A Nonlinear Reactivity Method with Application to Accident-Tolerant Fuels

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Abstract

A nonlinear reactivity model with thermal-hydraulic feedback is presented for analysis of PWR fuel with various cladding materials. The simplified, batch-wise neutronic model requires batch reactivities and migration areas as predetermined functions of burnup, temperature (fuel and coolant), and any design parameters having neutronic significance (e.g., enrichment or cladding composition). Here, such functions are found by using symbolic regression, a unique approach that finds both a functional form and any model coefficients simultaneously. Core thermal-hydraulics are modeled using single-channel, axially-averaged values. The models were implemented in an open-source, Python-based tool, used here to analyze fuel with Zr-based cladding having outer, protective layers of either FeCrAl or SiC, two materials proposed for use in next-generation, accident-tolerant fuel.

Keywords

nonlinear reactivity model, nodal parameter model, coupled physics, accident-tolerant fuel, educational tools

I. INTRODUCTION

Advanced cladding materials are of increasing interest for improved safety under a variety of planned and unplanned operating conditions.¹ Although high-resolution, coupled-physics models of these materials will be required before their adoption, a variety of parametric studies can be performed using simple, coupled-physics models to understand the gross impacts of a material on various reactor characteristics. This paper presents a coupled neutronics and thermal-hydraulics tool² based on a nonlinear reactivity model for analysis of PWR fuel and the results of its application to fuels with advanced SiC and FeCrAl cladding. While a full study would necessarily require inclusion of structural mechanics, the models presented here consider only neutronics and thermal-hydraulics. With certain extensions, the models described can easily be extended to other applications. Similar studies have recently been conducted that focused primarily on the neutronics³ and structural mechanics⁴ of FeCrAl and/or SiC cladding. Although the results presented herein for illustration are consistent with those previously reported,^{3,4} the methods developed here provide a simple way to incorporate core-level thermal-hydraulics into the neutronic analysis.

The rest of this paper is organized as follows. Section II presents a nonlinear reactivity method that provides batch-wise neutronic detail based on precomputed parameters from lattice-physics calculations. These temperature-dependent parameters, described in Section III, provide direct coupling to a simple thermal-hydraulics model, presented in Section IV. Section IV-C discusses the simple scheme used to couple the models, while Section V provides some illustrative results that demonstrate the potential utility of such simple models.

II. NEUTRONIC MODEL

A neutronic model that can capture core-level effects would be ideal for the analysis of cladding materials. Such models can provide assembly powers and, at

least approximately, pin powers. Unfortunately, even the simplest of these models, e.g., the classical FLARE nodal method,⁵ require an explicit geometry and other detail that would preclude their use in parametric studies.

As an alternative, a simple model is proposed, which is based in part on the linear reactivity model (LRM).⁶ The basic premise of the model is that a core is comprised of one or more “batches” of like fuel, and the neutronic properties of these batches can be found by simple approximations based essentially on average values. The output of this model includes cycle-averaged batch powers and burnups, which can be coupled to a thermal-hydraulics model. LRM has long been used for various parametric studies, and an LRM-like method was recently used to study the impact of FeCrAl cladding.³

A. Linear Reactivity Model

The linear reactivity model is based on the assumptions that a core is composed of one or more batches of like fuel and that the reactivity of the fuel varies linearly with burnup,⁶ i.e.,

$$\rho(B) = \rho_0 - AB, \quad (1)$$

where ρ is reactivity, B is burnup (usually in GWd/MTU), and ρ_0 and A are constants. Reactivity can also be defined as

$$\rho = \frac{k - 1}{k}, \quad (2)$$

where k is the multiplication factor, i.e., the ratio of gains from fissions to losses by absorption and, if applicable, leakage.

In the simplest LRM approximation, the core reactivity is taken to be the arithmetic average of the various fuel reactivities. Suppose the core is composed of N batches of equal size; for a typical PWR, $N \approx 3$. The core reactivity is then

taken to be

$$\bar{\rho} = \frac{1}{N} \sum_{i=1}^N \rho_i, \quad (3)$$

where ρ_i is the reactivity of the i th batch. Usually, the infinite multiplication factor k_∞ is used, so ρ_i represents the reactivity of an infinite reactor composed of the i th-batch fuel. To include losses due to leakage, the core reactivity can be redefined as

$$\bar{\rho} = \frac{1}{N} \sum_{i=1}^N \rho_i - \rho_L, \quad (4)$$

where ρ_L is the reactivity penalty due to leakage and is typically close to 4%.

The classical use of LRM is to estimate critical cycle lengths for various batching schemes. Consider an N -batch core at the end of cycle (EOC). The EOC reactivity of each batch is

$$\begin{aligned} \rho_1 &= \rho_0 - AB_c \\ \rho_2 &= \rho_0 - 2AB_c \\ &\vdots \\ \rho_N &= \rho_0 - NAB_c, \end{aligned} \quad (5)$$

where B_c is the cycle length, i.e., the (average) burnup each batch accumulates between fuel reloads. The corresponding core average reactivity is

$$\bar{\rho} = \frac{1}{N} \left(N\rho_0 - \frac{N(N+1)}{2} AB_c \right) = \rho_0 - \frac{N+1}{2} AB_c. \quad (6)$$

If the EOC reactivity is assumed to be zero, then

$$B_c = \frac{2\rho_0}{(N+1)A} = \frac{2B_s}{N+1}, \quad (7)$$

where $B_s = \rho_0/A$ is the single-batch cycle burnup. The batch burnup after N

cycles, often called the “discharge burnup,” is

$$B_d = NB_c = \frac{2NB_s}{N+1}. \quad (8)$$

A key observation is that by using multiple fuel batches, one can extract more energy from the fuel than if the reactor were fueled with just one batch. In the extreme of continuous fuel reloading, $N \rightarrow \infty$, and the resulting discharge burnup is doubled.

B. Nonlinear Reactivity Model

Even though the LRM assumes that ρ varies linearly with burnup, this assumption is unnecessary if numerical techniques are used to analyze fuel configurations. In other words, for N batches, the cycle length B_c can be found by solving the nonlinear equation

$$\frac{1}{N} \sum_{i=1}^N \rho(iB_c) = \rho_L, \quad (9)$$

where leakage is included explicitly. Once B_c is determined, batch-average properties can be evaluated for any burnup $B \in [0, B_c]$.

Of course, the reactivity ρ_i of the i th batch is a function not only of burnup but also of the cladding material (in the present study, a protective coating thickness), fuel and coolant temperatures, and boron concentration. Equation (9) (like Eq. (6)) is based on the implicit assumption that batch powers are equal. At any point during the cycle, the reactivity should be positive, and a corresponding critical boron concentration can be found by nonlinear iteration for any burnup of interest.

Nonlinear reactivity models (NRMs) have long been studied, usually with the assumption that ρ still has a reasonably tractable dependence on B , e.g., a polynomial.⁶ Such a model based on equal-power sharing was used to accelerate scoping studies of fluoride salt-cooled reactors.⁷ In addition, a NRM based on a simple linear-power sharing model was used to study pebble-bed, gas-cooled

reactors.⁸

1) *Unequal Power Sharing*: Although the model described above is adequate for some analyses, in reality the power of various batches should depend on the burnup. For instance, fresh fuel (if unpoisoned) should burn “hotter” than older, burned fuel, as it has more fissile material. In the following sections, a simple way to account for this observation is developed following the approach of Ref. 6.

Consider a core divided into N regions (e.g., assemblies or batches). The reactivity of the i th region is

$$\rho_i = \frac{F_i - A_i}{F_i}, \quad (10)$$

where F_i and A_i are the region-wise neutron production and absorption rates, respectively. The reactivity of the whole core is

$$\rho = \frac{\sum_{i=1}^N (F_i - A_i)}{\sum_{i=1}^N F_i} = \frac{\sum_{i=1}^N F_i \rho_i}{\sum_{i=1}^N F_i}. \quad (11)$$

To a very good approximation, the region-wise neutron production rates F_i can be replaced by the region-wise powers q_i , so that*

$$\rho \approx \frac{\sum_{i=1}^N q_i \rho_i}{\sum_{i=1}^N q_i} = \frac{\sum_{i=1}^N q_i \rho_i}{Q}, \quad (12)$$

where Q is the reactor power. Let

$$f_i = \frac{q_i}{Q} \quad (13)$$

denote the fraction of power generated in the i th region, subject to

$$\sum_{i=1}^N f_i = 1. \quad (14)$$

*Note that $F = \nu \Sigma_f \phi$ while $q = \kappa \Sigma_f \phi$, where ϕ is the flux, Σ_f is the fission cross section, ν is the average number of neutrons produced per fission, and κ is the average energy released per fission. Over a wide range of burnups, the ratio κ/ν is relatively constant, which implies that $F \propto q$ is a good approximation.

Note that f_i is a function of burnup within a cycle because the relative assembly powers change with burnup. With substitution of Eq. (13) into Eq. (12), the core reactivity (neglecting leakage) is

$$\rho = \sum_{i=1}^N f_i \rho_i. \quad (15)$$

2) *Determination of the Cycle Length:* Let the EOC burnup of the i th batch be denoted by B_i . This implies that $B_N = B_d$, i.e., the discharge burnup. Finally, let $B_0 = 0$. Then, the burnup accumulated by region i during the cycle is given by

$$B_i - B_{i-1} = \Delta B_i = B_c \times \frac{\bar{f}_i}{\bar{f}}, \quad (16)$$

where

$$\bar{f}_i = \frac{\int_{B_{i-1}}^{B_i} f_i(B) dB}{\Delta B_i}, \quad (17)$$

$$\bar{f} = \frac{1}{N}, \quad (18)$$

and the ratio $\bar{f}_i/\bar{f}$ is the cycle-averaged, region-wise, power peaking factor.

From Eqs. (16)–(18), the EOC reactivity of region i is found to be

$$\begin{aligned} B_i &= B_{i-1} + \Delta B_i \\ &= B_{i-2} + \Delta B_{i-1} + \Delta B_i \\ &\vdots \\ &= B_0 + \Delta B_1 + \Delta B_2 + \dots + \Delta B_{i-1} + \Delta B_i \\ &= \sum_{j=1}^i \Delta B_j \\ &= N B_c \sum_{j=1}^i \bar{f}_j. \end{aligned} \quad (19)$$

Because $B_N = B_d = NB_c$, the region- i burnup is

$$B_i = B_N \sum_{j=1}^i \bar{f}_j, \quad (20)$$

and for $i = N$, this result indicates that

$$\sum_{j=1}^i \bar{f}_j = 1, \quad (21)$$

which is consistent with Eq. (14).

For a fixed leakage reactivity penalty ρ_L , the power-weighted, core-averaged, EOC reactivity must satisfy

$$\bar{\rho} = \sum_{i=1}^N f(B_i) \rho(B_i) = \rho_L. \quad (22)$$

Together, Eqs. (17), (20), and (22) define a nonlinear system of equations for $\mathbf{B} = [B_1, B_2, \dots, B_N]$, i.e.,

$$\mathbf{r}(\mathbf{B}) \equiv \begin{pmatrix} B_1 - B_N \bar{f}_1 \\ B_2 - B_N (\bar{f}_1 + \bar{f}_2) \\ \dots \\ B_{N-1} - B_N (\bar{f}_1 + \bar{f}_2 + \dots + \bar{f}_{N-1}) \\ \sum_{i=1}^N f(B_i) \rho(B_i) - \rho_L \end{pmatrix} = \mathbf{0}, \quad (23)$$

which can be solved for the B_i by an appropriate numerical scheme, e.g., Newton's method.

3) Estimation of Power Fractions: All that remains to complete the model is to define the region-wise power fractions f_i in some way. The simplest approach is to assume values based on the results from a whole-core analysis. Such an approach was used in recent work on the assessment of FeCrAl cladding materials.³ Here, a way to estimate these power fractions directly from the neutronic properties of

the batches is developed following the presentation of Ref. 6.

Consider the two-group diffusion equations:

$$\begin{aligned} -D_1 \nabla^2 \phi_1(\mathbf{r}) + \Sigma_{r1}(\mathbf{r}) \phi_1(\mathbf{r}) &= \frac{1}{k} [\nu \Sigma_{f1}(\mathbf{r}) \phi_1(\mathbf{r}) + \nu \Sigma_{f2}(\mathbf{r}) \phi_2(\mathbf{r})] \\ -D_2 \nabla^2 \phi_2(\mathbf{r}) + \Sigma_{a2}(\mathbf{r}) \phi_2(\mathbf{r}) &= \Sigma_{s12}(\mathbf{r}) \phi_1(\mathbf{r}), \end{aligned} \quad (24)$$

where upscatter is neglected, fission neutrons are limited to the fast group, and $\Sigma_{r1} = \Sigma_{a1} + \Sigma_{s12}$ is the fast removal cross section. The remaining notation is standard.⁹

In the two-group approximation, the core reactivity is given by

$$\rho = \frac{k - 1}{k} = \frac{[\nu \Sigma_{f1} \phi_1 + \nu \Sigma_{f2} \phi_2] - [\Sigma_{a1} \phi_1 + \Sigma_{a2} \phi_2]}{\nu \Sigma_{f1} \phi_1 + \nu \Sigma_{f2} \phi_2}. \quad (25)$$

If thermal leakage is assumed to be negligible, i.e., $D_2 \nabla^2 \phi_2 \ll \Sigma_{a1} \phi_2$, then

$$\phi_2 = \frac{\Sigma_{12} \phi_1}{\Sigma_{a2}}, \quad (26)$$

which is sometimes referred to as the “one-and-a-half group” approximation.⁹ By combining Eqs. (24), (26), and, (25), one has

$$\nabla^2 \phi_1 + \frac{1}{M^2} \left(\frac{\rho}{1 - \rho} \right) \phi_1 = 0, \quad (27)$$

where the migration area M^2 is defined as

$$M^2 = \frac{D_1}{\Sigma_{s12} + \Sigma_{a1}}. \quad (28)$$

The power density is related to the fast flux by

$$q = \kappa \left(\Sigma_{f1} + \frac{\Sigma_{f2} \Sigma_{12}}{\Sigma_{a2}} \right) \phi_1, \quad (29)$$

and, hence, Eq. (27) can be rewritten as

$$\nabla^2 [q(1 - \rho)] + \frac{\rho q}{M^2} = 0. \quad (30)$$

However, if this equation is discretized over assemblies (or sub-assemblies), the local q_i for node i can be cast instead as the power fraction f_i times the total power Q . Because Q is constant, it may be eliminated, leading to

$$\nabla^2[f_i(1 - \rho_i)] + \frac{\rho_i f_i}{M_i^2} = 0. \quad (31)$$

Of course, the direct solution of this equation (via finite differences) would be about as difficult as solving the FLARE or similar nodal-diffusion equations. Moreover, such a model would require an explicit fuel map that requires input that would not likely exist in parametric scoping studies.

Here, a simpler approach is adopted. The Laplacian can be approximated based on the difference of the node i value with neighboring values, but to simplify the analysis, the neighbors will be taken to have core-averaged values. Consider the 1-D case, with node i surrounded by nodes $i - 1$ and $i + 1$. The Laplacian can be approximated by

$$\begin{aligned} \nabla^2[f_i(1 - \rho_i)] \\ \approx \frac{f_{i+1}(1 - \rho_{i+1}) - 2f_i(1 - \rho_i) + f_{i-1}(1 - \rho_{i-1})}{h^2}, \end{aligned} \quad (32)$$

where h is the width of the node. If the neighbor values, e.g., f_{i+1} and ρ_{i+1} , are core-averaged values, then

$$\frac{\bar{f}(1 - \bar{\rho}) - f_i(1 - \rho_i)}{\frac{1}{2}h^2} + \frac{\rho_i f_i}{M_i^2} = 0, \quad (33)$$

Furthermore, if the core reactivity $\bar{\rho}$ is zero, i.e., the reactor is critical, then

$$\frac{\bar{f} - f_i(1 - \rho_i)}{\frac{1}{2}h^2} + \frac{\rho_i f_i}{M_i^2} = 0. \quad (34)$$

and, hence,

$$f_i = \frac{\bar{f}}{1 - \rho_i \left(1 + \frac{\frac{1}{2}h^2}{M_i^2}\right)} = \frac{\bar{f}}{1 - \theta_i \rho_i} = \frac{1}{N(1 - \theta_i \rho_i)}, \quad (35)$$

where

$$\theta_i = 1 + \frac{\frac{1}{2}h^2}{M_i^2}. \quad (36)$$

It is easy to show the factor of $1/2$ in θ_i changes to $1/4$ for 2-D and $1/6$ for 3-D grids. In all results presented in Section V, a 2-D grid was assumed. Although this model for θ comes directly from a reasonable physical model, in practice, it might be better to adjust θ to match results of more detailed models that include explicit spatial dependence.

Equation (35) is correct only when the core reactivity is zero, i.e., at EOC without a leakage penalty. In any other case, the resulting power fractions, which are functions of burnup, are not guaranteed to satisfy Eq. (14) and, hence, they must be normalized before use. This includes the computation of the region-wise, cycle-averaged values $\bar{f}_i$.

III. NEUTRONIC DATA MODEL

The nonlinear reactivity method presented in Section II depends on the availability of two nodal parameters, ρ and M^2 , which are assumed to be assembly-specific functions of burnup, fuel temperature, coolant temperature, and boron concentration. Both of these (and other) parameters can be computed using standard lattice-physics tools.

Such nodal parameters are typically represented by functions of several historical variables (e.g., the average boron concentration up to an exposure point) and several instantaneous variables (e.g., the boron concentration at an exposure of interest, possibly different from past concentrations). For most production-level analyses, nodal parameters are tabulated for interpolation (e.g., PARCS¹⁰ or SIMULATE¹¹) or approximated by polynomial regression (e.g., NEXUS¹²).

For this work, the TRITON module of SCALE 6.1 was used to compute all nodal parameters. TRITON allows users to produce nodal parameters for baseline

conditions as a function of burnup and for a variety of branch cases (i.e., step perturbations in state parameters such as the fuel temperature).

Let a generic nodal parameter be denoted by p for a specific fuel assembly type. Then

$$p \equiv f(B, T_F, T_C, C_B), \quad (37)$$

where B is the burnup (GWd/MTU), T_F and T_C are the current fuel and coolant temperatures (K), and C_B is the current boron concentration (ppm). Dependence on historical values is neglected. For the present work, the data is also dependent on the thickness of either SiC or FeAlCr, as described below.

To represent these dependencies on state parameters and cladding features, symbolic regression was employed using the Eureqa tool,^{13,14} which appears to be the first use of symbolic regression for the nodal parameter problem. Whereas traditional regression models seek to fit data to a particular functional form with undetermined coefficients, symbolic regression determines the form *and* the values of the coefficients. This process can be very time-consuming, but the results tend to represent data with fewer coefficients and operations, which, in turn, helps users understand their data better by isolating key dependencies. Although this approach might not be useful for production-level analyses, the types of functions found for various parameter types might be useful starting points for advanced (i.e., non-polynomial) regression.

Eureqa was used to provide fits of ρ and M^2 to the data computed by TRITON. Two basic approaches were followed. The first applied Eureqa directly to fits having the form of Eq. (37). The second applied Eureqa to the approximate form

$$\begin{aligned} p \equiv & p_o(B) + \frac{\partial p}{\partial T_F}(T_F - T_{Fo}) \\ & + \frac{\partial p}{\partial T_C}(T_C - T_{Co}) + \frac{\partial p}{\partial C_B}(C_B - C_{Bo}), \end{aligned} \quad (38)$$

where $p_o(B)$ is a function of all non-state variables (e.g., burnup and cladding

attributes) at baseline conditions, $\partial p/\partial x$ is the partial derivative of p with respect to the state variable x at nominal conditions, and x_o is the baseline value of x . For both approaches, the objective was to minimize the average, absolute error between the model and data.

Experience with these two approaches suggests strongly that the latter approach based on partial derivatives leads to fits that are more accurate overall but suffer from increased complexity. Because Eureka tends to produce fits with a limited number of terms, subtle dependencies were easily lost when pursuing the first “fit all-at-once” approach. Consequently, all results presented in Section V are based on the second approach.

IV. THERMAL-HYDRAULICS MODEL

The thermal-hydraulic model developed is a simple, single-channel model.¹⁵ Assembly-averaged powers are used to define an axial-averaged, bulk coolant temperature for each assembly. Then, by using a very simple fuel pin model, the average fuel temperature is computed for each assembly. Coupling of the thermal-hydraulic and neutronic models is performed by fixed-point iteration.

A. Bulk Coolant Temperature

If pressure and friction losses are neglected, energy balance along an axial channel with single-phase flow is approximately described by¹⁵

$$\dot{m}c_p \frac{dT_C}{dz} = q'(z), \quad (39)$$

where T_C is the bulk coolant temperature, $\dot{m}$ is the coolant mass-flow rate, c_p is the specific heat capacity, which is assumed to be constant, and q' is the axial linear heat generation rate. Because the nonlinear reactivity method is based on an effectively two-dimensional representation, the z -dependence of q' must be

assumed. Here, that dependence is taken to be

$$q'(z) = q'_o \cos\left(\frac{\pi z}{H + 2\delta H}\right), \quad (40)$$

where q'_o is the axial peak linear heat generation rate, H is the active fuel height, and δH is the extrapolation length at either end of the core. The axial average linear heat generation rate is defined as

$$\begin{aligned} \bar{q}' &= H^{-1} \int_{-H/2}^{H/2} q'(z) dz \\ &= \left(\frac{2q'_o(H + 2\delta)}{\pi H} \right) \sin\left(\frac{\pi H}{2H + 4\delta}\right). \end{aligned} \quad (41)$$

If the assembly power q is known (from the neutronic model) then

$$\begin{aligned} q &= H\bar{q}' \\ &= \left(\frac{2q'_o(H + 2\delta)}{\pi} \right) \sin\left(\frac{\pi}{2H + 4\delta}\right), \end{aligned} \quad (42)$$

from which the axial peak linear heat generation rate is determined to be

$$q'_o = \frac{\pi q}{2(H + 2\delta)} \frac{1}{\sin\left(\frac{\pi}{2H + 4\delta}\right)}. \quad (43)$$

Substitution of Eq. 40 into Eq. 39 and integration of the result over the axial length leads to

$$\begin{aligned} &\dot{m}c_p(T_C(z) - T_{in}) \\ &= \int_{-H/2}^z q'_o \cos\left(\frac{\pi z'}{H + 2\delta H}\right) \\ &= \left[\sin\left(\frac{\pi H}{2H + 4\delta}\right) + \sin\left(\frac{\pi z}{H + 2\delta}\right) \right] \left(\frac{2\delta + H}{\pi} \right). \end{aligned} \quad (44)$$

or

$$T_C(z) = T_{\text{in}} + \left(\frac{2\delta + H}{\pi \dot{m} c_p} \right) \times \left[\sin \left(\frac{\pi H}{2H + 4\delta} \right) + \sin \left(\frac{\pi z}{H + 2\delta} \right) \right], \quad (45)$$

where $T_{\text{in}} \equiv T_C(-H/2)$. It follows that the average coolant temperature (equal here to the mid-plane temperature) is defined as

$$\begin{aligned} \bar{T}_C &= T_{\text{in}} + \left(\frac{q'_o(H + 2\delta)}{\pi \dot{m} c_p} \right) \sin \left(\frac{\pi H}{2H + 4\delta} \right) \\ &= T_{\text{in}} + \frac{\bar{q}' H}{2\dot{m} c_p}, \end{aligned} \quad (46)$$

where

$$\bar{q}' = \left(\frac{2q'_o(H + 2\delta)}{\pi H} \right) \sin \left(\frac{\pi H}{2H + 4\delta} \right). \quad (47)$$

B. Fuel Temperature

To compute the assembly-averaged fuel temperatures, a single, representative fuel pin model is used that assumes constant power and constant coefficients (e.g., thermal conductivity). The radial-averaged fuel pin temperature at a particular axial plane is defined as¹⁵

$$T_F(z) = \frac{q'_{\text{pin}}(z)}{8\pi k_F} + T_{Fo}(z), \quad (48)$$

where $q'_{\text{pin}} = q'/N_p$, N_p is the number of pins in an assembly, k_F is the fuel thermal conductivity, and T_{Fo} is the temperature at the outer surface of the fuel. The total temperature drop across the gas gap, cladding, and between the outer cladding surface and the bulk coolant is¹⁵

$$\begin{aligned} \Delta T(z) &= \frac{q'_{\text{pin}}(z)}{2\pi} \left(\frac{t_g}{r_g k_g} + \frac{\ln(r_{co}/r_{ci})}{k_c} + \frac{1}{r_{co} h} \right) \\ &\equiv \frac{q'_{\text{pin}}(z)}{k_{NF}}, \end{aligned} \quad (49)$$

where t_g is the gap thickness, r_g is the average gap radius, r_{ci} and r_{co} are the inner and outer cladding radii, k_g and k_c are the gap and cladding thermal conductivities, h is the coolant heat transfer coefficient, and k_{NF} is the effective thermal conductivity for all non-fuel components. Given the bulk moderator temperature $T_C(z)$, the radial-averaged fuel temperature reduces to

$$T_F(z) = \frac{q'_{\text{pin}}(z)}{8\pi k_F} + T_C(z) + \Delta T(z), \quad (50)$$

the axial average of which is defined as

$$\bar{T}_F = \bar{T}_C + \bar{q}'_{\text{pin}} \left(\frac{1}{4\pi k_F} + \frac{1}{k_{NF}} \right). \quad (51)$$

Thermal conductivities are generally functions of temperature and, in the case of fuel, burnup. Here, only the axially- and radially-averaged temperatures are used to evaluate conductivities. A straightforward extension to the model would admit radial and axial dependence of the temperature and, hence, conductivities.

C. Coupling Neutronics and Thermal-Hydraulics

Coupling of the nonlinear reactivity and thermal-hydraulics models is straightforward by using a fixed-point iteration. To perform the iteration, various parameters must be defined a priori, including the average assembly thermal power. Because each batch is normalized to single-assembly values, the average batch power is taken to be the average assembly power.

Initial values for the bulk coolant and fuel temperatures for each batch are assumed to be known. With these temperatures, the neutronic properties are evaluated, and the batch-wise cycle burnups and power-peaking factors are computed. The power-peaking factors are in turn provided to the thermal-hydraulics model. Based on these fixed batch-wise powers, new temperatures are computed, and the process repeats until temperatures are converged to within a user-defined tolerance.

For the problems studied, convergence to within 0.01 K was achieved in fewer than 10 iterations.

V. NUMERICAL DEMONSTRATION

Zirconium-based alloys (e.g., Zr-4) are currently used for PWR fuel cladding, but owing to their behavior under accident conditions, alternative, accident-tolerant cladding materials are of interest. Here, two such materials were considered: FeCrAl (21% Cr, 5.8% Al, 0.7% Si, 0.4% Mn, and 0.08% C by mass) and SiC. Both FeCrAl and SiC may offer enhanced damage resistance under accident conditions. However, each cladding has potential disadvantages. For instance, FeCrAl is less neutron transparent than Zr cladding. This means that more neutrons are absorbed in the FeCrAl, thus requiring increased enrichment to compensate for these losses. On the other hand, SiC is more neutron-transparent than Zr, but it is a ceramic and, thus, is more brittle and prone to cracking.¹⁶ As an alternative to single-material, monolithic cladding based on FeCrAl or SiC alone, it has been proposed to use a thin layer of either material on a Zr-based substrate. Here, thicknesses of 100 and 300 microns of either material on top of a Zr-4 substrate were considered. In addition, monolithic (570 micron) cladding of each of the three materials was considered. An assessment of the structural mechanics implications of such layering schemes is beyond the present scope but has been examined elsewhere.¹⁶ All material properties for the cladding materials are consistent with those previously reported.¹⁶

Several numerical examples are presented below using the Python-based, open-source NRM tool available online.² All files to produce the figures in this paper are included in the source code.

TABLE I. ASSEMBLY AND FUEL-PIN DIMENSIONS

Assembly pitch	21.5036 cm
Pin pitch	1.2598 cm
Fuel pellet OR	0.4096 cm
Clad IR	0.4180 cm
Clad OR	0.4750 cm
Guide/instrument tube IR	0.5610 cm
Guide/instrument tube OR	0.6120 cm

Generation of Model Data

The geometries considered are all based on a 17×17 Westinghouse-like design with dimensions and other characteristics drawn from the publicly-available literature and summarized in a publicly-available EPRI report.¹⁷ Fuel-pin dimensions are specified in Table I. All models were set to 4% initial enrichment with specific powers of 38.1 MWd kg^{-1} . Nominal conditions were taken to be 580 K ($\rho = 0.712 \text{ g cm}^{-3}$) for the coolant temperature, 900 K for the fuel temperature, and 900 ppm for the boron concentration. Branch cases consisted of coolant temperatures of 560 K ($\rho = 0.752 \text{ g cm}^{-3}$) and 600 K ($\rho = 0.660 \text{ g cm}^{-3}$), fuel temperatures of 800 K and 1000 K, and boron concentrations of 0 ppm and 1800 ppm.

The cladding temperature was taken to be

$$T_{\text{clad}} = 0.12T_F + 0.88T_C, \quad (52)$$

where T_F and T_C are the fuel and coolant temperatures, respectively.¹⁷ The gas gap was filled with dry air at a density of 0.001 g cm^{-3} and temperature of 580 K.

To minimize computational time, the TRITON models were simplified by depleting all fuel pins as lumped fuel. To quantify the error introduced by this approximation, a separate case was studied for which each fuel pin was depleted

individually. The error in k_∞ was less than 0.01% over a small range of burnups, which suggests the approximation is sufficiently accurate for the present study.

All of the fuel and cladding thermal conductivities used are consistent with those reported elsewhere¹⁶ except that the NFIR model¹⁸ for UO_2 conductivity was used. A major limitation of the model is its treatment of the gas gap, which uses the following approximation for the gap conductance h ($\text{W m}^{-2} \text{K}^{-1}$) based on Figure 8.24 of Ref. 15:

$$h = \begin{cases} 6000 + 166.7/B & B < 30 \\ 11000 & \text{otherwise} \end{cases} \quad (53)$$

A better approach would use a fuel performance code (e.g., BISON) to generate correlations for the gap conductance as functions of applicable state variables. Such correlations would be consistent with the approach taken for neutronics modeling.

Example 1: Effect of Cladding on Reactivity

As a first example, the effect of the cladding material on the reactivity was assessed. Figure 1 shows the infinite multiplication factor as a function of burnup for five different cladding configurations: pure Zr-4, two different FeCrAl thicknesses, and two different SiC thicknesses. The sharp drop in k_∞ at very low burnups results from inclusion of equilibrium xenon (at nominal specific power).

Evidently, by replacing a portion of Zr-4 with a Fe-based alloy, the reactivity is significantly reduced, as expected. Contrarily, an addition of SiC leads to a slightly increased reactivity. The relative impacts of FeCrAl and SiC are easily explained by noting the relative increase in Σ_a caused by replacing Zr-4 with FeCrAl is larger than the corresponding decrease caused by replacing Zr-4 with SiC. Figure 2 shows the reactivity difference due to 100 and 300 micron layers of either FeCrAl or SiC relative to Zr-4. The FeCrAl penalty ranges from approximately -1000 pcm

Fig. 1. Comparison of k_{∞} vs burnup for various cladding configurations.

to -4000 pcm, whereas the gain from SiC is much smaller by nearly an order of magnitude. Defects for either cladding material are reduced in magnitude over the cycle.

Example 2: Effect of Cladding on Cycle Length

Because FeCrAl reduces the reactivity, its use can be expected to reduce the cycle length, perhaps compensated only by an increased enrichment. Similarly, use of SiC might actually lead to an increased cycle length (based on neutronics alone). To quantify these impacts, the cycle length was computed as a function of FeCrAl and SiC for a three-batch core assuming both equal-weighted and

Fig. 2. Reactivity defect due to layer of FeCrAl or SiC.

reactivity-weighted power-sharing. A boron concentration of zero and a leakage penalty $\rho_L = 0.04$ was assumed. The results are shown in Figure 3.

Two observations can be made. First, the FeCrAl thickness has a much stronger effect on the cycle length than the SiC thickness, consistent with its larger impact on reactivity. Second, there is a marked difference in cycle lengths between the two power-sharing methods. Although parameters used in the reactivity-weighted approach are subject to tuning, the apparent sensitivity of the cycle length to the power-sharing method suggests that a realistic power profile (i.e., not uniform) may be important for capturing gross core behavior.

Fig. 3. Comparison of cycle lengths for various FeCrAl and SiC thicknesses.

Example 3: Effect of Cladding on Batch Temperatures

As a final example, the effect of cladding material on the batch-wise, cycle-averaged temperatures was studied. Reactivity-based power sharing leads to different batch-wise powers, and hence, temperatures. The batch-wise fuel temperatures for the same conditions as used in Example 2 were computed as a function of layer thickness. Results are shown in Figure 4. The corresponding coolant temperatures and power-peaking factors are shown in Figures 5 and 6, respectively.

From Figure 4, it is apparent that the FeCrAl cladding leads to a reduction in the average fuel temperatures. This effect is easily explained by the neutronic characteristics of FeCrAl: it reduces the batch reactivity and, hence, the batch

Fig. 4. Comparison of batch-wise, cycle-averaged fuel temperatures for various FeCrAl and SiC thicknesses.

power is also reduced. A very slight trend in the opposite direction is observed for thick SiC layers. The bulk coolant temperatures shown in Figure 5 generally follow the fuel-temperature trends, as do the power-peaking factors shown in Figure 6.

VI. CONCLUSION

The models presented are admittedly very simple. However, once the underlying neutronic and thermal-hydraulic parameters are defined for the fuel configurations of interest, parametric studies like those of Section V are straightforward to conduct. An obvious path forward is the inclusion of a fuel-performance model. Although the models presented could, in theory, be coupled to detailed models

Fig. 5. Comparison of batch-wise, cycle-averaged coolant temperatures for various FeCrAl and SiC thicknesses.

like BISON, it would seem more natural to use a detailed model to generate data for a simplified model, much like what has been done here for the neutronic model. Of course, further improvements in the neutronic and thermal-hydraulic models are also possible, including tuning the neutronic model to higher-fidelity results and numerically computing the temperatures, e.g., to capture gradients in the thermal conductivities.

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Fig. 6. Comparison of batch-wise, cycle-averaged power-peaking factors for various FeCrAl and SiC thicknesses.

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