

Modeling Validation and Its Design Relevance for NTP Fuel Elements

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The development of Nuclear Thermal Propulsion engines depends heavily on modeling and simulation of several disciplines—neutronic / fluid / thermal / structural are only a start. Further, these rockets involve extreme conditions, particularly high material temperatures in the nuclear fuel. This paper considers validation of the underlying physical models and simulations and how their accuracy influences several design challenges. Several issues are identified, where models, material data, could enable design solutions. In particular, thermal and CTE mismatch stresses are a concern, and stress predictions would benefit from improved mechanical property data at high temperatures. Nuclear inter-element heating causes propellant flow maldistribution and performance risks, but a simple model provides insights. High temperature chemical diffusion should be modeled to understand fuel element mass loss.

I. Nomenclature

A	=	area, m ²
CFD	=	computational fluid dynamics
C_p	=	specific heat, J/kg-K
CTE, α	=	coefficient of thermal expansion (secant method), m/m-K
C_{specie}	=	specie concentration
D	=	coolant channel diameter, m
D_I	=	interaction depth, mm
E	=	modulus of elasticity, Pa
E_a	=	activation energy of permeating species, J/mol
f_{turb}	=	turbulent Fanning friction factor, dimensionless
HEU	=	highly enriched uranium
I, I_0	=	particle beam intensity, initial intensity, number/s
I_{sp}	=	specific impulse (vacuum), s
J	=	index
k	=	coefficient of thermal conductivity, W/m-K
LEU	=	low enriched uranium
M	=	Mach number, dimensionless
MCNP	=	Monte Carlo n-particle transport, a neutronics simulation code
$\dot{m}$	=	mass flow rate, kg/s
n	=	surface normal direction, away from solid
N_a	=	number density of target particles, here U-235 nuclei, number/cc
NTP	=	nuclear thermal propulsion
$O()$	=	order of magnitude approximation
$P, \Delta P$	=	pressure, pressure drop, Pa
PPF	=	power peaking factor, ratio of local (channel) power density, Q , to fuel element average, dimensionless
Pr	=	Prandtl number, dimensionless
q	=	heat flux, W/m ²
Q	=	volumetric heat deposition rate, equivalently power density, W/m ³

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r, r_0, r_1	= radial distance to coolant channel center, borehole radius of fuel, maximum radius, m
R	= universal gas constant, J/mol-K
Re	= Reynolds number based on coolant channel diameter, dimensionless
s	= half coolant channel pitch, m; seconds, s
SNRE	= small nuclear rocket engine
t	= time, s
T	= temperature, K
T_{SF}	= stress-free temperature, or fabrication temperature, K
u, v	= axial, radial displacements, for stress-strain, m
U	= fluid velocity, m/s
z	= axial distance from channel inlet, m
α , CTE	= coefficient of thermal expansion (secant method), m/m-K
γ	= ratio of specific heats, dimensionless
Δ_J	= Sparrow equation coefficients, K
$\varepsilon_r, \varepsilon_\theta, \varepsilon_z$	= structural strain, in radial, circumferential, and axial directions, m/m
θ	= circumferential coordinate in polar coordinates, rad
ν	= Poisson's ratio, dimensionless
ρ	= density, kg/m ³
σ	= nuclear cross section, σ_f -fission, σ_e -elastic, σ_γ -radiative capture, cm ²
$\sigma_r, \sigma_\theta, \sigma_z$	= structural stress in radial, circumferential, and axial directions, Pa
τ_w	= shear stress at the wall, Pa
ψ	= thermoelastic displacement potential, for stress-strain
w/b	= wall / bulk conditions
in/out	= inlet / outlet
$0/1$	= inner / outer

II. Introduction

Modeling and simulation are appealing in a broad range of scientific and engineering fields. Predictions are valuable to designs, computers are fast, costs are low, and designs are becoming increasingly complex. Yet the gold standard remains experimental testing. In a test, Mother Nature gets all the physics right: all disciplines are tested together—plus their interactions, transients, controls and fabrication. Modeling and simulation are more piecemeal: even the best, foreseeable multidisciplinary simulations are unlikely to capture all the subtle disciplines, nor their interactions. Do we currently capture acoustic disturbances in coolant tubes with their structural consequences and importance? The more important question is: what physics do we need to capture for a viable design?

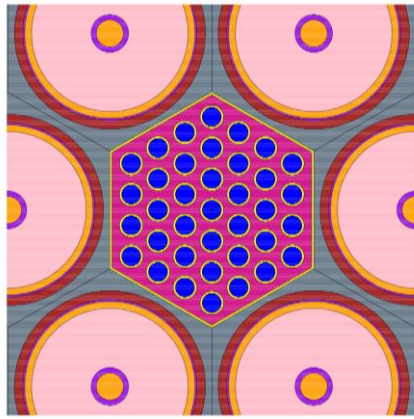


Figure 1: Simulations and their validation involve fuel element / moderator element reactor designs. Particle bed and ribbon fuels are not currently simulated.

The perspective of this paper is that validation is important in complex simulations but understanding a design's constraints is also important.

Aggressive, novel designs have design challenges. Nuclear Thermal Propulsion (NTP) rockets have the promise of high levels of thrust while efficiently using propellant. Uniquely for a rocket, nuclear heat is deposited in the solid fuel, diffuses to nearby coolant channels containing flowing propellant; fuel is cooled, propellant is heated. In contrast, chemical rockets and jet engines release heat *directly* into the gas phase; incidentally, walls are carefully cooled. For NTP rockets, propellant temperature is performance—higher temperature is better (I_{sp} increases by 17 s for every 100K increase in mean propellant temperature). Yet, when the heat originates in solid fuel, this reactor fuel presents new design issues. Not only material temperatures, but many disciplines are pushed to their limits. Further, other rocket components (nozzles, turbopumps, and valves) have been operationally proven, while NTP fuel elements are relatively unproven.

There are limitations to the scope of this work. Validation is specialized to NTP hexagonal fuel/moderator elements (Figure 1) and a reactor configuration which was first used in the Rover/NERVA program [1]. Other reactor types include the Russian ribbon fuel [2] and pebble bed

[3] reactor designs. This work does not consider many other pacing issues in NTP design, including: long term liquid hydrogen storage in space, valve leakage, material property changes in a reactor's radiation field.

The following sections break down current multidisciplinary simulations into their disciplines, the equations solved, and how these predictions are validated. Further, validations are emphasized according to important design issues. When limited testing and experimental data exists, validation is careful comparisons with other solutions.

III. Basic Validation and Verification

1. Conservation of Mass, Momentum and Energy

In fluid solutions, conservation of mass, momentum and energy are routinely verified. Further, convergence is carefully monitored to ensure the best practical convergence. Lastly, solutions are carefully examined and checked.

2. Propellant Outlet Mean Temperature

Propellant outlet mean temperature is validated readily, by comparing with an energy balance equation, Eq. (1). Heat is conserved by the numerical scheme, so all deposited heat, Q , is transferred to the propellant and exits at the fluid outlet boundary. Consequently, propellant outlet mean temperature is a material property: hydrogen specific heat, C_p . It is dependent solely on the specified total nuclear heat deposition and the specified propellant flow rate.

$$\int_{Fuel} Q dVol = \int_{out} \rho U \int_{T_{in}}^{T_{out}} C_p dT dA, \text{ in steady conditions} \quad (1)$$

IV. Disciplines, Equations & Solution Validation:

The author's multidisciplinary simulations for NTP [4] [5] [6] involve neutronic / fluid / thermal / structural simulations which solve 3D equations in complex, fuel element / moderator element geometries (Figure 1). The following sections consider each of these disciplines, with a focus on the equations solved, validation, and relevance to design challenges. Ideally, validation is typically comparison with a closed-form solution.

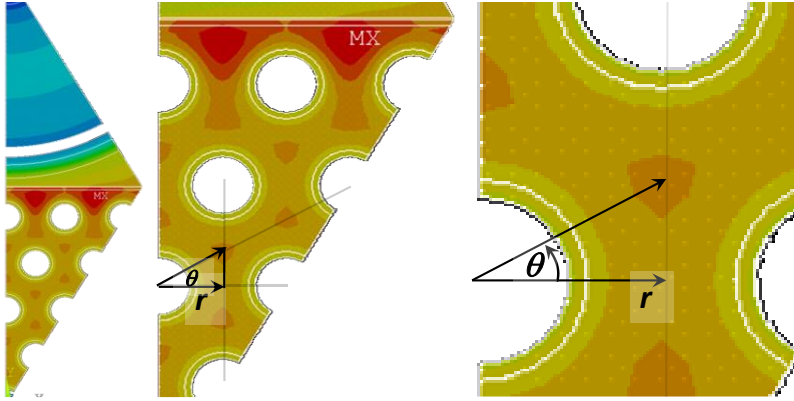


Figure 2: Temperature in a fuel element with symmetrical coolant tube spacing and uniform heating. The triangular region tiles or covers the section—reflecting over any face preserves the geometry. Temperature and 2D heat diffusion are predicted by the Sparrow equation [10], Eq. (3). Outside the tube array—at the fuel element edges—symmetry fails as does the closed-form temperature prediction.

$k(T)$, are measured [9], with consensus, to high temperatures for many materials, but not all. A closed-form solution, Eq. (3), exists [10] [11] for validation. This two-dimensional solution is specialized to the symmetry of a coolant tube array, as shown in Figure 2, with no coating or cladding, and uniform heating.

$$T(r, \theta) - T_{wall} = \frac{Q}{k} s^2 \left[\frac{\sqrt{3}}{\pi} \ln \left(\frac{r}{r_0} \right) - \frac{1}{4} \left[\left(\frac{r}{s} \right)^2 - \left(\frac{r_0}{s} \right)^2 \right] + \sum_{j=1} T_j(r) \cos 6j\theta \right] \quad (3)$$

A. Thermal Simulations

Fluid / thermal simulation and predictions come from ANSYS Multiphysics [7] [8], which combines FLOTRAN for the fluid analysis, ANSYS Thermal for the thermal analysis, and ANSYS Structural for the stress analysis.

1. Heat Diffusion in Solid

One important discipline is calculating heat flow through a solid material. The physics is thermal diffusion; the equation,

$$\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q \quad (2)$$

has a simple, stable numerical solution; and thermal conductivities,

$$T_j(r) = \frac{\Delta T}{6J} \left(\frac{r}{s}\right)^{6J} \left[1 - \left(\frac{r_0}{r}\right)^{12J}\right] \quad (3-b)$$

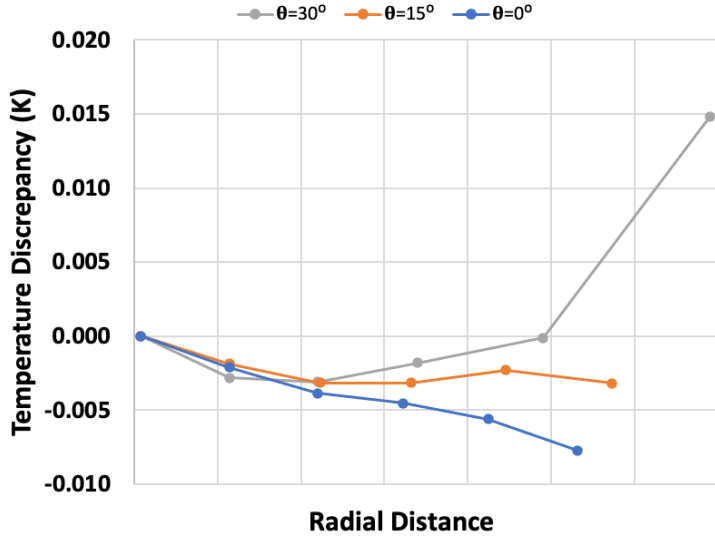


Figure 3: Comparison of thermal simulation and closed-form solution. The discrepancy or error is less than 0.015 K while the temperature range in the solution is ~170 K.

Figure 3 shows the disagreement (or error) between the closed form solution, Eq. (3), and simulation. The temperature range is order $O(170 \text{ K})$, and the error is less than 0.015 K throughout the triangular region. The simulation does not include channel coating or cladding—only homogenized fuel; thermal conductivity, k , and volumetric heat deposition, Q , are constant radially and axially.

One consideration is the composition of the fuel. Modeling prefers uniform, isotropic solid materials. In reality, a volume of fuel may contain many fuel particles in a distinct matrix material or be sintered from a powder mixture. Ideally, experimental measurements provide *homogenized* (averaged) material properties for these simulations; often, carefully devised mathematical methods can estimate these homogenized properties.

B. Fluid / Thermal Simulations

In an NTP rocket engine, nuclear heat is deposited in the solid fuel, and diffuses to nearby coolant channels containing flowing hydrogen propellant. Heat transfer at the wall is not trivial to model. As indicated in Figure 4, local heat transfer depends on the slope $\frac{\partial T}{\partial n}$ at the wall for solid, Eq. (2), and fluid. In the CFD fluid calculation, the boundary layer's velocity and temperature profiles must be accurately calculated. Heat transfer correlations exploit a mathematical trick: similarity solutions for the non-dimensionalized Navier-Stokes equations.

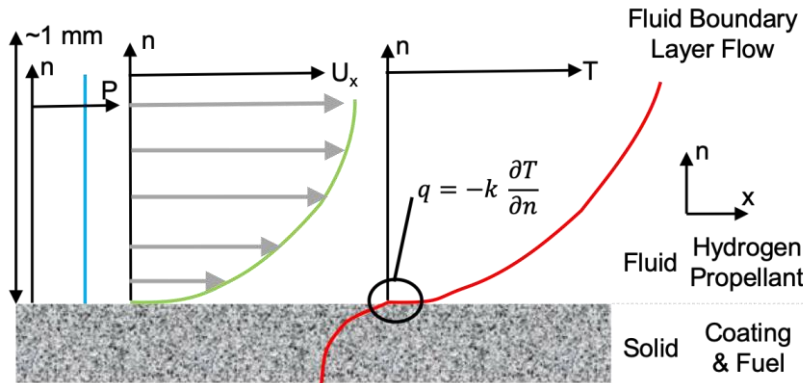


Figure 4: Heat transfer from solid to fluid depends on calculating the slope $\frac{\partial T}{\partial n}$ normal to the wall (circle) through a boundary layer—much harder than calculating the surface pressure, P , which is constant through a boundary layer.

1. Fluid / Solid Heat Transfer: Heat Transfer Correlations

Heat transfer correlations are a common method of calculating this local heat transfer (Figure 4). Equation (4) gives the SNRE standard formula [12, pp. 138, Vol 2], and there are a number of similar correlations [13].

It is helpful to understanding the origin of heat transfer correlations, like Eq. (4). The underlying idea is a similarity solution: scaling the non-dimensionalized Navier-Stokes equations. In this form, the momentum equations have only *one parameter*: Reynolds number, Re . Adding the heat equation adds

another parameter: Prandtl number, Pr . For two different problems (say flow in two different pipes, different radii, fluids, temperatures, pressures), if you match these two numbers (in similar geometry), the solutions are the same—

heat flow too². If experiments measure heat flux, q , over many values of Re and Pr , then q is a function of Re and Pr . Fitting this experimental data [14] will reveal the exponents and coefficient in Eq. (4). Note that the experimental data [14] is hydrogen and helium in a tube at NTP temperatures—custom data from the NERVA/Rover program. Note Eq. (4) is very similar to the Dittus-Boelter equation; exponents and coefficients are very different for other geometries like flat plate heat transfer.

$$q = 0.023 \frac{k_b}{D_b} Re_b^{0.8} Pr_b^{0.4} \left(\frac{T_w}{T_b} \right)^{\left[-0.57 - \frac{1.59}{D_b} \right]} \quad (4)$$

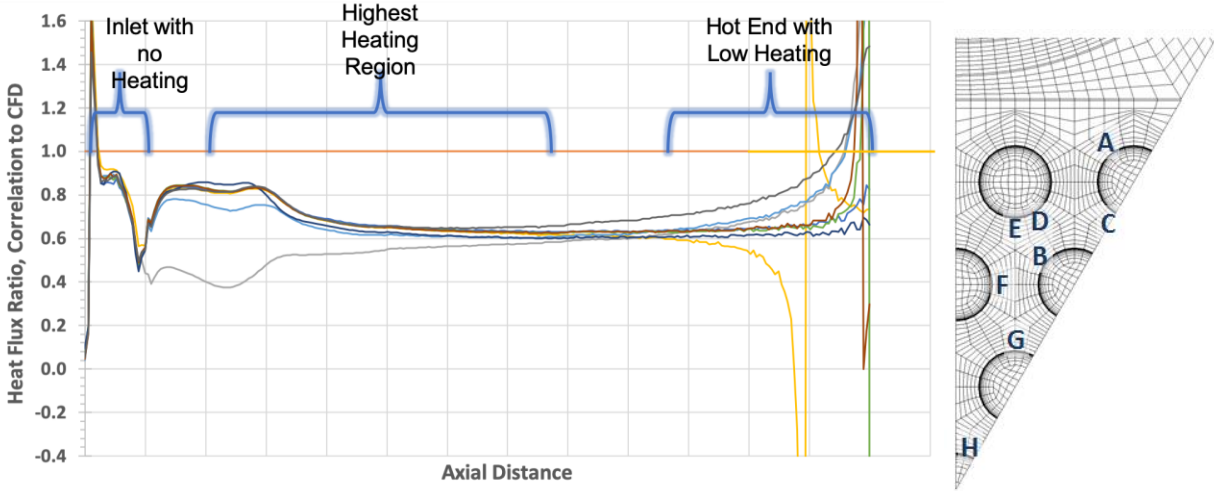


Figure 5: Comparison (left) between heat transfer correlations and CFD [6] by plotting the heat flux, q , ratio,

2. Fluid / Solid Heat Transfer: Validation

Comparison of CFD and the heat transfer correlation Eq. (4) is a strong validation—these starkly independent methods should make similar predictions. Figure 5 graphs the ratio of heat fluxes, q , given by correlation, Eq. (4), and numerical simulation [6] axially along multiple wall locations. Figure 5 suggests general agreement to ~25%, with CFD predicting more heat transfer than the correlation.

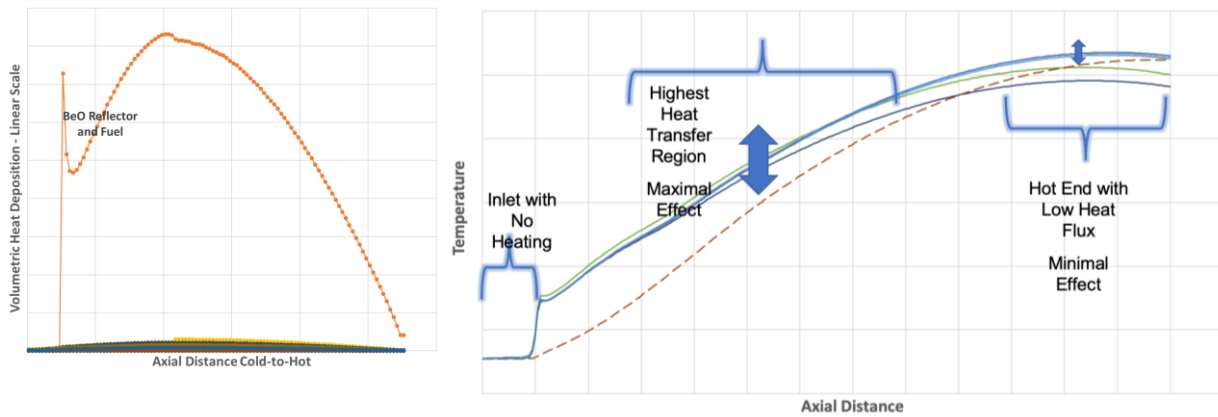


Figure 6: Peak heat deposition (left) occurs mid fuel element. Over/under predictions of solid/fluid heat flux may decrease/increase the wall and fuel temperature.

² There is fine print. Typically, the pipe flow scaled solution is fully developed flow—~20 diameters from an inlet—otherwise it is not truly a scaled solution, only an approximation. If flow accelerates due to high heating and expansion, is it still a scaled solution?

A rule of thumb in CFD is that surface pressure (lift and drag) can be predicted to within 1%, but heat transfer within 10% is doing well. The operational conclusion is agreement to 25% for a difficult calculation, while looking for a more satisfactory resolution.

What are the consequences of inaccurate fluid/solid heat flux predictions from CFD? It could be worse. Heat is conserved numerically, so all heat is transferred to the fluid and exits at the fluid outlet boundary. However, wall and fuel temperatures (Figure 6) are likely over/under predicted, particularly in *high* heat flux locations and *not likely* where the fuel is hottest. Where fuel temperatures are hottest—at the hot end with low nuclear heat deposition—heat flux is low, and temperatures are dominated by the propellant temperature.

3. Coolant Channel Pressure Drop Verification

Coolant channel pressure drop is traditionally predicted with Eq. (5); here the first RHS term. The Fanning friction factor, f_{turb} , is given by a correlation Eq. (6), and was fitted [15] so that 90% of experimental data falls within $\pm 10\%$.

$$\Delta P = -\frac{1}{2}\Delta\overline{\rho U^2} - f_{turb} \left(\frac{1}{2}\overline{\rho U^2}\right) \frac{2\Delta z}{D_b} \quad (5)$$

$$f_{turb} = \frac{\tau_w}{\frac{1}{2}\rho U^2} = \left(0.0014 + \frac{0.125}{Re^{0.32}}\right) \left(\frac{T_b}{T_w}\right)^{1/2} \quad (6)$$

A comparison between this correlation and CFD results is not yet complete.

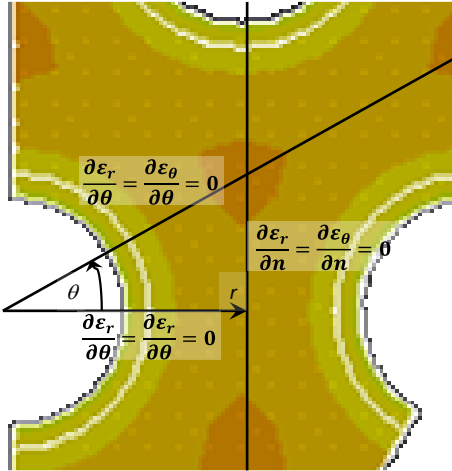


Figure 7: Boundary conditions for stress-strain equations. Hexagonal symmetry is ensured by the condition $\frac{\partial \epsilon_r}{\partial \theta} = \frac{\partial \epsilon_\theta}{\partial \theta} = 0$ on the two radial lines. Currently, the condition $\frac{\partial \epsilon_r}{\partial n} = \frac{\partial \epsilon_\theta}{\partial n} = 0$ is not satisfied.

C. Stress and Strain Simulations in Fuel Elements

For NTP fuel and fuel elements, large stresses accompany high nuclear heat deposition, large temperature ranges and gradients. Also, coatings (coolant channels and exterior) introduce CTE mismatch stresses. Russian NTP designs (no coatings) also emphasize the relevance of thermal stresses [2, p. 306] and there is considerable Russian research [16].

Multidisciplinary simulations [4] capture these stresses, and closed-form solutions can *almost* validate them; yet, these solutions do provide valuable insights.

1. Closed-Form Stress-Strain Solutions for Fuel

Timoshenko and Goodier [17, pp. 481, 443] give a closed-form solution, Eq. (7), for stress/strain equations (plane strain) with arbitrary temperature distributions in polar coordinates. Figure 7 shows the intended domain and boundary conditions³.

$$\psi(r, \theta) = \psi_0(r) + \sum_{j=1}^{\infty} \psi_j(r) \cos 6j\theta \quad (7-a)$$

$$u = \frac{\partial \psi}{\partial r}, \quad v = \frac{1}{r} \frac{\partial \psi}{\partial \theta}, \quad (7-b, -c)$$

$$\epsilon_r = \frac{\partial u}{\partial r}, \quad \epsilon_\theta = \frac{u}{r} + \frac{1}{r} \frac{\partial v}{\partial \theta} \quad (7-d, -e)$$

The radial solution, $\psi_0(r)$, gives the dominant radially dependent stresses of Eq. (8), [17, p. 444],

$$\sigma_r(r) = -\frac{\alpha E}{1-\nu} \frac{1}{r^2} \int_{r_0}^r (T(r) - T_{SF}) r dr + \frac{E}{1+\nu} \left(\frac{C_1}{1-2\nu} - C_2 \frac{1}{r^2} \right) \quad (8-a)$$

$$\sigma_\theta(r) = \frac{\alpha E}{1-\nu} \frac{1}{r^2} \int_{r_0}^r (T(r) - T_{SF}) r dr + \frac{E}{1+\nu} \left(\frac{C_1}{1-2\nu} + C_2 \frac{1}{r^2} \right) - \frac{\alpha E(T-T_{SF})}{1-\nu} \quad (8-b)$$

$$\sigma_z(r) = -\frac{\alpha E(T-T_{SF})}{1-\nu} + \frac{2\nu E C_1}{(1+\nu)(1-2\nu)} + C_3 \quad (8-c)$$

³ Currently, these solutions satisfy all boundary conditions but one, as explained in Figure 7. Applicable remote from axial ends.

based on the temperature, $T(r)$, given by the radial component of Eq. (3). The constants C_1, C_2, C_3 must satisfy boundary conditions. The $r - \theta$ solutions, $\psi_j(r) \cos 6j\theta$, are given by Eq. (9).

$$\psi_j(r) = -\frac{1+\nu}{1-\nu} \frac{\alpha}{12j} \left[r^{6j} \int_r^{r_1} T_j(\rho) \rho^{1-6j} d\rho + r^{-6j} \int_{r_0}^r T_j(\rho) \rho^{1+6j} d\rho \right] \quad (9)$$

where $T_j(r)$ are the radial terms in Eq. (3-b); ρ is a dummy integration variable. These functions are polynomials in radial distance, r . Note that the $\cos 6j\theta$ term ensures hexagonal symmetry.

A factor which aids validation and analysis is linearity of the stress-strain equations. In the linear elastic region, $\varepsilon_r - \alpha(T - T_{SF}) = \frac{1}{E}[\sigma_r - \nu(\sigma_\theta + \sigma_z)]$ (similarly for $\varepsilon_\theta, \varepsilon_z$; E, ν, α constant), solutions can be added. Hence, different stresses—including thermal and CTE mismatch stresses—can each be analyzed and compared in isolation, then added together for the net stress. For example and comparison, Roark [18, p. 376] gives, for a thin cylindrical shell, the thermal stress term $\frac{\alpha ET}{1-\nu}$ balanced between $\sigma_\theta = \sigma_z = \frac{T_1 - T_0}{2} \frac{\alpha E}{1-\nu}$ at inner and outer radii, tension and compression respectively for $T_1 > T_0$.

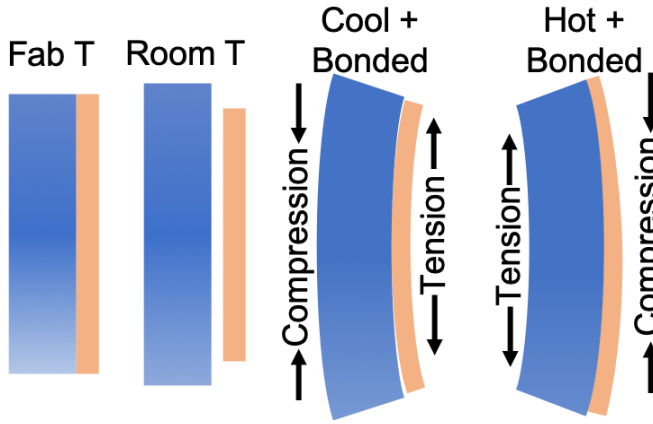


Figure 8: CTE mismatch stresses are a dominant fuel element stress, and can cause coating failure [1]. Tension and compression depend on $\alpha_{fuel}, \alpha_{coating}$, fabrication temperature.

2. CTE Mismatch Stress

When different materials are bonded, and temperature differs from the fabrication temperature, the result is thermal expansion differences and CTE mismatch stresses (Figure 8). Since they occur at the fuel/coating interface (and coating is generally weaker), they are more likely to cause coating fracture and failure. Depending on coating, cracking or blistering is possible.

Equation (8) can accommodate CTE mismatch stresses. In particular, Eq. (8) applies to both coating(s) and fuel individually with, of course, different properties, E, α, ν , and constants, C_i . At interfaces, strains $\varepsilon_r, \varepsilon_\theta$ must be continuous.

3. Stress / Strain Validation Conclusions

Equation (8) is insightful in understanding the importance of design choices, including heat deposition level, coating material and thickness. Currently, one boundary condition (Figure 7)

cannot be satisfied, so validation is out of reach, for now.

D. Neutronic Analysis: Code Verification and Cross Section Validation

Neutronic analysis [6] is done with MCNP6 [19] [20] using ENDFB-VII.1 cross section data [21]. MCNP is used extensively in the United States and the international community, and the MCNP development team takes code verification and validation very seriously [22]. In particular, benchmark problems and results are published [22] [23] [24]. These benchmarks compare against both analytical solutions and experimental results.

1. Cross Section Validation

The nuclear community is focused on nuclear cross-section validation and improvement. Reference [25] explains contemporary issues in U235 cross section data validation.

2. Validation Conclusions

Realistically, errors are more likely to come from the user, rather than the code.

3. NTP Design Relevance: Axial and Radial Nuclear Heat Deposition

MCNP simulations confirm design details including nuclear criticality, fuel loading, drum worth. However, for multidisciplinary simulations, they also generate reactor axial (Figure 6 (left)) and fuel element radial (Figure 9) nuclear heat deposition profiles. Axial profiles are scaled to the reactor design power, and become the Q term in the thermal equation, Eq. (2).

With ~20% of the fissionable U-235 atoms of HEU, LEU designs must increase fission probabilities to achieve criticality. Using low absorption materials helps, but the dominant trick is using U-235's higher fission cross section for lower energy, thermal neutrons. Fission probability increases by a factor of $O(10)$ as neutron energies drop from epithermal to thermal. Practically, more moderator elements are added to the reactor, compared with an epithermal reactor like the SNRE [4] [12].

4. Inter-Element Heating

An important design issue is non-uniform, radial heating of fuel elements (Figure 9), or inter-element heating [26, p. 529]. The thermal neutrons that return to fuel elements—after losing fission energy to collisions in the moderator—preferentially fission near the edges of fuel elements. This non-uniform heat deposition is apparent in Figure 9.

Inter-element heating is important for high performance of NTP engines. In a rocket, performance (specific impulse, I_{sp}) requires the highest possible mean outlet temperatures. With maximum temperature limited by fuel materials, the hottest channel (highest PPF) becomes the limiter, and broad heat deposition variations impede performance.

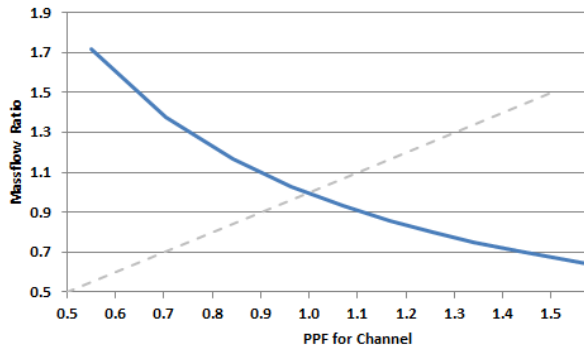


Figure 10: The Rayleigh equation (10) compares coolant tubes with different heat deposition or PPF —all tubes are at a common pressure ratio. ‘Hot’ tubes are starved of coolant, while ‘Cold’ tubes are over-supplied with coolant. The ideal response is shown by the dashed line.

5. A Neutronic Model for Inter-Element Heating

There is a helpful model of inter-element heating; it provides both design guidance and code validation. From the definition of a nuclear cross section, σ , [26, p. 20], the interaction of particles with target particles is given by

$$\sigma N_a dx = -\frac{dI}{I} \quad (12-a)$$

For a beam of intensity I_0 incident on a material (Figure 11), the solution is,

$$I(x) = I_0 e^{-\sigma N_a x}, \quad x \geq 0 \quad (12-b)$$

The material properties are cross section, σ , and number density of target particles, N_a .

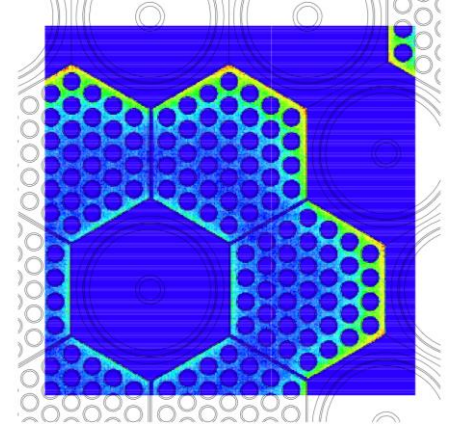


Figure 9: TMESH/MCNP plot of power density near reactor's central axis. Results are qualitative; linear color scale is a factor of ~3, extreme values are cutoff—to blue.

There is also a design challenge for fluid dynamics. For a common pressure drop across all coolant channels, the ones draining different amounts of heat have very different mass flows and outlet temperatures. In fact, channels with more heating are starved for coolant, while tubes with less heat are flooded with coolant. Analytically, Rayleigh flow [27] is a very good model, Eq. (10), namely, a constant area duct, with heat addition, and frictionless flow. Figure 10 shows Eq. (10) solutions for a constant pressure drop and a range of channel $PPFs$. Further, it shows that high PPF channels are starved for coolant flow—the ideal response curve has a slope of opposite sign.

$$\frac{P_{out}}{P_{in}} = \frac{1+\gamma}{1+\gamma} \frac{M_{in}^2}{M_{out}^2} \quad \frac{T_{out}}{T_{in}} = \left[\frac{M_{out}}{M_{in}} \frac{1+\gamma}{1+\gamma} \frac{M_{in}^2}{M_{out}^2} \right]^2 \quad (10)$$

$$PPF_{chan} = \frac{\int_{chan} Q dVol}{\int_{avg chan} Q dVol} = \frac{(T_{out}-T_{in})_{chan} M_{in}}{(T_{out}-T_{in})_{avg} M_{in}} \quad (11)$$

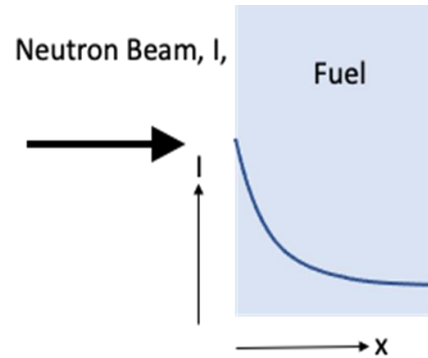


Figure 11: Fission distribution due to neutrons incident on a fuel face.

Importantly, Eq. (12-b) includes a characteristic length, $\frac{1}{\sigma N_a}$. As the particle beam enters and transits the material, 63% of incident particles will interact from surface to depth $\frac{1}{\sigma N_a}$; before two depths, $\frac{2}{\sigma N_a}$, 86% of incident particles will interact. In a reactor, the particles of interest are neutrons, and their flux is not normal to the fuel's surface; if neutron direction is a uniform random distribution, the heating or interaction depth, D_I , is slightly less.

$$D_I = \frac{4}{\pi^2} \frac{1}{\sigma N_a} \quad (13)$$

This nuclear cross section model describes several interactions between neutrons and atoms: elastic σ_e and inelastic scattering, including absorption cross sections: fission, σ_f , and radiative capture σ_γ .

For inter-element heating, fission is the appropriate particle interaction. Of the fission heat released, 83% is released within μm of the fission site; the balance is more uniformly distributed. Equation (13) uses the U-235 fission cross section, σ_f , and number density of U-235 target nuclei, N_a . These two parameters can be determined from MCNP and input data. The fission cross section, σ_f , depends on the incident neutron's energy, so a range of values of interaction depth, D_I , will result.

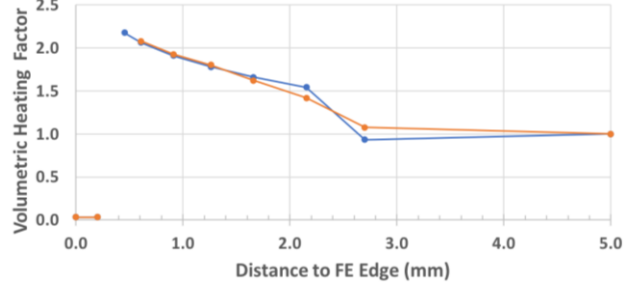


Figure 12: Local *PPF* near fuel element (FE) edge, based on MCNP calculations for an alternate reactor design. Calculated from MCNP tallies of hexagonal shells of varying thickness on FE edge. Equation (13) predicts 1.1 mm for 0.025 eV neutrons and 6.0 mm at 0.625 eV.

Reactor	Nuclei Density, N_a	Predicted Heating Depth, D_I (mm)		Neutron Fission Spectrum (%)		
	(atom/cc)	@ 0.025 eV	@ 0.625 eV	<0.0625 eV	0.625 < 100 keV	> 100 keV
SNRE	1.14E+21	6.7	35.5	39.2	54.1	6.6
Alt Design	6.76E+21	1.1	6.0	59.8	31.6	8.6

Table 1: Predictions of interaction or heating depth, D_I , using Eq. (13) for fuel elements of two reactors. Given the SNRE's flat-to-flat dimension of 19 mm and the reactor's neutron spectrum, the heating depth is as large or larger than the fuel element dimension. This confirms the narrow distribution of channel *PPF* shown in Figure 13.

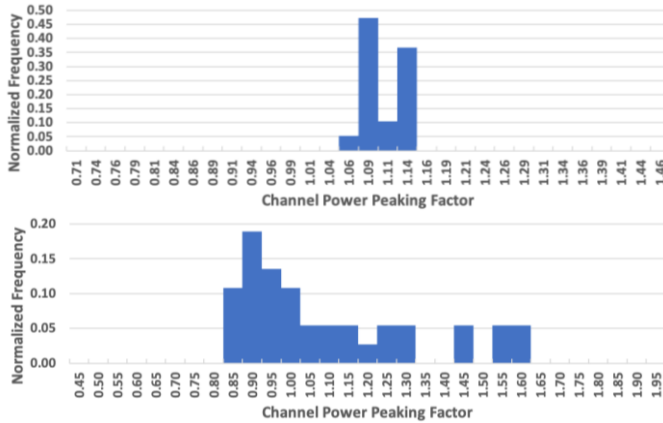


Figure 13: Distribution of *PPF* for channels in a single fuel element in each of two designs. The upper distribution is for the SNRE [12], while the lower distribution is for the alternate design. The channel tally is heat deposition in a hexagonal region surrounding each coolant channel.

6. Validating the Neutronics of Inter-Element Heating

Comparison of this model for heating depth, D_I and MCNP simulations is a valuable validation, which also provides design insights. Figure 12 shows the measured *PPF* profile near the fuel element edge in a LEU cermet reactor which will be denoted as the alternate reactor design. The heating depth of ~ 2 mm is very close to the thickness predicted by Eq. (13) as shown in Table 1. The measurement of Figure 12 exploits MCNP tallies in a variable thickness shell on the outer edge of each fuel element. Consequently, it is a highly averaged value, that would not capture the extremes apparent in Figure 9.

Table 1 compares interaction or heating depth, D_I , predictions of Eq. (13) for two reactors with different fuel types: the HEU SNRE reactor [12] and an LEU alternate reactor design—a typical cermet reactor. The listed

neutron fission spectrum shows the SNRE is an epithermal reactor, while the alternate design is thermal. This shift to lower neutron energies will increase σ_f in Eq. (13) and accounts for some of the reduced heating depth, D_I .

However, a significant factor—at least five—in the D_I differences is the U-235 nuclei density, N_a , which is six times higher here. Cermet NTP reactors typically require five to ten times more U-235 mass to reach criticality.

The SNRE reactor has a flat-to-flat dimension of 19 mm. With the large predicted heating depth, severe inter-element heating would *not* be expected in this reactor. While in the alternate cermet design it would be expected. Figure 13 shows measurements which confirm this prediction. The MCNP measurements show typical *PPF* distributions for channels in single fuel element from each of the two reactors. In particular, tallies measure nuclear heat deposition in hexagonal regions surrounding each coolant channel. The narrow SNRE distribution indicates much more uniform heating across the fuel element, while the broad distribution of the alternate reactor indicates the non-uniform heating of inter-element heating, as in Figure 9.

E. Chemical Species Diffusion and Fuel Element Mass Loss

As fuel temperatures increase, specie diffusion (permeation) rates through fuel and coating increase exponentially, in particular, an Arrhenius form, $\exp\left(\frac{-E_a}{RT}\right)$. Figure 14, from Reference [28], shows measured rates. This diffusion is mass loss, which is isolated to the fuel elements' hot end, but, in some cases, it is a significant issue in reactor life [12, pp. 87, 111 Vol 3].

Figure 15 shows how chemical species diffuse through fuel and cladding, and convect/diffuse from the wall into the hydrogen of the coolant channel, where the hydrogen flow convects it downstream.

Transfer of specie atoms at the wall is a balance between surface vaporization and condensation—atoms escaping from and returning to the solid surface. Saturated vapor pressure is the specie partial pressure where a balanced equilibrium occurs with no convection. Clearly, predicting specie concentration through the boundary layer—in particular, within a mean free path of the wall—is important to predicting this equilibrium.

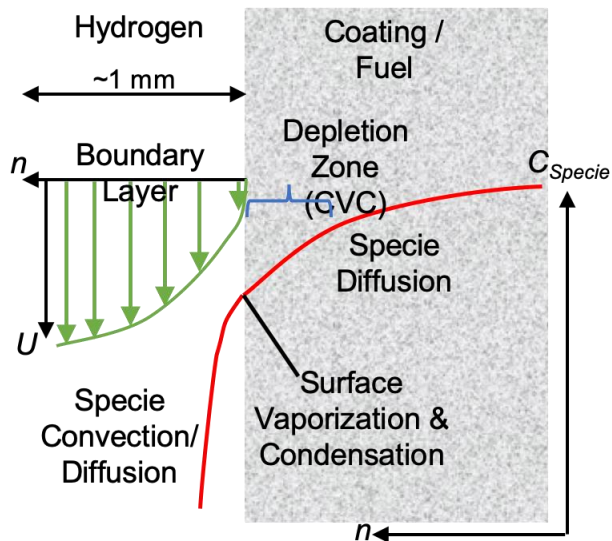


Figure 15: Species diffusion through fuel and coating couples with convection/diffusion in the coolant channel. Mass loss results at high temperatures. Hydrogen can diffuse into hot fuel.

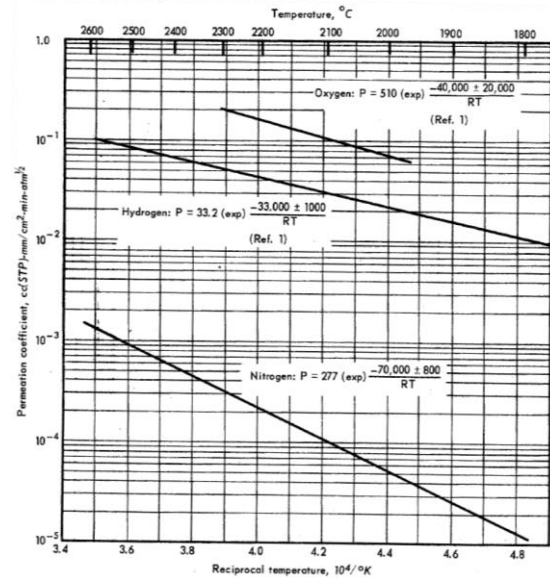


Figure 14: Comparison of permeation coefficients for nitrogen, hydrogen, and oxygen through arc-cast tungsten. Diagram from [28]. Ref 1 refers to [32].

In the Rover/NERVA program, mass loss due to species diffusion was carefully studied. Storms [29] suggested that mass loss leads to an erosion region (CVC) near the coolant channel surface. Mass loss slows as the rate limiting process becomes specie diffusion from deeper within the fuel.

For both carbide and cermet fuels, coating or cladding on coolant channel surface can reduce this process by either reducing the diffusion rate with a coating, or by displacing the erosion region. Cermet fuel testing [30] showed that cladding reduced mass loss by an order of magnitude. For these fuels, cladding is a requirement. Some fuels have less of a need for coatings, and Russian fuel is apparently not clad [2, pp. 306, 316]. Eliminating CTE mismatch stresses is an advantage.

V. Conclusion

Validation of NTP simulation results is an important part of numerical simulation and prediction of NTP performance. There is strong validation of thermal solutions, and moderate validation of fluid and neutronic solutions. Stress / strain solutions need further attention. No significant inconsistencies have been found.

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