Parametric Trade Space Investigation of Particle Bed Reactors for Nuclear Thermal Propulsion

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Nuclear thermal propulsion (NTP) systems utilizing particle bed reactors (PBR) offer performance advantages over traditional NTP propulsion system designs. In addition to low pressure drop requirements through the reactor, PBRs can deliver high power density, potentially leading to lower mass designs. This work seeks to investigate various design points of PBR-based NTP systems. The DOD Space Nuclear Thermal Propulsion (SNTP) PBR design is a template for the trade space investigation. Parameter sweeps of core length, particle radius, system mass flow rate, packing fraction, bed thickness, and many other variables inform point design definitions. Coupled multiphysics modeling methodology yields data on the performance of design points, while ruling out any infeasible configurations. This study captures the mass and performance trades of feasible PBR designs.

A PBR trade space database is generated and reveals that for a given thrust class, the SNTP-derived designs offer low mass, critical reactor options with reduced pressure drop requirements while using high-assay low-enriched uranium fuel. A comparison of the trade space summarizes the performance capabilities of PBR NTP reactors.

I. INTRODUCTION

The United States has invested in advancing the technology readiness of nuclear propulsion systems over the past seventy years through independent and collaborative efforts from the National Aeronautics and Space Administration (NASA), Department of Energy (DOE), and Department of Defense (DOD). In particular, a majority of the funded research centered around nuclear thermal propulsion (NTP) aims to enable efficient in-space transportation between the Moon and Mars. These government entities made significant advancements in NTP technology maturation, yet most of the legacy research relied on highly enriched uranium (HEU) fuel forms to minimize mass without sacrificing performance. Modern regulatory restrictions on HEU decrease the applicability of the past reactor designs to the current goal of a near-term NTP demonstration test. However, the years of research and development into the fuel forms and general reactor configurations allow for simpler adaptation to meet the high-assay low-enriched uranium (HALEU) threshold. In this work, AMA led an investigation of the parametric trade space of the former DOD Space Nuclear Thermal Propulsion (SNTP)[1] configuration with a HALEU fuel form.

As seen in Figure 1, the SNTP design, in principle, leverages particle bed fuel assemblies interspersed in a moderator block. Given its use of a moderator, the adaptability from a HEU to HALEU design is simplified in comparison to other legacy HEU variants. Nevertheless, the key reactor components, such as the active core and reflector region, must scale in geometrical size (e.g., length and radius) to accommodate the reduction in enrichment. This problem introduces several parametric variables to investigate the neutronic and thermal hydraulic trade space while still identifying optimal regions of interest for the engine performance metrics and system mass.

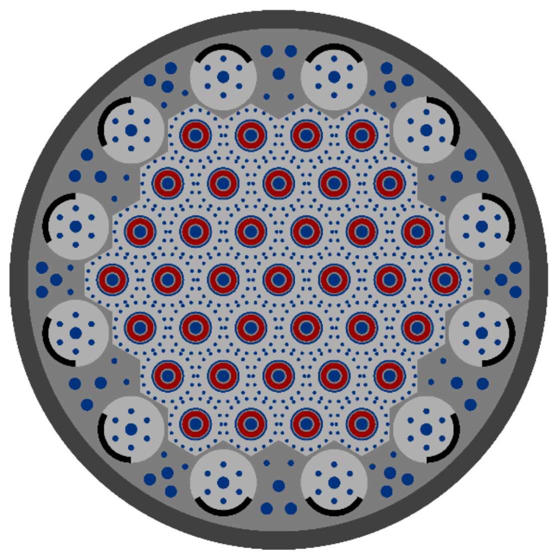

Fig. 1. Cross section of an SNTP-derived design which features particle bed fuel assemblies.

II. METHODOLOGY

II.A. Reduced Order Thermal Hydraulics

In general, assessment of the reactor physics and engine performance relies on proper modeling of the heat transfer and fluid mechanics to determine boundary conditions as well as temperature and density profiles within the system. Most NTP designs utilize cylindrical internal cooling channels which have been investigated at length and are simplistic to model. However, the difficulty with modeling the SNTP design falls on the thermal hydraulics (T/H) of multidimensional flow within the fuel assemblies.

The T/H calculation in this work is a three-step process. First, the T/H code solves the discretized, 1D, area-averaged, steady-state Navier Stokes equations to determine the flow temperature distribution, assuming that the frits and fuel assembly design are such that there is little flow velocity in the axial direction. Eqs. 1-3 show the mass, momentum, and energy conservation equations respectively where A is flow area, ρ_f is fluid mass density, u is bulk flow velocity, P is static pressure, E_f is internal energy, $\dot{Q}$ is heat added to the flow, $\dot{m}$ is mass flow rate, and c_p is specific heat capacity. Second, a Nusselt number correlation is used to determine the heat transfer coefficient which is then used by the T/H code to solve for the surface temperature of a particle. Finally, the T/H code determines the solid temperature profile by solving the heat conduction equation for a sphere with constant heat generation with the assumption of a smeared particle material.

$$\frac{\partial}{\partial x}(A\rho_f u) = 0 \quad (1)$$

$$\frac{\partial}{\partial x}(A\rho_f u^2 + AP) = LOSS \quad (2)$$

$$\frac{\partial}{\partial x}\left(Au(\rho_f E_f + P)\right) = \frac{\dot{Q}}{\dot{m}c_p} \quad (3)$$

The T/H model slices the fuel element into numerous axial sections to capture the axial variations in the temperature profile. The total mass flow rate for the fuel assembly is divided into each section based on pressure convergence. While this approach offers some form of axial variation, the assumption is that there is no axial flow velocity, and therefore no flow shift. The results made with these assumptions can provide insights into the trends in the T/H performance but are not able to fully identify hotspots caused by flow shift. Figure 2 shows the discretized computational domain.

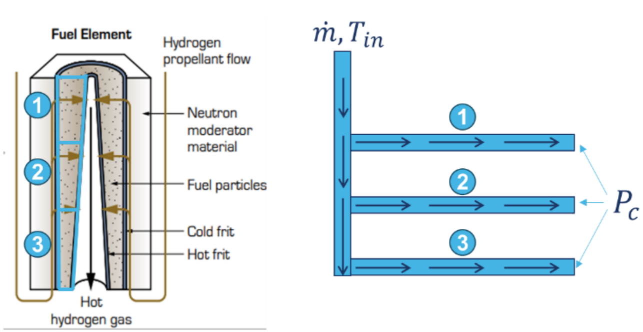

Fig. 2. Spatial discretization of reduced order PBR T/H model. Original image from Ref. 2.

II.A.1. Momentum Loss Term

The reduced order T/H modeling methodology for PBRs varies slightly from the methodology for traditional NTP systems. The source term added to the momentum equation is the most obvious difference. While traditional NTP T/H must account for friction wall effects with its momentum equation, PBR T/H must account for the momentum loss through a packed bed. The T/H models developed for this work contain multiple options for modeling this momentum sink. Eq. 4 shows the Ergun equation where $\frac{\Delta P}{L}$ is pressure drop per unit distance, μ is dynamic viscosity, ϵ is the bed porosity (flow volume divided by total volume), V is the bulk flow velocity, d_p is particle diameter, and ρ is the fluid mass density. Eq. 5 shows the pressure drop-flow rate correlation presented by Erdim.[3] Eq. 6 defines the Modified Reynolds Number (Re_m) where Re is the traditional Reynolds number and Eq. 7 defines the friction factor.

$$-\frac{\Delta P}{L} = 150\mu\frac{(1-\epsilon)^2}{\epsilon^3}\frac{V}{d_p^2} + 1.75\rho\frac{(1-\epsilon)}{\epsilon^3}\frac{V^2}{d_p} \quad (4)$$

$$f_v = 160 + 2.81\, Re_m^{0.904} \quad (5)$$

$$Re_m = \frac{d_p \rho V}{\mu(1-\epsilon)} = \frac{Re}{(1-\epsilon)} \quad (6)$$

$$f_v = -\frac{\Delta P d_p^2}{\mu V L}\frac{\epsilon^3}{(1-\epsilon)^2} \quad (7)$$

The trade space study initially used the Ergun equation as a pressure drop correlation. However, the Erdim correlation replaced the Ergun equation[4] since it has been shown that the Ergun equation should not be used for problems with a modified Reynolds Number above $Re_m = 500$.

II.A.2. Particle Temperature Distribution

In the second and third steps of the T/H calculation, the T/H code calculates the surface and maximum temperatures as a function of radial position. Eq. 8 shows the Achenbach correlation[5] which provides the Nusselt number in this study. Eq. 9 shows the relationship between local Nusselt number and local heat transfer coefficient at any radial node where h is the local heat transfer coefficient and k is the thermal conductivity of the fluid. Eq. 10 then utilizes the heat transfer coefficient to calculate the surface temperature of the particle where T_{surf} is the particle surface temperature, $\dot{Q}_p$ is the heat generated by a single particle, A_{surf} is the surface area of a single particle, and T is the bulk fluid temperature. Finally, the T/H code uses Eq. 11 to analytically solve for the maximum particle temperature where T_{max} is the maximum particle temperature, $\dot{Q}'''$ is the volumetric heat generation rate, and k_{solid} is the smeared thermal conductivity of the particle.

$$Nu = [(1.18Re^{0.58})^4 + (0.23Re_m^{0.75})^4]^{0.25} \quad (8)$$

$$h = \frac{Nu \cdot k}{d_p} \quad (9)$$

$$T_{surf} = \frac{\dot{Q}_p}{h \cdot A_{surf}} + T \quad (10)$$

$$T_{max} = T_{surf} + \frac{\dot{Q}''' \cdot d_p^2}{24k_{solid}} \quad (11)$$

II.B. Neutronics Modeling

A simulation of continuous energy neutron transport provides insight into the power deposition shape and the nuclear feasibility of a PBR point design. A fully defined neutron transport problem requires reactor design dimensions, material identifiers, and an array of multiphysics coupling data such as spatially varying fuel temperature and propellant density. CSV files hold the large number of input parameters required to fully define the neutron transport problem.

An extensive SNP OpenMC Generator code then reads the CSV files and uses the input parameters to create an individual neutron transport case for OpenMC[6]. The SNP OpenMC Generator code discretizes many regions of the core to vary the local neutron cross sections based on temperature. Since the fuel temperature is expected to vary largest in the direction of the propellant flow, the generator code discretizes the reflector (with 12 control drums) and the moderator in the axial direction, while the packed particle bed is discretized in the radial direction. The T/H calculations provide a volume-averaged temperature for each discretized region. A smeared material represents each discretized region in the packed particle bed in lieu of discrete particle modeling. OpenMC cannot natively model two isotopes with different fuel temperatures in one material, therefore, the generator does not include the propellant isotopes in the packed particle bed. Initially, the model included the propellant with the assumption that its temperature was the same as the fuel; however, preliminary findings from the T/H model showed that this assumption is poor for large diameter particles.

OpenMC then stochastically solves the neutron transport problem using the ENDF/B-VII.1 Evaluated Nuclear Data Library to obtain the temperature-dependent neutron cross-sections for all isotopes.[7] OpenMC is configured to record fuel assembly-dependent tallies. A post processing script reads the raw tally data and then records k_{eff}, power deposition shape, reactor mass, and many other values to an output CSV file.

II.C. Coupling Algorithm

The T/H code and the SNP OpenMC Generator code are linked together in a tightly coupled iteration loop.[8] A coupling script shares data between the two codes. The T/H code provides the volume averaged material temperatures to the SNP OpenMC Generator code, which in turn provides the power deposition shape to the T/H code. The coupling script continues the data sharing process until the values of all coupling data match the values of the previous iteration within some tolerance. Figure 3 shows the coupling loop.

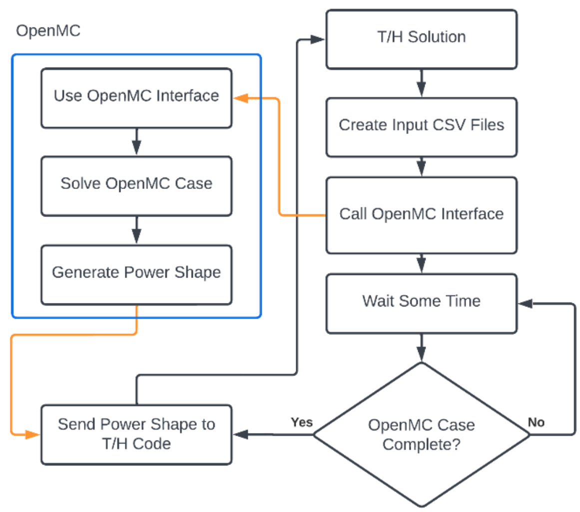

Fig. 3. Multiphysics coupling between neutronics and T/H.

II.D. Database Generation and Parameters of Interest

The coupling algorithm solves a parametric sweep of cases to create a representative trade space database. The variation of many design variables fully captures the corners of feasible PBR design configurations. Table I summarizes the varied parameters and their bounds. The bed modifier parameter is a value multiplied by the fuel assembly's inner channel radius and outer hot frit radius, effectively increasing the thickness of the particle bed.

TABLE I. Varied parameters for PBR trade study.

Parameter	Range
Core Length	50 – 200 cm
Packing Fraction	0.53 – 0.74
System Mass Flow Rate	5 – 20 kg/s
Particle Radius	0.15 – 0.5 mm
Bed Modifier	0.25 – 1

This study narrows the trade space by holding other design parameters constant from case to case. This includes the reactor materials, the propellant, and some geometry parameters. The general layout of the core, including the reflector, control drums, moderator, and the fuel assembly configuration remains unchanged. Table II shows a summary of the reactor material assumptions and Table III design parameters that are considered constant.

TABLE II. Material assumptions for PBR trade study.

Region	Material
Fuel	UN (HALEU)
Frit	Be
Moderator	ZrH
Reflector	Be
Control Drum	Be
Poison Vane	B4C
Propellant	H2

TABLE III. Constant parameters for PBR trade study.

Parameter	Value
Core Inlet Temperature	200 K
Fuel Assembly Pitch	9.1 cm
Reflector Thickness	10 cm
No. of Control Drums	12
Poison Vane Thickness	1 cm

For each case, the database stores many calculated values, including required power level, chamber temperature, k_{eff} (with control drums at 180 deg from full in), control drum worth, reactor mass, and others. The power level is calculated iteratively such that no material temperature limits are violated. A datapoint is considered valid if the k_{eff} is above 1.00 when the control drums are fully out.

III. TRADE SPACE RESULTS

III.A. Neutronics Performance Investigation

The database described in Section II.D. is generated from 640 converged multiphysics cases using the varying design parameters. The first objective is identifying whether a critical ($k_{eff} > 1$) design can be obtained using HALEU fuel. Figure 4 shows all design points, their criticality factors, and the resulting reactor mass.

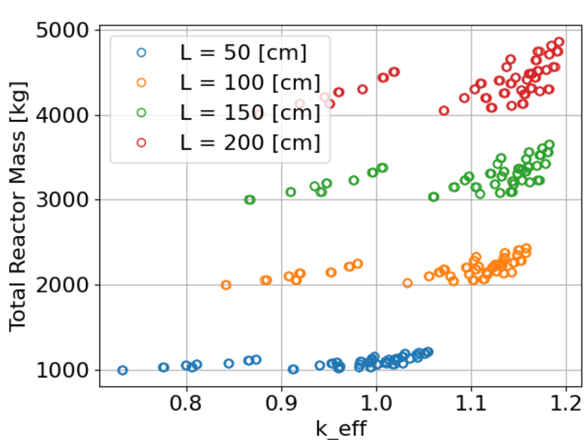

Fig. 4. Criticality factor vs total reactor mass.

The initial results reveal that achieving a critical reactor design using HALEU fuel is possible inside of the limited trade space of this study. From a mass perspective, the dataset is separated into four distinct sections that are directly correlated to the reactor length parameter. The implication is that the total reactor mass is sensitive to the length parameter. While increasing the length increases the bed volume (and thus, increases k_{eff}), the volume of other reactor components such as the moderator, reflector, and control drums also increase, significantly increasing the reactor mass.

The trade space database shows that there are parameters that can affect the criticality factor while having a smaller impact to the reactor mass. Figure 5 and Figure 6 show the impact of the particle radius on the criticality factor and the mass respectively. The assumption for the particle design is that the particle coating thickness remains constant, which means that as the particle radius increases, the ratio of the fuel to coating increases, which increases the criticality factor.

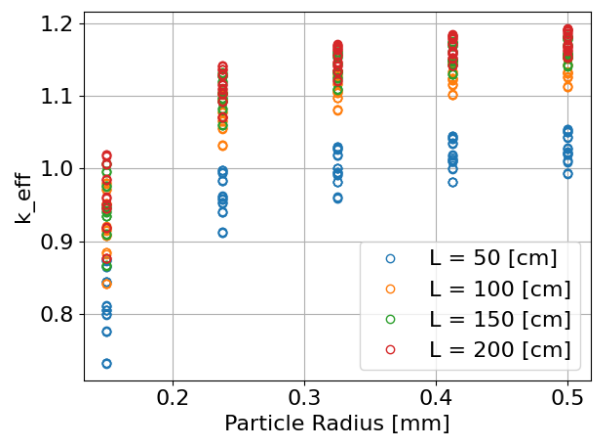

Fig. 5. Particle radius vs criticality factor.

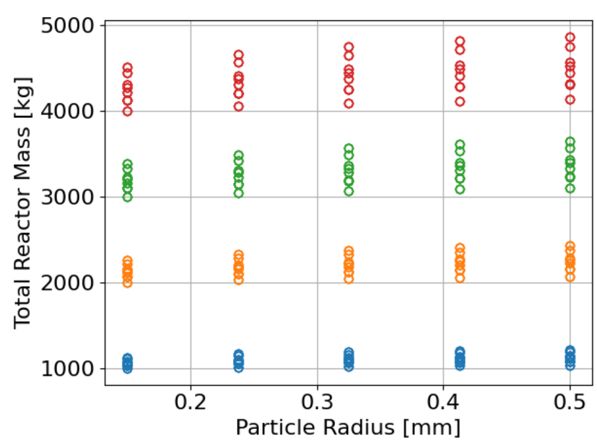

Fig. 6. Particle radius vs total reactor mass. The different plot colors indicate the reactor length in a similar fashion to Figures 4 and 5, but the legend is not shown for clarity.

III.B. T/H Results

The particle radius emerges as a promising design parameter to achieve a low mass, critical HALEU PBR reactor design. However, there are T/H implications for large particle radii. Specifically, maximum temperature gradient, and thus, the stress in the particle due to thermal expansion, increases as the particle radius increases. This means that while an increase of the particle radius can assist a design from a criticality perspective with minimal impact to the reactor mass, the particle radius is limited by the maximum thermal stress allowed by the fuel material. Figure 7 shows this effect but limits the results to cases where the $k_{eff} > 1$, the packing fraction is 0.74 (maximum possible packing fraction) and the bed modifier is 1.0 (the inner chamber's geometry is not impacted) for clarity.

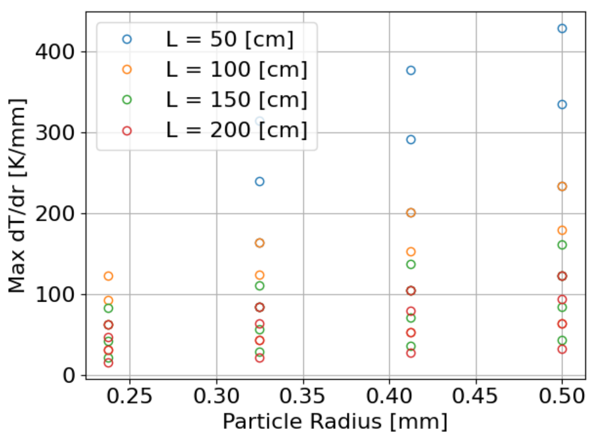

Fig. 7. Particle radius vs maximum temperature gradient in a particle for cases where $k_{eff} > 1$, packing fraction = 0.74, and bed modifier = 1.0.

In addition to the thermal stress in the particle, the reactor power level and the pressure drop through the particle are T/H outputs of interest. Figure 8 shows the power level as a function of the pressure drop through the bed. It's important to note that the pressure drop is only modeled through the particle bed, with no consideration of the pressure drop through the inlet plenum, the frits, or any other fuel assembly component. With the assumption that all the power generated in the reactor is transferred to the propellant, a higher reactor power level is proportional to a higher thrust class propulsion system.

While the power level is important, it does not provide any indication to the size of the reactor providing it. The mass specific power level gives a better indication of the thrust to weight trends in this trade space. Figure 9 shows the mass specific power level by taking the results shown in Figure 8 and dividing by the corresponding total reactor mass.

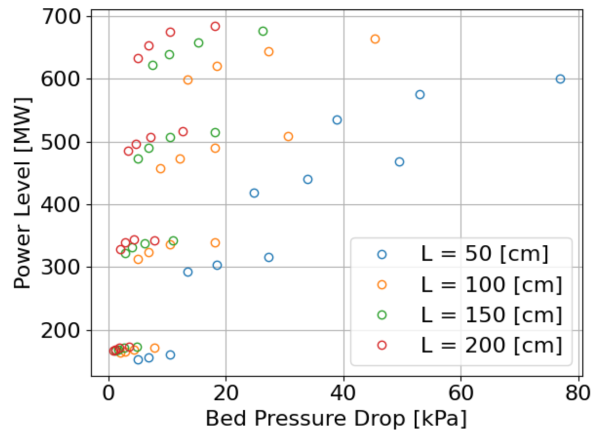

Fig. 8. Bed pressure drop vs power level for cases where $k_{eff} > 1$, packing fraction = 0.74, and bed modifier = 1.0.

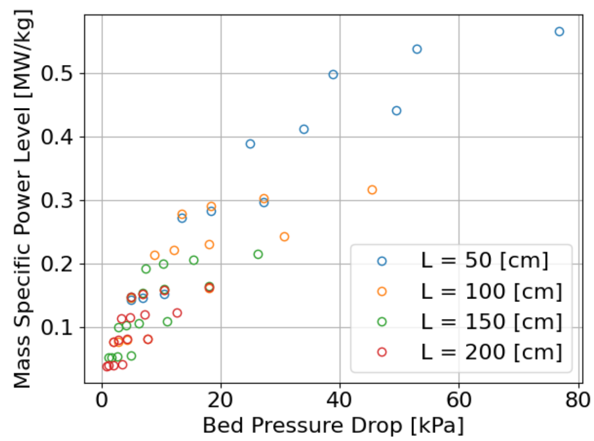

Fig. 9. Bed pressure drop vs mass specific power level power level for cases where $k_{eff} > 1$, packing fraction = 0.74, and bed modifier = 1.0.

IV. CONCLUSIONS

The neutronics results from this limited PBR trade space analysis has revealed that a critical design using HALEU fuel is possible with small modifications to the particle bed volume or the particle radius. The lowest mass, critical design had a reactor mass of 1063 kg (this only includes fuel particles, frits, moderator, core insulator, reflector, control drums, poison vanes, and pressure vessel along active core length).

The criticality factor is impacted by many of the design parameters in this trade space. The length of the reactor impacts the criticality factor by increasing the particle bed volume; however, the reactor mass is sensitive to this parameter. The particle radius value can impact the criticality factor without having the same level of influence on the reactor mass, but with the added complication of affecting the maximum thermal stress seen in the particles.

There are many areas marked for forward work. The T/H models used in this study do not capture many phenomena required for accurate modeling of PBR designs, such as axial flow shift, frit pressure drop, and mass flow rate pressure convergence. The replacement of the basic T/H models used here with a porous flow model that can capture these phenomena is a priority, especially for comparing the pressure drop between PBR designs and any other NTP point design. In addition, the design process used in this study must be modified to combat the fuel assembly power peaking seen in the neutronics model. This will provide a better understanding of the specific impulse and thrust levels that are possible from a PBR. The design process can accomplish this by varying the packing fraction, particle radius, or fuel enrichment in each assembly to achieve a flatter power distribution. With these model enhancements, the trade space can be expanded to vary other parameters such as number of fuel assembly rings, fuel materials, and propellant types.

ACKNOWLEDGMENTS

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