (6.15)$$

$$\Delta H = \text{Specific energy [kWh/kg-H}_2\text{]}. \quad (6.16)$$

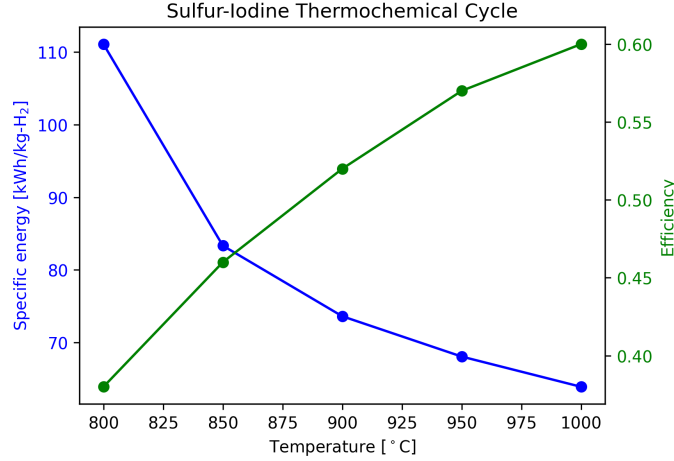


Figure 6.5: Energy required by the Sulfur-Iodine Thermochemical Cycle.

## 6.5 Microreactors and SMRs

These reactor concepts share several features. The reactors require limited on-site preparation as their components are factory-fabricated and shipped out to the generation site. This feature reduces up-front capital costs, enables rapid deployment, and expedites start-up times. This reactor concept allows for black starts and islanding operation mode. They can start up from an utterly de-energized state without receiving power from the grid. They can also operate connected to the grid or independently. Moreover, these types of reactors are self-regulating. They minimize electrical parts and use passive safety systems to prevent overheating and safely shutdown.

Microreactors have the distinction that is transportable. Small designs make it easy for vendors to ship the entire reactor by truck, shipping vessel, or railcar. These features make the technology appealing for a wide range of applications, such as deployment in remote residential locations and military bases.

The DOE defines a microreactor as a reactor that generates from 1 to 20 MWt [?]. The IAEA describes an SMR as a reactor whose power is under 300 MWe. It defines, as well, a very small modular reactor as a reactor that produces less than 15 MWe [?]. As the definitions of these reactor concepts overlap, we will consider reactors of less than 100 MWt regardless of their specific classification.

## 6.6 Methodology

In this analysis, the energy source (electric and thermal) is a nuclear reactor with co-generation capabilities. The nuclear reactor supplies the grid with electricity  $P_E$  while providing a hydrogen plant with electricity  $P_{EH2}$  and thermal energy  $P_{TH2}$ , see the diagram in Figure 6.6.  $\beta$  and  $\gamma$  determine the distribution of the reactor thermal power  $P_{th}$  into  $P_E$ ,  $P_{EH2}$ , and  $P_{TH2}$ , see Equations 6.17 to 6.22.

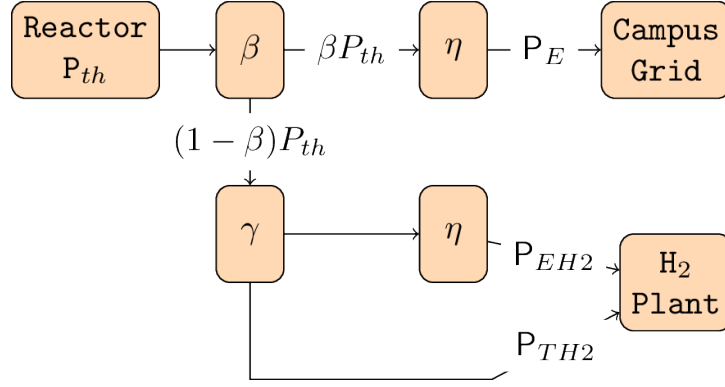


Figure 6.6: Diagram of a reactor coupled to a hydrogen plant.

$$P_E = \eta \beta P_{th} \quad (6.17)$$

$$P_{EH2} = \eta \gamma (1 - \beta) P_{th} \quad (6.18)$$

$$P_{TH2} = (1 - \gamma)(1 - \beta) P_{th} \quad (6.19)$$

where

$$\eta = \text{thermal-to-electric conversion efficiency} \quad (6.20)$$

$$\beta = \frac{P_E / \eta}{P_E / \eta + P_{TH2} / (1 - \gamma)} \quad (6.21)$$

$$\gamma = \frac{P_{EH2} / \eta}{P_{EH2} / \eta + P_{TH2}}. \quad (6.22)$$

If  $\beta = 1$ , the reactor only supplies the grid with electricity  $P_E$ , and the hydrogen plant does not produce  $H_2$ . If  $\beta = 0$ , the reactor only supplies the hydrogen plant, and no electricity goes into the grid. Table 6.1 summarizes the values that  $\gamma$  takes for the different methods.

Method	$\gamma$	$P_{EH2}$	$P_{TH2}$
LTE	1	$\neq 0$	0
HTE	$0 < \gamma < 1$	$\neq 0$	$\neq 0$
SI	0	0	$\neq 0$

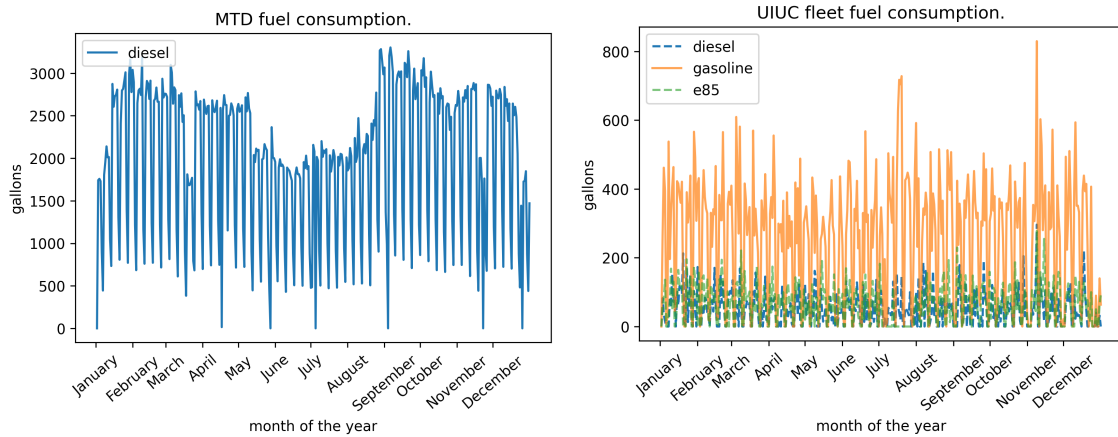
Table 6.1: Energy requirements of the different methods.

## 6.7 Results

This section holds the results of the different analyses.

### 6.7.1 Transportation

This subsection centers its focus on the transportation sector. Figure 6.7 displays the fuel consumed per day by MTD and UIUC fleet. Using the values shown in Table 6.2, we calculate the  $H_2$  requirement for MTD and UIUC fleets, Figure 6.8. Table 6.3 summarizes the results.



(a) MTD fleet. Data go from July 1, 2018, until June 30, 2019 [?]. (b) UIUC fleet. Data go from January 1, 2019, until December 31, 2019 [?].

Figure 6.7: Fuel consumption data.

Table 6.2:  $H_2$  necessary to replace a gallon of fuel [?] [?].

	Hydrogen Mass [kg]
Gasoline	1
Diesel	1.13
E85	0.78

Table 6.3:  $H_2$  requirement for MTD and UIUC fleets.

Total [tonnes/year]	943
Average [kg/day]	2584
Average [kg/h]	108
Maximum in one day [kg]	4440

Using Table 6.4, we calculate the  $CO_2$  savings caused by replacing all the fossil fuels by  $H_2$ . Table 6.5 displays the  $CO_2$  savings for both fleets.

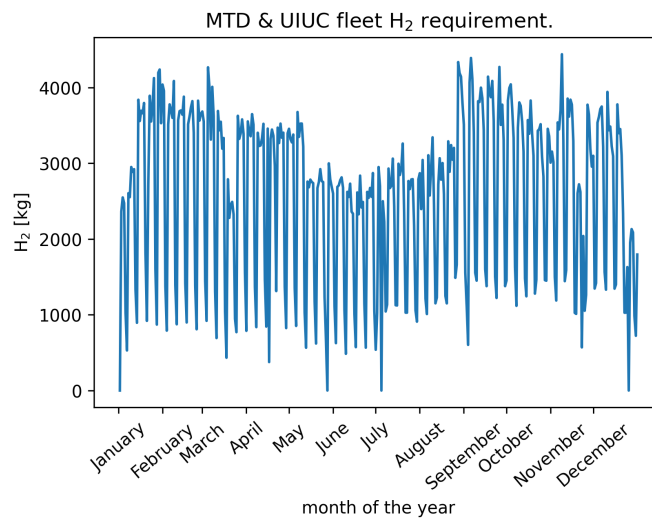


Figure 6.8: H<sub>2</sub> requirement for MTD and UIUC fleets.

Table 6.4: CO<sub>2</sub> savings in lbs per gallon of fuel burned [? ].

	CO <sub>2</sub> produced [lbs/gallon]
Gasoline	19.64
Diesel	22.38
E85	13.76

Table 6.5: CO<sub>2</sub> yearly savings.

	CO <sub>2</sub> mass [tonnes/year]
MTD	7306
UIUC	1143
Total	8449



We have determined the  $H_2$  requirement by the fleets, and now we seek a microreactor design capable of meeting such demand. For our analysis, we chose a few microreactor designs summarized in Table 6.6. Further studies could include other designs as well.

Figure 6.9 shows the hourly production rates for the different reactors and the  $H_2$  production processes. The figure includes a continuous line that represents the hydrogen requirement of both fleets. Note that the SI process' required high temperatures allow for the coupling with only one microreactor design, which has an outlet temperature of more than  $800^\circ\text{C}$ .

Table 6.6: Microreactor designs.

Reactor	P[MWt]	$T_o[^\circ\text{C}]$
MMR [?] ]	15	640
eVinci [?] ]	5	650
ST-OTTO [?] ]	30	750
U-battery [?] ]	10	750
Starcore [?] ]	36	850

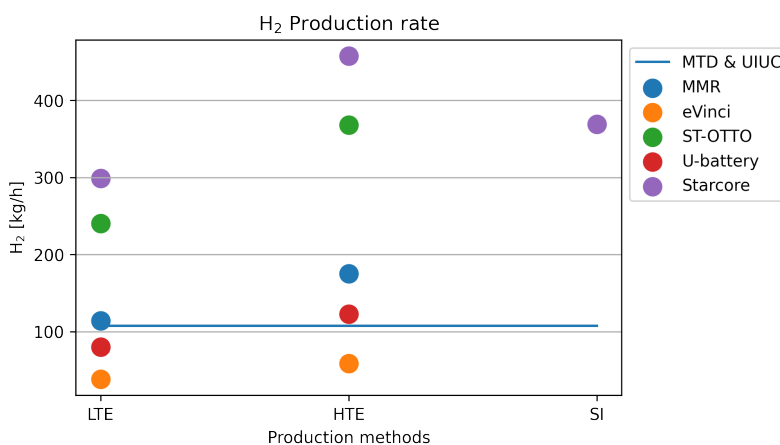


Figure 6.9: Hydrogen production rate by the different microreactor designs.

## 6.7.2 Electricity Generation

This subsection centers its focus on the electricity generation sector and the duck curve problem. To quantify the duck curve's magnitude, we have to predict the UIUC grid's load and the expected electricity production from solar. As the iCAP's main objective is to become carbon neutral before 2050, we make our prediction for that year. UIUC solar farm is relatively new, and the data available is not enough for producing a reliable forecast. To go around this barrier, we use the available data for the whole US. Figure 6.10 displays the prediction for 2050. We carry out the prediction using a linear regression that produces the worst-case scenario. In such a scenario, the total load does not increase considerably, whereas the solar generation does.

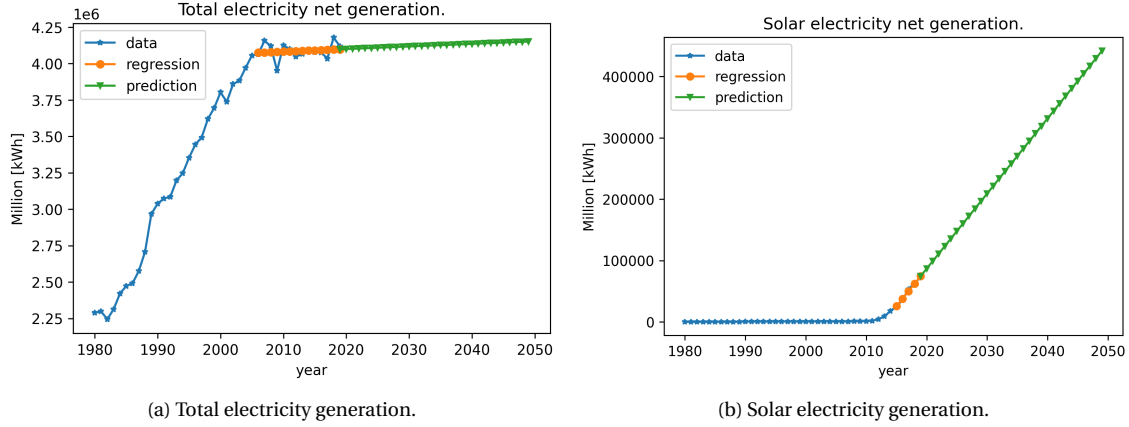


Figure 6.10: Prediction of the electricity generation in the US for 2050. Data from [? ].

The next step was to apply the same growth factor from the predictions to the UIUC grid's load and solar electricity. To obtain a prediction for 2050, we apply the growth factor to the hourly data. We choose a spring day when solar production is higher, as it is sunny, but the total load is low since people are not using electricity for air conditioning or heating [? ]. Finally, we subtract the solar production from the total load, obtaining the net load or demand ( $D_{NET}$ ).

We narrowed our analysis' focus to April 4th, when the net demand reached the lowest value in the 2019's spring. Figure 6.11 shows these results. In 2050, the peak net demand will be 46.9 MWh at 5 PM. The lowest net demand will be 15 MWh at 11 AM. These results yield a demand ramp of 31.9 MWh in 4 hours. These results show that the grid requires an available capacity of dispatchable sources of at least 31.9 MW.

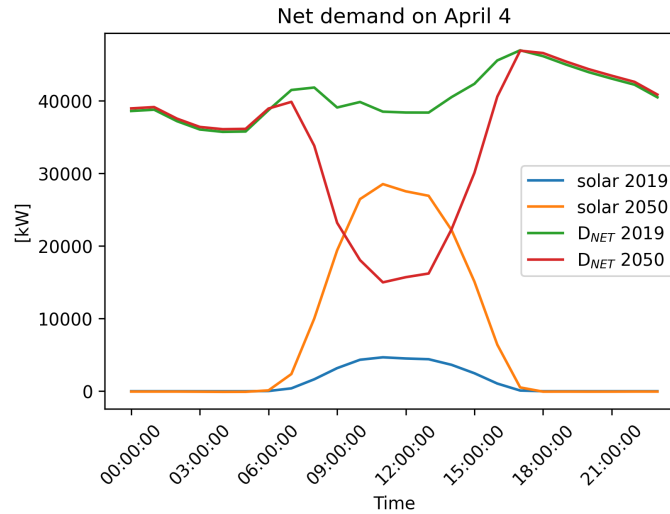


Figure 6.11: Prediction of UIUC's net demand for 2050.

Once we calculated the net demand, the next step was to figure the over-generated electricity. For that purpose,

we arbitrarily chose a reactor of 25 MW. For the LTE case, any reactor is a valid option. We chose an  $\eta$  of 33%, which yields a reactor power of 75.8 MWt. For the HTE case, the reactor's choice is an HTGR with an outlet temperature of 850°C. We consider an  $\eta$  of 49.8%, which yields a reactor of 50.2 MWt.

The reactor operates at full capacity at all times. However, the reactor electricity ( $P_E$ ) equals the net demand ( $D_{NET}$ ) once smaller than 25 MW. Note that  $P_E$  has power units while  $D_{NET}$  has energy units. We chose time steps of 1 hour for our analysis, hence  $P_E$  and  $D_{NET}$  differ by the constant  $h$ . As  $P_E$  is lower than 25 MW, and the reactor is at full thermal capacity, the hydrogen plant takes the excess of thermal energy. We use equation 6.23 with equations 6.17 to 6.22 to calculate the hydrogen produced. Figure 6.12 displays the results. The total  $H_2$  production reaches 660, 1009, and 815 kg for LTE, HTE, and SI.

$$P_E = D_{NET}$$

$$\frac{P_E}{25MW} = \frac{\eta\beta P_{th}}{\eta P_{th}} = \beta \quad (6.23)$$

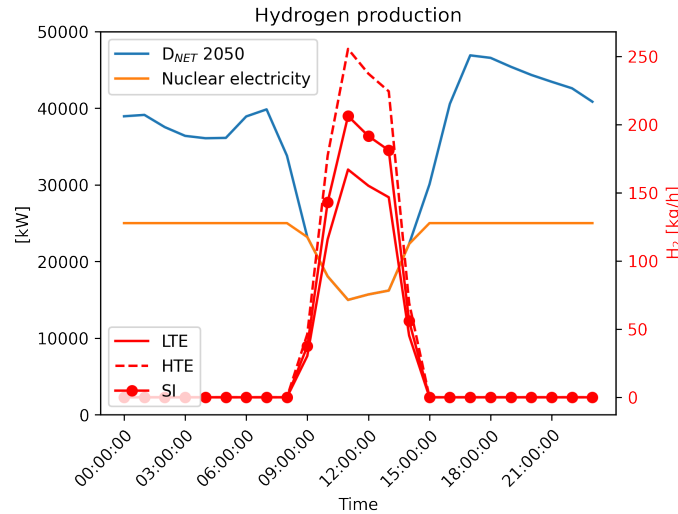


Figure 6.12:  $H_2$  production.

Our analysis last step is to calculate the peak demand reduction by using the hydrogen to produce electricity. The energy produced by hydrogen is  $285\text{ kJ/mol}$ , equal to  $40\text{ kWh/kg}$  [?]. However, conventional fuel cells can use up to 60% of that energy [?]. Knowing the mass of hydrogen produced, we calculate the total electricity produced. We now reduce the peak demand by distributing the electricity over a specific range of hours. We chose to distribute the electricity for over 6 hours. We calculate the new peak using equation 6.25. Figure 6.13 shows these results. The different  $H_2$  processes can generate 15.84 MWh, 24.2 MWh, and 19.6 MWh, respectively. This generation accounts

for a peak reduction of 5 MW, 6.4 MW, and 5.6 MW, respectively.

$$NP = \frac{\sum_{i=0}^N D_{NET,i} - TH}{N} \quad (6.24)$$

$$(6.25)$$

where

$$NP = \text{New peak magnitude} \quad (6.26)$$

$$D_{NET,i} = \text{Hourly net demand} \quad (6.27)$$

$$TH = \text{Total mass of hydrogen} \quad (6.28)$$

$$N = \text{Total number of hours when we use the H}_2 \quad (6.29)$$

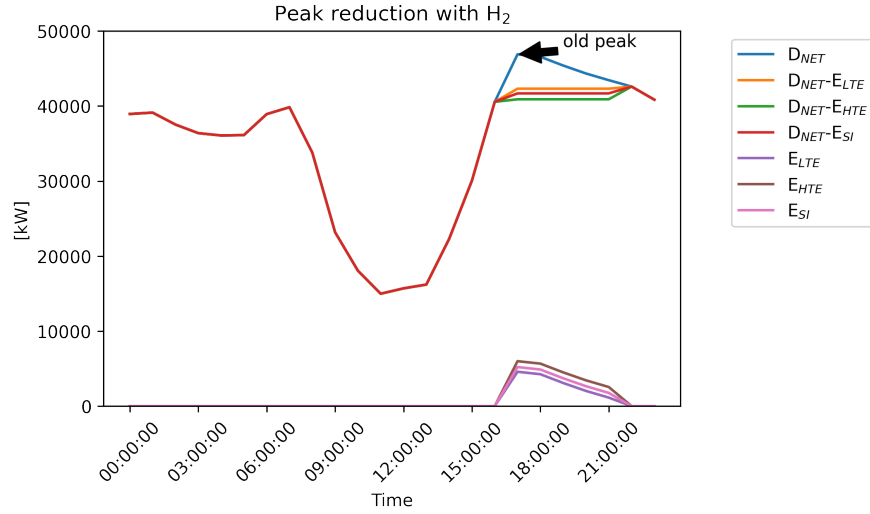


Figure 6.13: Peak reduction by using the produced H<sub>2</sub>.

## 6.8 Conclusions

The world faces energy challenges that compromise the efforts to stop climate change. The electricity generation and transportation sectors are the largest issuers of GHGs and, hence, the major contributors to climate change. These challenges underscore the need for cleaner sources. Nonetheless, the common belief that renewable energy is the solution to the problem presents several drawbacks. The duck curve is an example of such drawbacks. Moreover,

a carbon-neutral electric grid will be insufficient to halt climate change. The transportation sector needs to survey some possible alternatives to become carbon-free as well. In this work, we proposed combining nuclear energy and hydrogen production that represents a possible solution to these challenges.

To seek a solution for the challenge described above, we narrowed down our focus on a more particular case, the University of Illinois. Through the implementation of the iCAP, the University of Illinois is actively working to reduce GHG emissions on its campus. This work's objective aligns with the efforts in two of the six target areas defined on the iCAP, electricity generation, and transportation.

Regarding hydrogen production methods, we surveyed three different processes: LTE, HTE, and SI. We developed a tool to calculate their energy requirements, regarding electricity and heat, and hydrogen production rates. This tool is applicable to a stand-alone hydrogen plant and a nuclear power plant that produces both electricity and hydrogen.

In the transportation sector analysis, we quantified the fuel requirements of MTD and UIUC fleets. We calculated the mass of hydrogen necessary to replace 100% of the fleet's fossil fuel usage. Finally, we chose several microreactor designs, and we calculated their hydrogen production rates. The microreactors that can meet both fleet hydrogen needs are the MMR, ST-OTTO, U-battery, and Starcore. Starcore design is the only one that could use the SI process.

In the electricity generation sector analysis, we predicted the duck curves' magnitude in UIUC's grid in 2050. This result exhibits how an increased solar penetration into the grid worsens the duck curve. We proposed a mitigation strategy that uses a microreactor of 25 MWe. For such a reactor, we calculated the mass of hydrogen produced by the different methods during the day. Finally, we estimated a peak demand reduction by using the hydrogen produced during the day. This last result highlights that hydrogen introduces a means to store energy that reduces the reliance on dispatchable sources. This analysis emphasizes how nuclear energy and hydrogen production are an approach to mitigate climate change.

# **Chapter 7**

## **Conclusions**

### **7.1 Contribution**

This section will summarize the contributions of this thesis.

### **7.2 Future Work**

This section will introduce some possible future work as a continuation of this thesis.

# Appendix

Appendix.

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