Coupled Reactor and Engine Nuclear Thermal Propulsion Modeling Methodology

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The design and development process of a Nuclear Thermal Propulsion (NTP) system requires extensive multiphysics modeling to couple the neutron physics and thermal feedback effects to determine the reactor's power shape. Propulsion system performance codes utilize this power shape to determine NTP key performance parameters. While the power shape is heavily dependent on the temperature profile and geometry of the reactor, many analyses either assume a constant power shape, or use neutronics analysis to determine a power shape for a specific reactor configuration. The development of a coupling interface for a propulsion system performance code and a Monte Carlo neutron transport code (OpenMC) allows for the reactor power shape to be calculated in an iteration loop.

The interface utilizes a file share system to transfer geometry dimensions, temperatures, and material identifiers to OpenMC, which is used to perform a neutron transport simulation of a design like the government Testing Reference Design reactor. The interface is then able to post-process the results from OpenMC and use the same file share system to share a power shape and other important neutron transport parameters to the system performance code. Initial results show that neglecting the changes to power shape when comparing reactor configurations can yield inaccurate results. Furthermore, utilizing propellants other than hydrogen gas can cause significant changes to the power shape, and thus, the thermal performance of a specific reactor design. This methodology is being expanded to allow for multiple families of NTP reactors to be analyzed, including block moderator, particle bed, and NERVA-derived reactors.

I. INTRODUCTION

The National Aeronautics and Space Administration (NASA) has released strategic goals for extending human presence to the Moon and Mars. The pursuit of expanding humanity's presence beyond earth and cislunar space requires the utilization of advanced propulsion methods due to the relatively long transit times and risks involved with deep space travel. Nuclear Thermal Propulsion (NTP) emerges as a candidate propulsion system, promising double the specific impulse of conventional chemical rockets. However, successful design and development of such a system demands a comprehensive understanding of the thermal performance and the physics governing the nuclear reactions within the reactor core. These underlying multiphysics effects are also extremely dependent upon one another, thus a routine that iteratively converges on desired reactor performance metrics is imperative for proper system-level modeling.

This work introduces a novel methodology developed by Analytical Mechanics Associates that seamlessly connects a Simulink-based NTP system performance code[1-2] with the open-source Monte Carlo neutron transport code, OpenMC[3]. The Simulink tool converges on all state points of the NTP engine from propellant tank exhaust to the exit nozzle exhaust through physics-based solvers of all internal components, including the reactor subsystem. Following initial convergence, the thermal hydraulic solver provides axial and radial temperature and density distributions of all in-core solid materials as well as the flowing propellant to OpenMC for higher fidelity neutronics analyses. Results of the neutronics analysis include static core-specific performance metrics, such as the neutron multiplication factor, and power distributions for each region of thermal importance that are readable for the next Simulink iteration. This process is repeated until desired engine convergence metrics are reached, typically the thrust, specific impulse, and reactor thermal power.

II. METHODOLOGY

II.A. NTP System Power Balance Model

The thermal hydraulic performance of the NTP system is determined by a power balance engine modeling suite coded in Simulink, known as the X-NTP model[1-2]. This code analyzes various engine cycles, including expander and bleed cycle configurations. Propellant state points (temperature, pressure, and mass flow rate) communicate the performance of the NTP system and allow for easy connection of various components to form different engine cycles. Figure 1 shows a typical flow cycle for the government Testing Reference Design (TRD).[4]

The X-NTP model is formed as a modular engine design suite with the capability to pick and choose the engine cycle, flow schedule, and components utilized. Figure 2 shows a general schematic of a component model. Each component block houses equations that govern the state points that are connected to it and the system performance parameters that it calculates.

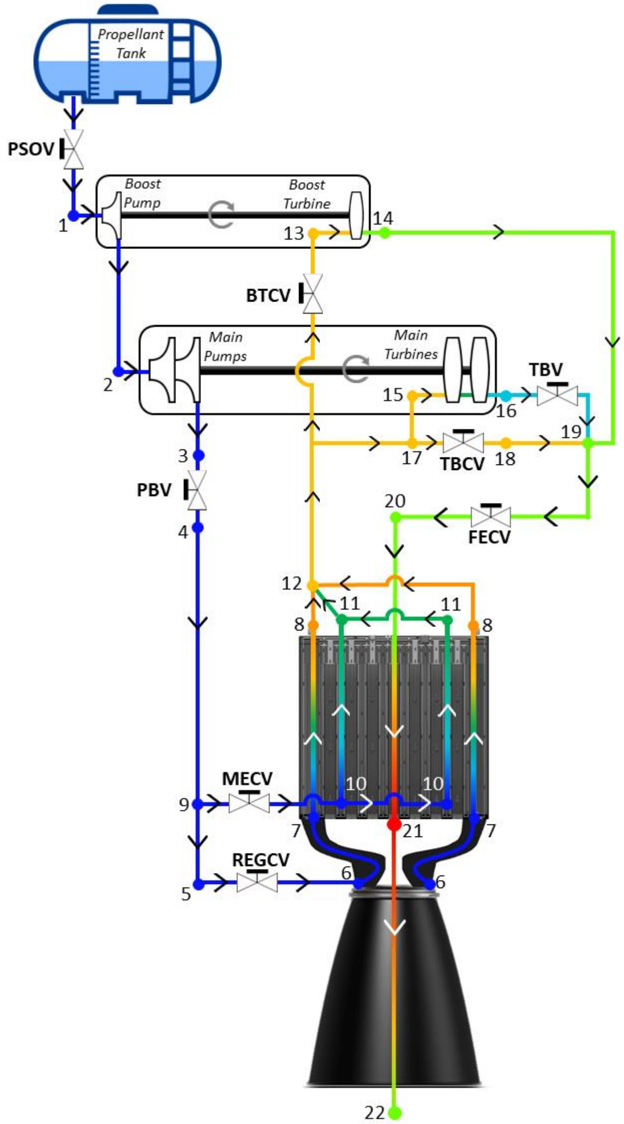

Fig. 1. H-NTP Testing Reference Design Schematic[1].

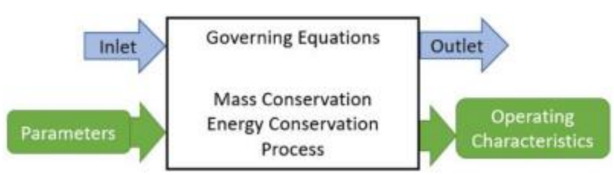

Fig. 2. Arbitrary Engine Component Schematic

The engine components use various user input parameters and the power shape for the reactor (provided by neutronics analysis) to determine the thermal performance of the reactor. Eq. 1 shows the calculation for the surface temperature of a small section of a cooling channel, where δQ is the differential heat added to node i, $\hbar$ is the convective heat transfer coefficient, ΔA_s is the node wall area, and T_s is the surface temperature. Eq. 2 shows the calculation for maximum temperatures in any solid surrounding a cooling channel in the reactor, where d_{c_o} is the outer diameter of the representative solid, d_{c_i} is the inner diameter of the representative solid, k_f is the thermal conductivity of the solid, and Δx is the length of the channel node. The maximum temperature is averaged with the wall temperature to determine a representative temperature for the material. This temperature then informs which cross-section library is selected in the neutronics analysis for the given material. Further, the neutronics analysis also uses the propellant temperatures and pressures to determine the cross-section library and the propellant atom density.

$$\delta Q_i = \hbar \Delta A_s \left[T_{s_i} - \frac{T_i + T_{i+1}}{2}\right] \tag{1}$$

$$T_{f_{max_i}} = \frac{\delta \dot{Q} \ln\left(\frac{d_{co}}{d_{ci}}\right)}{2\pi k_f \Delta x} + T_{s_i} \tag{2}$$

II.B. Neutronics

A Python script uses OpenMC's Python API to build a representation of the TRD for neutronics analysis. The general configuration of the TRD is used; however, all dimensions are provided by the user input files, easily allowing for parametric sweeps on various geometry parameters. The ENDF/B-VII.1 Evaluated Nuclear Data Library[5] provides the neutron cross-sections for all isotopes. The materials attached to the TRD-like geometry are provided by a material card generator. This algorithm allows for an optional porosity correction factor to the material from Eq. 3, where ρ_{TD} is the theoretical density and P is the porosity of the material. The density for all solids is taken as the room temperature density because thermal expansion is ignored for the neutronics analysis. The number of values provided in each temperature row defines the axial temperature discretization of each component in the active core.

$$\rho = \rho_{TD}(1 - P) \tag{3}$$

Two sensitivity studies inform the run-time settings for OpenMC. Eq. 4 defines Shannon Entropy, where S_i is the fraction of fission sites in the i-th element. Figure 3 shows a Shannon Entropy convergence study which illustrates that with a course mesh, the fission site distribution converges after 10 iterations. Since it is impossible to have an infinitely fine mesh for the sensitivity study, this study uses 50 inactive cycles to assure that the error from the source term convergence is minimized. Figure 4 shows a separate sensitivity study where the maximum relative uncertainty in any heating tally was found by varying the particle count. A particle count of 50,000 allows the maximum relative uncertainty to stay below 5% which has been common practice for NTP system models.

$$H = -\sum_i S_i \log_2 S_i \quad (4)$$

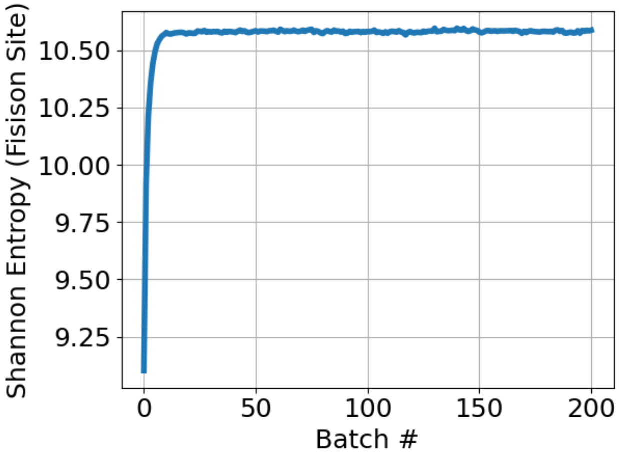

Fig. 3. Convergence of Shannon Entropy from fission sites during inactive batching.

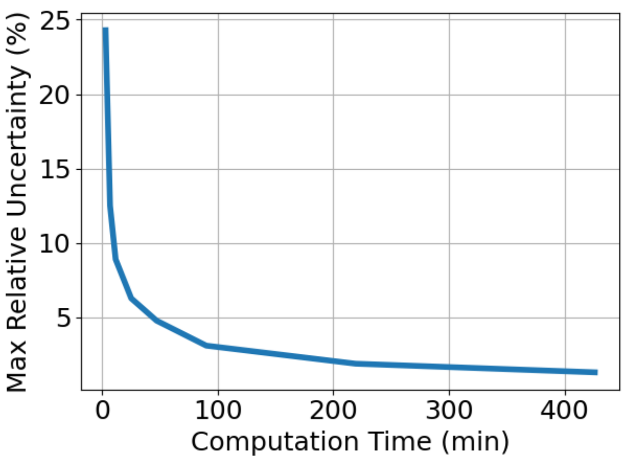

Fig. 4. Maximum relative uncertainty in heating tallies by varying particle count.

OpenMC records the heat shape, flux shape, and criticality of the reactor during the neutron transport simulation. The magnitude of the heating and flux values are determined by the reactor design and is driven by the temperature limits of the materials used in the active core. The heating shape is then provided to the X-NTP model to complete the Picard iteration loop.

II.C. X-NTP Model and OpenMC Coupling

A coupling interface allows for seamless, on-the-fly communication between the X-NTP model and OpenMC for use of a TRD-like design. Figure 3 shows the solution flow diagram as seen from the coupling interface.

The coupling interface takes parameters from the X-NTP model through three input files, summarized in Table I. Developers selected Comma Separated Value (CSV) files as the format for all inter-code communication due to their ease of reading and writing in different codes. These files are written by the X-NTP model and supplied to the coupling interface.

TABLE I. Coupling Interface Input Files

Static Inputs	Dynamic Inputs	Axial Inputs
Geometry Dimensions	Core Power	Solid Temperatures
Material Identifiers	N/A	Fluid Temperatures
Solver Options	N/A	Fluid Pressures

The interface then takes the values from the input files while using additional information from the material card generator and material properties module to build the TRD-like case in OpenMC. The results from the OpenMC case are manipulated by the post-processor to create a useable file for the X-NTP model. This forms an output file, summarized in Table II. Figure 5 illustrates the entire solution flow.

TABLE II. Coupling Interface Output File

Output File
Axial Power Shapes
Axial Flux Shapes
Effective Neutron Multiplication Factor

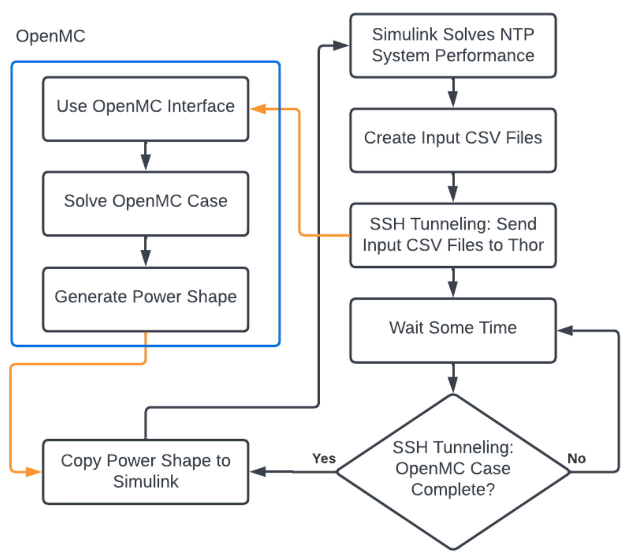

Fig. 5. Solution Flow Diagram of Coupling Interface

The X-NTP model is the driver of the entire iteration loop. It is responsible for creating the input files for the coupling interface and instructing the coupling interface to start. It then enters a waiting loop until OpenMC has completed its simulation where it then reads the resulting output files to receive the new power shape.

III. RESULTS

Two cases illustrate the effect of the decoupled vs. coupled analysis with this tool. The decoupled case was performed with a power shape calculated manually from a single OpenMC iteration. This power shape was used in every iteration of the X-NTP model and never updated to account for a new temperature profile. Thus, the effect of temperature on the power shape is not considered. For the coupled case, the calculation utilized the methodology outlined in Section II.C where the temperature profile is fed back into OpenMC. This coupling effect ensures that both the temperature and power profiles are converged upon.

Figure 6 shows the heat fraction deposited per axial node in the centermost fuel element. This fuel element offers a comparison point between the coupled and the decoupled case. The normalized axial position of 0 corresponds to the top of the core, while 1 corresponds to the bottom of the core. Visually, the power fractions nearly overlap, indicating that the constant power shape used in the decoupled approach was accurate enough to yield similar results. Figure 7 is a calculation of the relative error in the axial heat deposition fraction for the centermost fuel element, using the coupled case as truth data.

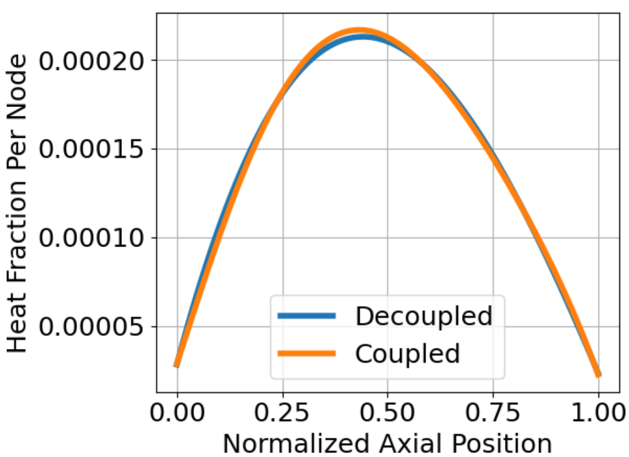

Fig. 6. Axial heat deposition of centermost fuel element for coupled and decoupled cases.

In a similar fashion, the fuel temperature profile offers an additional comparison between the coupled and decoupled case. For the decoupled case, the last iteration of the X-NTP model provides the temperature profile without using OpenMC to update the power profile at any point. Meanwhile, the temperature profile found in the coupled case is the result of the X-NTP model converging the power profile through multiple iterations.

Figure 8 shows the resulting temperature profiles. The values are reported as the axial temperature normalized to the maximum axial temperature for the centermost fuel element. Figure 9 is a calculation of the relative error between the two cases, using the coupled case as truth data.

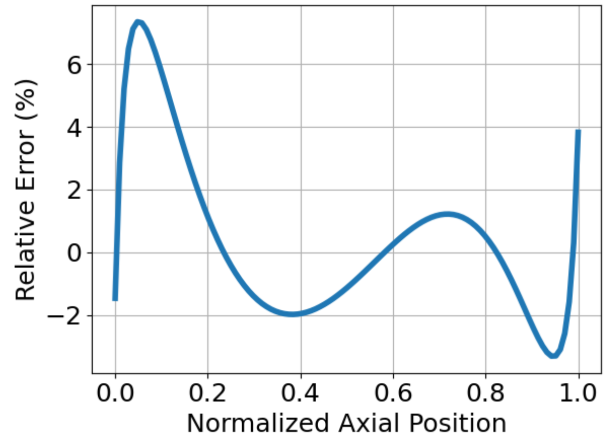

Fig. 7. Relative error in the axial heat deposition of the centermost fuel element for coupled and decoupled cases.

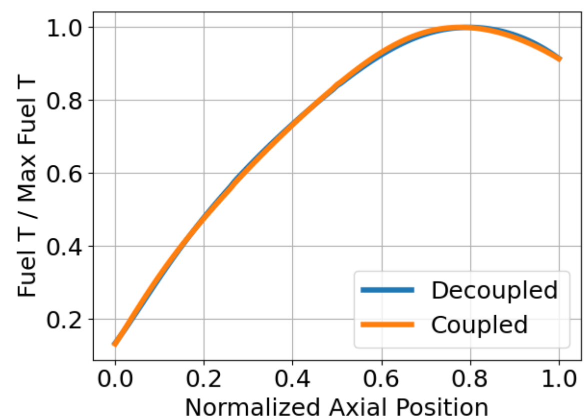

Fig. 8. Normalized fuel temperature of the centermost fuel element for coupled and decoupled cases.

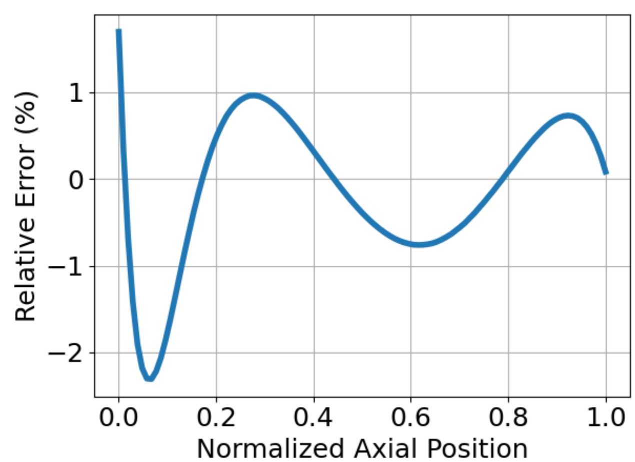

Fig. 9. Relative error in the temperature profile of the centermost fuel element for coupled and decoupled cases.

The sample analysis between the coupled and decoupled cases shows great agreement, with the maximum change in the heating profile of the centermost fuel element being less than 8% and the maximum change in the temperature profile being less than 2.5%. The highest temperature region observes some of the lowest error between the two cases which is likely due to the 2500 K temperature upper-limit for the cross-section libraries. Since the heat profile error is above the 5% acceptable error commonly used in NTP analysis, this example illustrates the importance of direct coupling between thermal hydraulic and neutronics analysis.

The shape of the error in the temperature and heating profile illustrates where the temperature assumptions are most incorrect in the initial model used for calculating the decoupled power shape. Since the initial guess for the power shape in the decoupled case was reasonable, the error is not as significant. The biggest advantage of the coupled approach comes from future analysis where a good power shape assumption does not already exist. This is particularly useful for parametric studies of reactor geometry where the power shape will vary from case to case. Transient analyses will also require a coupled approach as the power shape will change significantly as the fuel temperature increases.

The error seen in this sample analysis can be attributed to a variety of sources. The largest source being the stochastic nature of Monte Carlo neutron transport simulations. Since the flux magnitude is smallest near the top and bottom of the core, the uncertainty in these heating tallies is also the highest. While Figure 4 illustrates that this uncertainty is being driven down below 5% for this calculation configuration, the error still exists and propagates through the X-NTP model.

IV. CONCLUSIONS

The AMA-developed methodology allows for the direct interfacing of two dissimilar codes. The X-NTP model and OpenMC are connected and actively trade information with the objective of learning how the results of an NTP system performance model are impacted by a converged reactor power shape. The use of CSV files for both inputs and outputs makes the tool modular enough to be further connected to other models in the future if the model in question has the capability of reading and interpreting a CSV file.

A more comprehensive modeling suite based on the X-NTP model, and the methodology described in this paper is already in progress. The capabilities of the modeling suite will extend past TRD-like designs and include other families of NTP reactor designs. These include, but are not limited to, NERVA-derived designs, fast reactor designs and particle bed reactor designs. The capability to design and analyze a reactor based on a design family and a few key input variables will allow for quick turnaround evaluation of design decisions such reactor size scaling.

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