

Impact of Real Gas Properties on Multiphysics Modeling of a Nuclear Thermal Propulsion Fuel Element

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INTRODUCTION

Advanced nuclear reactors are under investigation as a possible solution to a large array of modern challenges. These areas of research span from microreactors for remote cities or military bases to small modular reactors to support the sizable energy requirement of training artificial intelligence algorithms. Additional applications of current interest are space reactors to provide large amounts of electric power on the surface of celestial bodies and to propel spacecraft for crewed and science missions. The National Aeronautics and Space Administration (NASA), in particular, presently researches three primary nuclear reactor technologies: nuclear thermal propulsion (NTP), nuclear electric propulsion (NEP), and fission surface power (FSP). NASA is interested in NTP as a near-term solution for crewed interplanetary space travel to reach Mars by 2039. This research is led through the Space Nuclear Propulsion (SNP) project at NASA's Marshall Space Flight Center (MSFC). This technology uses an extremely high temperature nuclear reactor (~3000 K) as a heat exchanger to increase the temperature of the propellant to peak values. Hydrogen is the most desirable propellant for NTP since it enables the highest specific impulse (i.e., "fuel efficiency"). Specific impulse is directly proportional to the effective molecular weight of the propellant as well as its temperature in the nozzle chamber. Yielding these extreme fluid temperatures presents numerous challenging multiphysics problems for the reactor to handle during nominal and transient operation.

Risk reduction for the engine, spacecraft, and crew are the paramount concern for NASA's technology maturation efforts. Traditional technology maturation involves an intensive development strategy that includes testing each component until failure prior to incorporation in the final product. However, technology advancement for space reactor technologies requires high-fidelity multiphysics and system-level models given the harsh environment for experimental testing, significant cost burden, and regulatory hurdles for nuclear safety. Reduced order and higher fidelity models are both utilized depending on the application. This work aims to investigate how a finite element model for a reference NTP fuel element performs when the fluid property database assumption is varied. Many research fields use ideal gas fluid properties given their availability, ease of use, and validity in the operability region of interest. NTP, in contrast, experiences large temperature and pressure variations throughout the reactor and engine cycle, necessitating a better

data repository that includes real gas and dissociation effects. To simulate these effects on overall thermal hydraulic system performance, a reference reactor configuration and a robust modeling framework must be established. Subsequent sections of this introduction discuss the requirements for modeling this test case to achieve the desired results.

SNRE Reference Design

The most reputable and documented heritage NTP research occurred during the Nuclear Engine for Rocket Vehicle Applications (NERVA) program which spanned from the mid-1950s through early 1970s. These reactors included highly enriched uranium (HEU) fuel elements in a hexagonal supercell with zirconium hydride moderated structural tie-tubes. Modern regulatory requirements limit the uranium enrichment from HEU to high-assay low enriched uranium (HALEU) with a maximum weight fraction of 20% U-235. Thus, recent efforts from NASA and the Idaho National Laboratory (INL) sought to develop a benchmark case around the NERVA reactor configurations within the HALEU restriction. This effort yielded the Small Nuclear Rocket Engine (SNRE) which serves as a common reference reactor for benchmarking thermal hydraulic and neutronic simulation results¹⁻³. SNRE is a lower thrust variant comparable with modern demonstration reactor efforts and utilizes a hydrogen working fluid to maximize specific impulse. The SNRE fuel element mesh under investigation in this work is included in Fig. 1 below.

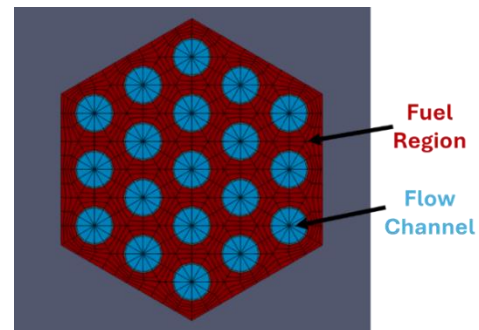


Fig. 1. Reference Mesh of the SNRE Fuel Assembly⁴

Incorporation of the SNRE into the modeling analysis for this work requires geometric and system operating parameters, such as element length, inlet and outlet flow conditions, and thermal power level. The case-specific boundary conditions and unit cell geometry are taken from the Space Propulsion Optimization Code (SPOC)

benchmark¹ covering the analysis of the SNRE and are listed within Table I. Additionally, a solid solution carbide (SSC) fuel form of (U, Zr)C with a 35% volume loading of UC is implemented, and a reference NTP power deposition curve is held constant for all runs. The reactor is comprised of 564 fuel elements, so the total thermal power and mass flow rate are divided by this value to simulate average fuel conditions in the SNRE core. Engine turbomachinery and the regenerative nozzle are excluded from this exercise.

TABLE I. Test Case Geometry and Boundary Conditions¹

Input Parameter	Value
Active Core Length	89 cm
Channel Radius	0.13 cm
Channel Pitch	0.41 cm
Engine Specific Impulse	899.9 s
Engine Thrust	16,406 klbf
Pressure Drop	360 kPa
Outlet Pressure	3.64 MPa
Inlet Temperature	372.1 K
Thermal Power	357.49 MW
Maximum Fuel Temperature	2861.85 K

MOOSE Methodology

With known reference geometry and system conditions, the multiphysics modeling suite can be tailored to simulate the thermal hydraulic performance. Numerous finite element multiphysics suites are explored within literature; however, the Multiphysics Object Oriented Simulation Environment (MOOSE) software developed by INL is under investigation for other NTP modeling projects and will be utilized in this work. MOOSE can handle complex geometries to assess neutronics, thermal hydraulics, and thermal mechanics modeling cases. In particular, this work utilizes the Thermal Hydraulics Module⁵ (THM) and Reactor Module⁶ that come pre-loaded within the open-source version of MOOSE for incorporation of the physics-based solvers and the necessary meshing routines for the hexagonal fuel element. The resulting model has all physics of interest for this work which includes 3D volumetric heat generation with a representative axial power shape, heat conduction in solids, and heat removal to convective flow channels. The channel models utilize a 1D area-averaged Navier Stokes approximation.

The remaining action to simulate the conditions needed for this work included implementation of the kernels for ideal gas and custom tabulated fluid properties. Past work focused on the use of ideal gas properties for simplicity, so these models existed from prior research^{4,7}. Tabulated properties are required instead of empirical correlations given the structure of the reference real gas database, as discussed in the next section. Based on the SNRE reference, a hydrogen working fluid is implemented for all results. Required properties include the fluid density, thermal conductivity, viscosity, enthalpy, and isobaric specific heat. The Churchill⁸

and McCarthy & Wolf⁹ (M&W) empirical correlations for friction factor and Nusselt number, respectively, are included as a means of calculating the frictional pressure losses and convective heat transfer coefficient. Additional solid material properties are implemented for the SSC fuel form and cladding to inform the 3D fuel temperature distribution.

Parahydrogen Properties Database

Assessment of the thermal hydraulic performance of the SNRE fuel element requires temperature- and pressure-dependent fluid properties of the working fluid. Given that the hydrogen is stored cryogenically to minimize propellant loss, the spin isomer of interest is parahydrogen^{10,11}. The transition time between parahydrogen and orthohydrogen is significantly longer than the time inside the engine, so it is assumed that the fluid remains as parahydrogen at all state points. Thermophysical and transport properties of parahydrogen are documented through published NASA-funded work and are included in this analysis to investigate the real gas effects^{10,11}. As mentioned in the MOOSE section above, prior analysis utilized hydrogen as the working fluid but simply implemented ideal gas assumptions for the high-temperature properties. The parahydrogen dissociation region occurs near the mid-plane of the SNRE fuel channels and yields significant variations in all required properties. The results of this work will focus on the thermal hydraulic impact of these real gas properties and compare them to the results that used ideal gas assumptions.

RESULTS

A collection of thermal hydraulics results is gathered following implementation and simulation of the SNRE fuel element in MOOSE. The physical impacts of interest include property-induced variations on the fluid pressure drop, axial bulk temperature, convective heat transfer coefficient, and maximum fuel temperature. These output parameters are all strongly dependent on fluid choice and the properties utilized while also showcasing the impact of modeling assumptions on key system performance parameters. To exemplify the 3D nature of the MOOSE simulation, the radial fuel temperature at the axial hotspot and axial temperature profile are included using ideal gas properties in Fig. 2 and Fig. 3.

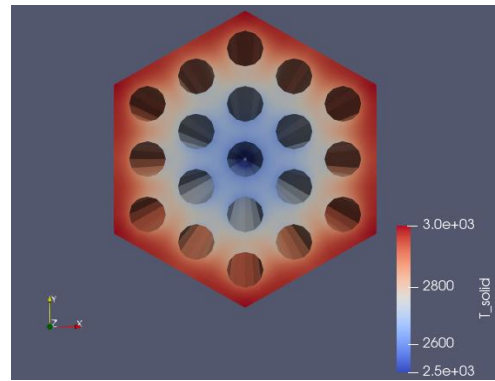


Fig. 2. Fuel Element Temperature Distribution at the Axial Hotspot using Ideal Gas Properties

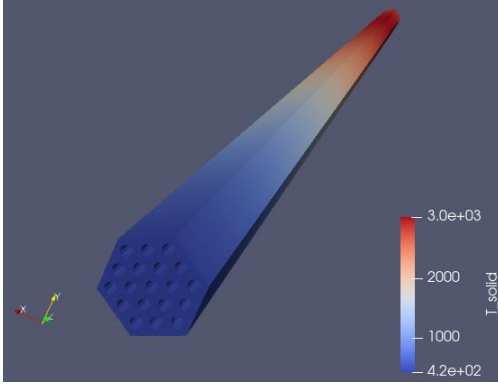


Fig. 3. Fuel Temperature Contour Plot using Ideal Gas Properties

The set of comparison results focus on the average axial variation of the fluid, channel wall, and peak fuel temperatures for each database, as shown in Fig. 4 and Fig. 5. Fig. 6 provides a visual of the percent difference (ϵ) of each of these three curves between the two methodologies which are calculated using Eq. 1. Additional flow results are included in Fig. 7 to show the differences in Reynolds and Prandtl numbers, convective heat transfer coefficient, and friction factor using the same error calculation. Table II includes a summary of the simulated output conditions, including the total pressure drop, exit velocity, and maximum fuel temperature for each case.

$$\epsilon = 100\% * \left(\frac{\text{Real Gas} - \text{Ideal Gas}}{\text{Real Gas}} \right) \quad (1)$$

TABLE II. Summary of Output Conditions

Output Parameter	Ideal Gas Results	Real Gas Results
Pressure Drop	310 kPa	330 kPa
Max Fuel Temperature	2955.4 K	2849.7 K
Exit Velocity	434.2 m/s	439.6 m/s

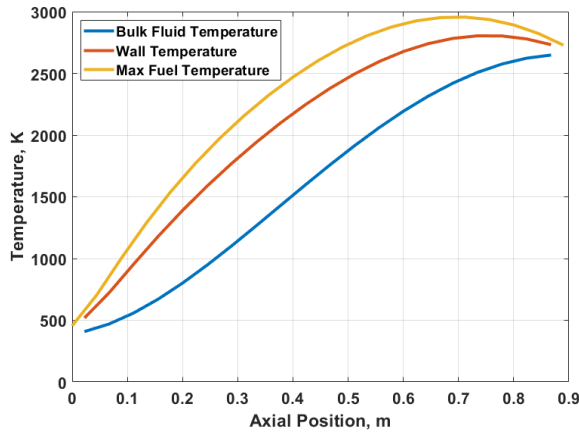


Fig. 4. Axial Fluid and Solid Temperature Distribution using Ideal Gas Properties

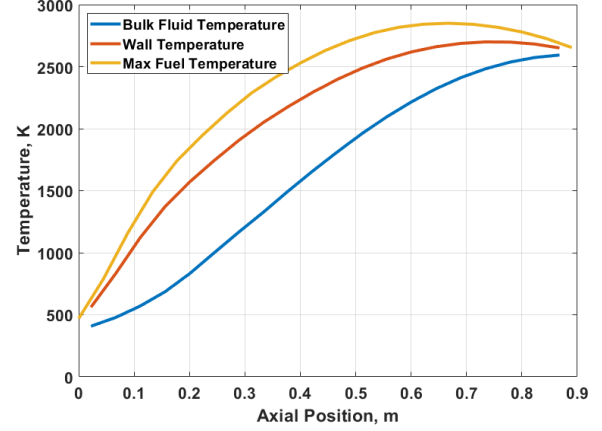


Fig. 5. Axial Fluid and Solid Temperature Distribution using Real Gas Properties

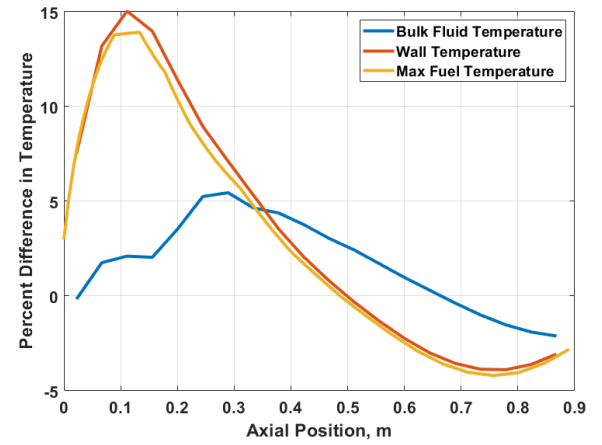


Fig. 6. Percent Difference in Axial Temperatures between the Real and Ideal Gas Property Approaches

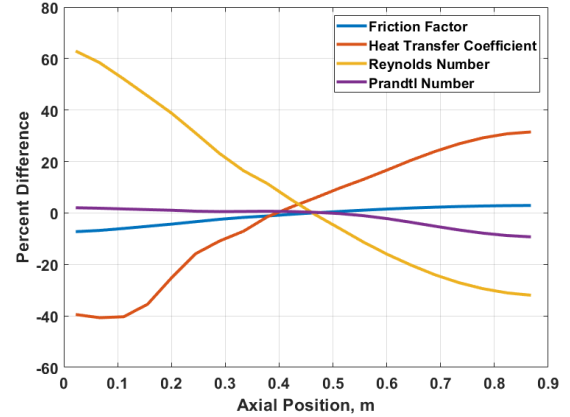


Fig. 7. Percent Difference in Relevant Flow Conditions

The primary takeaways from these output plots are the strong deviation in flow conditions and the effect on maximum fuel temperature. The inclusion of real gas properties strongly impacts the heat transfer coefficient which drives a higher fuel temperature near the flow inlet and a lower fuel temperature at the axial hotspot. This effect is beneficial for the safe operation of an NTP reactor since the maximum fuel temperature is pulled toward the average fuel

temperature as a result of the decreasing heat transfer coefficient. The heat transfer coefficient, in this example case, is driven by the strong deviation in Reynolds number since the Prandtl number does not vary strongly as a function of axial position. Another observation is that the bulk fluid temperature of the real gas case is higher in the first half of the axial channel in comparison to the ideal gas simulation. Specific heat capacity is a strong function of temperature and pressure which leads to this significant deviation as well as some variation in the exit conditions.

CONCLUSIONS

Modern modeling efforts of NTP reactor systems involve numerous assumptions given the minimal amount of experimental data, especially for empirical correlations and thermophysical property libraries. Proper inclusion of underlying modeling assumptions, such as fluid properties, is imperative for uncertainty calculation and risk assessment as NTP technologies are matured. This work highlights the impact of using real gas parahydrogen fluid properties when compared to the common ideal gas assumption. While bulk fluid conditions are impacted, the comparison of peak fuel and channel wall temperatures due to variations in the convective heat transfer coefficient are of utmost concern. The introduction of real gas properties captures high-temperature effects that were not previously captured by the ideal gas assumption, resulting in a higher accuracy wall temperature calculation and a reduction in modeled maximum fuel temperature. Future analysis will expand on this work to investigate thermal effects at the full core level with radial power distributions and variable fuel loadings.

NOMENCLATURE

3D = Three Dimensional

AMA = Analytical Mechanics Associates

ϵ = Percent Difference

FSP = Fission Surface Power

HEU = Highly Enriched Uranium

HALEU = High-Assay Low Enriched Uranium

INL = Idaho National Laboratory

M&W = McCarthy & Wolf

MOOSE = Multiphysics Object Oriented Simulation Environment

MSFC = Marshall Space Flight Center

NASA = National Aeronautics and Space Administration

NERVA = Nuclear Engine for Rocket Vehicle Applications

NEP = Nuclear Electric Propulsion

NTP = Nuclear Thermal Propulsion

SNRE = Small Nuclear Rocket Engine

SNP = Space Nuclear Propulsion

SPOC = Space Propulsion Optimization Code

SSC = Solid Solution Carbide

THM = Thermal Hydraulics Module

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