Using the Neutron Excess Concept to Determine Starting Fuel Requirements for Minimum Burnup Breed-and-Burn Reactors

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Title:

Using the Neutron Excess Concept to Determine Starting Fuel Requirements for Minimum-Burnup Breed-and-Burn Reactors

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ABSTRACT

In a breed-and-burn (B&B) reactor, the reactor is first started with enriched uranium or other fissile material, but can be thereafter refueled with natural or depleted uranium. B&B reactors have the potential to achieve >10% uranium utilization in a once-through fuel cycle, versus <1% for LWRs. A newly developed method for analyzing B&B reactors – the “neutron excess” concept – is used to determine the minimum amount of startup fuel needed to establish a desired equilibrium cycle in a minimum-burnup B&B reactor. Here a minimum-burnup B&B reactor is defined as one in which neutron leakage is minimized and feed fuel can be discharged at uniform burnup. The neutron excess concept reformulates the k-effective of a system in terms of material depletion quantities: the total number of neutrons absorbed and produced by a given volume of fuel, which are termed “neutron excess quantities”. This concept is useful because neutron excess quantities are straightforward to estimate using simple 1D and 0D models. A set of equations is developed which allows the quantity of starter fuel needed to establish a given B&B equilibrium cycle to be expressed in terms of neutron excess quantities. A simple 1D example of a sodium cooled, metal fuel reactor with a startup enrichment of 15% is used to illustrate how the method is applied. An estimate for the required amount of starter fuel based on a 0D depletion model is found to differ by only 3% from the actual amount computed using the 1D example model.

Key Words: Breed-and-burn; traveling wave reactor; neutron excess
I. INTRODUCTION

Breed-and-burn reactors are reactors that are able to run on non-multiplying ($k_e < 1$) fertile material by breeding it into usable fissile fuel. This newly-bred fuel can be subsequently burned in the same reactor, which produces neutrons that can be used to breed additional fertile fuel. An equilibrium cycle can be established in which neutron leakage from the burning region produces new bred fuel, which is able to continually replace the neutron-producing ($k_e > 1$) fuel in the core. Therefore, once a breed-and-burn equilibrium cycle is started by an initial loading of fissile starter fuel, it can operate indefinitely in an equilibrium cycle in which the only fuel input is fertile feed material. Examples of possible fertile feed include low enrichment, natural, or depleted uranium, light water reactor spent fuel, and thorium. Breed-and-burn reactors are also known as traveling wave reactors and convert-and-burn reactors. Past examples of breed-and-burn reactor concepts and analysis are given in references [1] through [4].

The neutron excess concept and its applicability to studying breed-and-burn (B&B) reactors were first introduced in an earlier paper by the authors [5]. The paper showed how to determine the minimum burnup and fluence required to sustain breed-and-burn operation for a given core composition. The minimum burnup is a function of its depletion-dependent neutron excess quantities. These were defined to be $\Delta P$, the total number of neutrons produced per volume of fuel, $\Delta A$, the total number of neutrons absorbed per volume, and $\Delta N$, the net number of neutrons absorbed or produced per volume, equal to the difference between $\Delta P$ and $\Delta A$. This quantity $\Delta N$ is termed the “neutron excess” of a material. Figure 1 shows a schematic figure of how $\Delta N$ evolves with increasing fluence for a B&B reactor feed fuel composition (consisting of fertile fuel, structure, and coolant). In region I, between points A and B, the fuel is a neutron absorber: it absorbs neutrons at a higher rate than it produces neutrons. In region II, between points B and D, the fuel has enough fissile material bred in it to become a neutron producer; it produces neutrons faster than it absorbs them. In region III, the accumulation of fission products causes the fuel to become an absorber of neutrons again. The minimum burnup of the feed fuel corresponds to point C, the point at which $\Delta N$ first becomes positive, i.e. the fuel has given back as many neutrons as it
has absorbed. Point E corresponds to the maximum theoretical burnup, which for most core compositions occurs at extremely high levels of burnup and fluence (> 40% fissions per heavy metal atom). Since neutron excess quantities are easily estimated using 1D models for the hard spectrum in a B&B reactor, accurate estimates of equilibrium cycle $k$-effective can be made without needing to construct detailed 3D reactor models.

Achieving the theoretical value of minimum burnup requires that neutron losses to leakage and control are minimized while all the feed fuel is discharged at a uniform burnup. To accomplish this in practice would require a unique reactor configuration in which fuel elements could be shuffled in three dimensions, to maintain a blanket of neutron-absorbing feed fuel in all directions while allowing each fuel element to be uniformly depleted. Using a reactor with conventional axially-connected assemblies would result in higher burnup because of axial peaking. A B&B reactor that allows fuel shuffling in three-dimensions is referred to in this paper as a “minimum-burnup B&B reactor.” Currently, high burnup and fluence are limiting design factors in B&B reactors using natural or depleted uranium as feed fuel. Therefore, minimum-burnup B&B reactors are interesting because they can reduce the technical challenge associated with high burnup and fluence, exchanging it for the alternative challenge of engineering a system that allows three-dimensional shuffling.

Even though a B&B reactor can in principle operate indefinitely on fertile-only feed fuel, some amount of external fissile material is required at startup for reactor criticality and to establish a B&B equilibrium cycle. In addition to achieving minimum burnup, it is also desirable to minimize this amount of starter fuel. The amount of starter fuel is important because it has implications for both the cost and fuel cycle performance (e.g. reactor doubling time) of B&B reactors. A method for determining the minimum starting fuel requirement using the neutron excess concept has been developed and is described in Section II. An example transition-to-equilibrium-cycle case for a 1D slab reactor is given in Section III, together with an infinite-medium depletion prediction for the required amount of starter fuel. Section IV gives an example of how the infinite-medium depletion approximation can be used to compare the
value of different types of starter fuel, such as different uranium enrichments. Concluding remarks are given in Section V.
II. USING NEUTRON EXCESS THEORY TO CALCULATE STARTER FUEL REQUIREMENTS

As discussed in an earlier work by the authors [5], the neutron excess ($\Delta N$) is defined as the net number of neutrons per unit volume produced or absorbed by a given material, as defined in Equation 1. This quantity is useful because it the way it evolves with burnup or fluence in a B&B reactor can be easily predicted.

$$\Delta N = \int_{t=0} \phi (\Sigma_f - \Sigma_a)$$

(1)

For a critical system, the rates of neutron production and absorption are equal, so neutron excess is conserved, stemming from the criticality relation:

$$k = 1 = \frac{\int dV \phi \Sigma_f}{\int dV \phi \Sigma_a}$$

(2)

$$\int dV \phi (\Sigma_f - \Sigma_a) = 0$$

(3)

$$\int dV \frac{d\Delta N}{dt} = \frac{d}{dt} \int dV \Delta N = 0$$

(4)

The volume integral in Equation 3 is taken over any volume that absorbs neutrons, including fueled regions, control elements, and leakage regions outside the core. The fact that neutron excess is conserved can be used to calculate how much starter fuel is required to start a given B&B equilibrium cycle. Conceptually, this is done by comparing the amount of positive neutron excess provided by the starter fuel and balancing that with the negative neutron excess contained in the equilibrium cycle, while also accounting for neutron absorptions in control and leakage. To accomplish this, it is useful to first define another quantity called $k_{fuel}$, which is described in Section II.A. Sections II.B discusses how neutron
excess theory can be applied to a simple idealized system with constant equilibrium-cycle $k_{\text{fuel}}$, and Section II.C describes the more general case in which $k_{\text{fuel}}$ can change over an equilibrium cycle.

II.A. Definition of $k_{\text{fuel}}$

To make the neutron excess concept simpler to apply, it is useful to first define a quantity $k_{\text{fuel}}$, equal to the total neutron production rate in fuel divided by the total neutron absorption rate in fuel, as shown in Equation 5.

$$k_{\text{fuel}} = \frac{\int dV \phi \Sigma_f}{\int dV \phi \Sigma_a} = \frac{\int dV \phi \Sigma_a}{\int dV \phi \Sigma_a + \int dV \phi \Sigma_a} + \int dV \phi \Sigma_a$$

In Equation 5, the numerators of the two right hand terms can be equated because the total neutron production and absorption rates in a controlled critical system are equal (see Equation 2). In the rightmost term, total neutron absorptions are explicitly broken up into absorptions in fuel, leakage, and control regions. Here “leakage region” is a generic term for any non-fuel, non-control material, including interstitial regions such as gas expansion modules or test positions, as well as all regions outside the core include shielding, reflector, gas plena, and the reactor vessel. In a minimum-burnup B&B reactor, it is possible reduce neutron leakage to nearly zero by surrounding the burning region of the core with a sufficiently thick blanket of feed fuel on all sides. For such a reactor, $k_{\text{fuel}}$ can be approximated by modeling an uncontrolled (or all-rods-out) $k$-effective, since a model with no control or leakage will have $k_{\text{fuel}}$ equal to $k$-effective. This approximation is used through the remainder of this paper, since explicitly modeling control introduces additional complexity and isn’t critical to the idea being studied.

The quantity $k_{\text{fuel}}$ is useful because it associates all the neutron absorptions in a system (in fuel, leakage, and control) with the neutron absorptions in the fuel alone, which simplifies the equations for neutron excess balance. Section II.B and II.C described how these equations are derived.
II.B. Case with Constant Equilibrium-Cycle $k_{\text{fuel}}$

First, a case is considered in which a hypothetical B&B equilibrium cycle has a constant value for $k_{\text{fuel}}$, designated $k_{eq}$. Such a case represents the (unrealistic) limit in which at equilibrium, the cycle length is shortened to zero, so there is no cycle reactivity swing. During the equilibrium cycle, $k_{\text{fuel}}$ is equal to $k_{eq}$, so one can substitute $k_{\text{fuel}}$ with $k_{eq}$ in Equation 5 and rearrange to yield:

$$
\int_{\text{fuel}} dV \left( \phi \Sigma_f - k_{eq} \phi \Sigma_a \right) = 0
$$

(6)

The neutron absorption and production rates in Equation 6 can be expressed as time derivatives of neutron excess quantities:

$$
\int_{\text{fuel}} dV \left( \frac{d\Delta P}{dt} - k_{eq} \frac{d\Delta A}{dt} \right) = 0
$$

(7)

Bringing the time derivative outside the volume integral yields:

$$
\frac{d}{dt} \int_{\text{fuel}} dV (\Delta P - k_{eq} \Delta A) = \frac{d}{dt} \int_{\text{fuel}} dV (\Delta N_{\text{adj}}) = 0
$$

(8)

$$
\Delta N_{\text{adj}} = \int_{t=0} dV \phi \Sigma_f - k_{eq} \Sigma_a = \Delta P - k_{eq} \Delta A
$$

(9)

Equation 8 introduces a new quantity $\Delta N_{adj}$, called the “adjusted neutron excess”, which is defined in Equation 9. The definition for $\Delta N_{adj}$ resembles that for the normal neutron excess ($\Delta N$), except that neutron absorptions are weighted by the constant term $k_{eq}$. Unlike the normal neutron excess, the adjusted neutron excess is only defined for fueled regions in the core. By weighing neutron absorptions in fuel by $k_{eq}$, $\Delta N_{adj}$ implicitly accounts for the neutron absorptions occurring outside of fuel (i.e., in control and leakage regions). In this remainder of this paper, $\Delta N_{adj}$ is also referred to as just “neutron excess” for simplicity, in places where the “adjusted” connotation is evident.
Equation 8 states that when $k_{\text{fuel}}$ equals $k_{eq}$, the total adjusted neutron excess \((\int dV \Delta N_{\text{adj}})\) of a system is constant. This is the same as Equation 3, except restated in terms of $\Delta N_{\text{adj}}$, which allows the volume integral to be performed over fueled regions only.

Once the equilibrium cycle is established, $k_{\text{fuel}}$ by definition equals $k_{eq}$, so the total $\Delta N_{\text{adj}}$ of the system becomes constant. In addition, if the system is designed such that its $k_{\text{fuel}}$ equals $k_{eq}$ over the entire life of the reactor (i.e. from startup through transition to the equilibrium cycle), then the total $\Delta N_{\text{adj}}$ is constant and equal to zero over the life of the system (since $\Delta N_{\text{adj}}$ by definition starts at zero for fresh fuel).

If one removes the assumption that $k_{\text{fuel}}$ is constant over the life of the reactor (i.e., if it varies during the transition from startup to the equilibrium cycle), then one can rearrange Equation 5 in a similar manner as Equation 6, but without substituting $k_{\text{fuel}}$ with $k_{eq}$:

\[
\int_{\text{fuel}} dV (\phi \Sigma_f - k_{\text{fuel}} \phi \Sigma_a) = 0
\]  

(10)

Shifting the $k_{\text{fuel}}$ term to the right and subtracting a $k_{eq}$ term yields Equation 11:

\[
\int_{\text{fuel}} dV (\phi \Sigma_f - k_{eq} \phi \Sigma_a) = \int_{\text{fuel}} dV (k_{\text{fuel}} \phi \Sigma_a - k_{eq} \phi \Sigma_a)
\]  

(11)

\[
\frac{d}{dt} \int_{\text{fuel}} dV (\Delta N_{\text{adj}}) = (k_{\text{fuel}} - k_{eq}) \frac{d}{dt} \int dV \Delta A
\]  

(12)

Equation 12 is the same as Equation 11, except written in terms of neutron excess quantities. The left side of Equation 12 is the time rate of change of the total amount of adjusted neutron excess in the system. Because the time rate of change of the total $\Delta A$ in the right hand term is always positive, when $k_{\text{fuel}}$ is higher than $k_{eq}$, the total adjusted neutron excess in a system increases. A higher $k_{\text{fuel}}$ means that there are more neutron absorptions in leakage and control, so the fuel has to supply additional excess neutrons.
To obtain the total adjusted neutron excess contained in a system, one can integrate Equation 12 over time to yield Equation 13, where the time integral is taken from the startup of the reactor:

\[
\int_{t=0}^{t} dt \left( k_{\text{fuel}} - k_{\text{eq}} \right) \frac{d}{dt} \int dV \Delta A
\]

Equation 13 shows that if \( k_{\text{fuel}} \) is greater than \( k_{\text{eq}} \) during the transition to the equilibrium cycle, then the total adjusted neutron excess would be positive, meaning that additional fissile fuel would be needed to supply excess neutrons. Conversely, if \( k_{\text{fuel}} \) is lower than \( k_{\text{eq}} \), then the total adjusted neutron excess decreases, reducing the fissile requirement.

II.C. Case with Varying Equilibrium-Cycle \( k_{\text{fuel}} \)

In a realistic reactor with finite cycle length, \( k_{\text{fuel}} \) will vary over an equilibrium cycle as the uncontrolled \( k \)-effective (i.e. amount of control required) varies over a cycle. In such a case, it is useful to first define a cycle-averaged value for \( k_{\text{fuel}} \):

\[
\overline{k_{\text{fuel}}} = \frac{\int_{\text{cycle}} dt \left( k_{\text{fuel}} \int dV \phi \Sigma_a \right)}{\int_{\text{cycle}} dt \left( \int dV \phi \Sigma_a \right)}
\]

In Equation 13, the bar superscript for \( \overline{k_{\text{fuel}}} \) denotes an averaged quantity, with the average being weighted by total neutron absorptions. The value of \( \overline{k_{\text{fuel}}} \) for an equilibrium cycle is referred to as \( \overline{k_{eq}} \).

For a constant power level (or an integral over EFPY instead of time), the integrals in Equation 13 can be rewritten in terms of the total power \( P \), by converting from the total number of neutrons absorbed to the total number of fissions:
In Equation 16, it is assumed that the average number of neutrons per fission ($\bar{\nu}$) and average energy per fission ($\bar{Q}$) do not change appreciably over each cycle. Equation 16 shows that the appropriate value to use for the average $k_{fuel}$ is the harmonic mean of $k_{fuel}$ over a cycle. For a small change in $k_{fuel}$ over a cycle, the harmonic mean can be approximated as the arithmetic mean, and for a linear reactivity swing, can be further approximated as the middle-of-cycle value of $k_{fuel}$.

Using the definition of $\bar{k_{fuel}}$ in Equation 14, it is possible to derive an expression analogous to Equation 13 but for discrete cycles. First, Equation 10 is rearranged and integrated over one cycle to yield:

$$\int_{cycle} dt \int_{fuel} dV (\phi \Sigma_f) = \int_{cycle} dt \left( \frac{\bar{\nu}P}{\bar{Q}k_{fuel}} \right)$$

The right-hand side of Equation 17 is equal to the numerator in Equation 14, allowing it to be rewritten as:

$$\int_{cycle} dt \int_{fuel} dV (\phi \Sigma_f) = \bar{k_{fuel}} \int_{cycle} dt \int_{fuel} dV (\phi \Sigma_a)$$

Subtracting a $\bar{k_{eq}}$ term from each side yields Equation 19:
\[
\int dt \int dV \left( \phi \Sigma_f - \overline{k_{eq}} \phi \Sigma_u \right) = \left( \overline{k_{fuel}} - \overline{k_{eq}} \right) \int dt \int dV \left( \phi \Sigma_u \right) \tag{19}
\]

\[
\int dV \left( \Delta N_{adj} \right)_{fuel} \left|_{cycle} \right. = \left( \overline{k_{fuel}} - \overline{k_{eq}} \right) \int dV \left( \Delta A_{adj} \right)_{cycle} \tag{20}
\]

Equation 20 is the same as Equation 19, except written in terms of neutron excess quantities. The left side of Equation 20 is the change of the total amount of adjusted neutron excess over a cycle. Since there is no single value of \( k_{eq} \) for a case with discrete cycles, \( \Delta N_{adj} \) is defined with \( \overline{k_{eq}} \) in place of \( k_{eq} \).

As with the continuous case, when \( \overline{k_{fuel}} \) for a cycle is greater than \( \overline{k_{eq}} \), the total adjusted neutron excess in a system increases, with the converse being true as well. When \( \overline{k_{fuel}} \) equals \( \overline{k_{eq}} \), such as over an equilibrium cycle, then total adjusted neutron excess is conserved; i.e. it has the same value at the beginning and the end of the cycle. Summing Equation 20 over all cycles from the reactor startup gives an expression for the total adjusted neutron excess in a system:

\[
\int dV \left( \Delta N_{adj} \right)_{fuel} = \sum_{cycles} \left( \overline{k_{fuel}} - \overline{k_{eq}} \right) \int dV \left( \Delta A_{adj} \right)_{cycle} \tag{21}
\]

**II.B. Computing Starting Fuel Requirements**

Equation 21 can be used to form an estimate for the minimum fissile requirement for a desired equilibrium cycle. From examining an equilibrium cycle, parameters such as peak feed discharge burnup, minimum reactivity, reactivity swing, and minimum core size can be measured. Other parameters, such as reactivity coefficients, can also be calculated based on the equilibrium cycle state. For the purposes of computing the needed amount of starter fuel, another significant parameter that can be measured is the total \( \Delta N_{adj} \) of the feed fuel in the equilibrium cycle. This value does not change from cycle to cycle once the equilibrium cycle is established, because the terms being summed in Equation 21 are zero over the
equilibrium cycle. Let one assume that the average $k_{\text{fuel}}$ for the transition cycles is approximately equal to that of the desired equilibrium cycle, which is reasonable because it is desirable to have the same minimum reactivity and reactivity swing over the life of the reactor. Under this assumption, it follows from Equation 21 that the total system $\Delta N_{\text{adj}}$ is equal to zero at the beginning and end of each cycle. Therefore, the total $\Delta N_{\text{adj}}$ of the feed fuel in the equilibrium cycle (which is negative) must be balanced by the positive $\Delta N_{\text{adj}}$ of the starter fuel, and any contribution from feed fuel that occurs during the transition period:

$$\int dV(\Delta N_{\text{adj}})_{\text{eq-cycle}} + \int dV(\Delta N_{\text{adj}})_{\text{starter fuel}} + \int dV(\Delta N_{\text{adj}})_{\text{transition feed fuel}} = 0$$

(22)

In Equation 22, the leftmost term can be measured directly from the equilibrium cycle of interest, by summing over the adjusted neutron excess of all the fuel contained in the equilibrium cycle. If the transition feed fuel is discharged at the same burnup as the equilibrium-cycle feed fuel, then its contribution to the total neutron excess will be small. Equilibrium-cycle feed fuel is by definition discharged with an average $\Delta N_{\text{adj}}$ of zero, so transition feed fuel burned to the same discharge burnup will have a $\Delta N_{\text{adj}}$ of approximately zero. Small deviations from zero arise due to different spectral histories for the transition feed fuel and the equilibrium-cycle feed fuel; these are generally positive because transition feed fuel is bred in the harder neutron spectrum present around the starter fuel. Since the third term in Equation 22 is small, the first and second terms must cancel each other out, meaning that the positive adjusted neutron excess of the starter fuel must equal the negative adjusted neutron excess contained in the equilibrium cycle. To find the amount of starter fuel needed, one would divide the total neutron excess needed by the average neutron excess per unit volume of the starter fuel used:

$$V_{\text{starter fuel}} = \frac{\int dV(\Delta N_{\text{adj}})_{\text{starter fuel}}}{\Delta N_{\text{starter fuel}}} \approx \frac{\int dV(\Delta N_{\text{adj}})_{\text{eq-cycle}}}{\Delta N_{\text{starter fuel}}}$$

(23)
The actual neutron excess obtained from a unit of starter fuel depends on its specific depletion history, which would be obtained by explicitly modeling the transition from startup to the desired equilibrium cycle. Designing and modeling such a transition is a complex fuel management problem, which makes it difficult to analyze a variety of starter fuel options. Fortunately, neutron excess is straightforward to estimate using simple models, such as an infinite-medium (0D) depletion model. The estimate is made by performing an infinite-medium depletion calculation to the burnupfluence limit of the starter fuel and measuring the resulting neutron excess. With this result, an estimate for the needed quantity of starter fuel can be made by dividing the total neutron excess contained in the equilibrium cycle by the average neutron excess predicted by the 0D model.

If cycle-averaged $k_{\text{fuel}}$ deviates from its equilibrium cycle value during the transition to the equilibrium cycle, the needed $\Delta N_{\text{adj}}$ is adjusted either upward or downward, as shown on the right-hand side of Equation 24, which matches the right-hand side of Equation 21. As a consequence, it is desirable to minimize excess reactivity during transition to reduce neutron losses to control and therefore lower the needed amount of starter fuel.

\[
\int_{\text{eq-cycle}} dV(\Delta N_{\text{adj}}) + \int_{\text{starter fuel}} dV(\Delta N_{\text{adj}}) + \int_{\text{transition feed fuel}} dV(\Delta N_{\text{adj}}) = \sum_{\text{transition cycles}} (k_{\text{fuel}} - k_{\text{eq}}) \int_{\text{cycle}} dV(\Delta A_{\text{adj}}) \quad (24)
\]
III. EXAMPLE TRANSITION MODEL

The concepts discussed in Section II are applied to an example transition case for a one-dimensional infinite slab model. Subsection III.A describes the target equilibrium cycle, III.B shows how to estimate the needed quantity of starter fuel, III.C discusses how the transition to equilibrium was modeled, and III.D compares the results from the transition model to the estimate made using an infinite medium calculation. Simulations were primarily run using a version of MCNPX-CINDER90 modified by TerraPower LLC to improve performance and parallelization and to add additional features [6]. A combination of ENDF-B/V and ENDF-B/VII cross section libraries were used. Some additional fuel management simulations were run using REBUS with DIF3D [7].

III.A. Equilibrium Cycle Description

The equilibrium cycle that is started up in this example uses a simplified core composition (50% U, 20% Fe, 30% Na by volume) and consists of fifty 5cm-thick infinite slabs, with a reflective boundary at the center line and a vacuum boundary at the other. The feed material is assumed to be depleted uranium with 0.3 mol% U-235. The large size of the model (5m total thickness) is to reduce leakage to effectively zero; only the inner 20 zones are important neutronically. The zones are numbered sequentially from 1-50, starting from the reflective boundary center of the model. The equilibrium-cycle shuffling sequence is a convergent-divergent pattern with the discharge zone being the eighth from the center: i.e. fuel is first shuffled sequentially from zone 50 to zone 9 (convergent), skips from zone 9 to zone 1, then is shuffled sequentially from zone 1 back out to zone 8 (divergent), where it is discharged. Convergent-divergent shuffling schemes are an interesting class of equilibrium shuffle sequences because they provide a much flatter power distribution than strictly convergent shuffling while retaining high reactivity and a small change in power distribution over an equilibrium cycle. The power level and cycle length are chosen to be 60 MW/m² and 900 days respectively, which corresponds to an equilibrium-cycle discharge burnup of
11.6% Fraction of Initial heavy Metal Atoms, or FIMA. Multiplying the burnup in FIMA by a factor of approximately 975 gives the burnup in MWd/kgHM.

The equilibrium-cycle configuration can be formed by starting from any starting fuel configuration and repeatedly applying the equilibrium-cycle shuffling sequence until an equilibrium state develops. The resulting equilibrium-cycle burnup and power distributions are shown in Figures 2 and 3. The power shape in seen in Figure 3 is a result of zones one through eight having the most Pu-239 bred in them, which causes the flux and power to concentrate there.

Equilibrium-cycle reactivity values are given in Table I; these values are the uncontrolled $k$-effective results from an MCNPX simulation. Since no control is modeled, it is assumed that these values for $k$-effective are approximately equal to the $k_{\text{fuel}}$ of a controlled system. The small number of zones in the burning region of this simple equilibrium cycle as well as the relatively low burnup result in a fairly large reactivity swing, nearly 5% (the last significant digit does not add exactly due to rounding).

The equilibrium cycle values for $\Delta N$ and $\Delta N_{\text{adj}}$ as a function of burnup are plotted in Figure 4. The value of $\Delta N$ is positive for fuel nearing discharge, which is necessary because a fraction of neutrons are absorbed in control (these control absorptions are virtual, since control is not explicitly modeled). Accounting for these losses yields the $\Delta N_{\text{adj}}$ curve, which is computed according to Equation 9, using the value of $\bar{k}_{eq}$ given in Table I. The discharge value of $\Delta N_{\text{adj}}$ is zero, so as the equilibrium cycle proceeds and more discharged feed fuel is created, the total value of $\Delta N_{\text{adj}}$ in the system does not change. This is illustrated in Figure 5, which shows the value of $\Delta N_{\text{adj}}$ as a function of zone index during the equilibrium cycle. Because the fuel has a zero $\Delta N_{\text{adj}}$ at discharge, the total $\Delta N_{\text{adj}}$ contained in the equilibrium is the same at the beginning of cycle and end of cycle.

**III.B. Estimating the Needed Amount of Starter Fuel**

By integrating $\Delta N_{\text{adj}}$ of Figure 5 over all zones, one obtains the total $\Delta N_{\text{adj}}$ of the chosen equilibrium cycle: $-6.20E-02$ mol/cm$^2$. For total $\Delta N_{\text{adj}}$ to be conserved (Eq. 20), a positive contribution of $6.20E-02$
mol/cm² is needed either from feed fuel burned past the breakeven value of 11.6%, or from enriched starter fuel. It is assumed that feed fuel cannot be burned much beyond this breakeven value, which is reasonable if one wishes to minimize burnup and cladding fluence. Therefore, nearly all the excess neutrons must come from the starter fuel. For this example, the starting fissile fuel is assumed to be 20 cm
(4 zones) of 15% enriched material, with the same composition (U, Fe, and Na) as the feed fuel. The ΔN and ΔN_adj of the starter fuel as a function of burnup are estimated by depleting an infinite medium of starter fuel, with the results shown in Figure 6. Dividing the required neutron excess (6.20E-02 mol/cm²) by the amount of feed fuel (20 cm), yields the needed neutron excess per unit of feed fuel (3.10E-03 mol/cm³), which from Figure 6 corresponds to an average burnup of 12.3%. Note that in this case, a given amount of starter fuel was assumed and the needed burnup estimated, but it is equally possible, and usually more practical, to choose a starting fuel composition and for a given burnup limit determine what volume of starting material is needed.

III.C. Modeling a Transition Case

Starting from 20 cm of 15% enriched starter fuel (4 5-cm zones) and 0.3% enriched feed fuel, the target equilibrium cycle was established by shuffling the fuel according to the sequence given in Table II. Only the innermost 20 zones are shown because the zones farther out are effectively isolated neutronically. This model simulates the transition from startup to equilibrium and is referred to as the “transition model” in this paper.

In this transition sequence, the starter fuel is initially in zones one through four but is shuffled to zones 1, 3, 4, and 7 before the first cycle. Depleted uranium feed fuel occupies all other zones. The starter fuel moves outward with each cycle and is rearranged to keep the lowest burned zones toward the center, while the feed fuel is kept in order of burnup. By cycle 7, the feed fuel is bred sufficiently that the starter fuel zones can be completely discharged while still leaving the feed fuel in a critical state. At this point, beginning of cycle reactivity is minimized by reversing the order of the five innermost feed zones. At the start of cycle 8, the innermost eight feed zones are reversed, forming a state close to the final
equilibrium cycle. After cycle 8, the equilibrium-cycle shuffling scheme is used, with spent feed fuel being discharged from zone number 8, and the equilibrium-cycle is quickly established.

This transition sequence was designed to satisfy the following goals:

1) Prevent $k$-effective from falling below unity
2) Keep the cycle-average $k$-effective close to $\bar{k}_{eq} = 1.0375$
3) Keep the peak feed burnup close to the required burnup of 11.6%
4) Discharge the starter fuel at roughly uniform burnup (i.e. minimize peaking)

One can also replace the feed and starter burnup goals with goals for total fluence or radiation damage and obtain similar results. To achieve goal number 2 while minimizing the number of shuffles (or maximizing the cycle length), it is desirable to minimize the beginning-of-cycle positive reactivity for each cycle. For more realistic systems, additional goals can be added, such as a peak power density constraint, or a goal to minimize the number of assembly movements per shuffle.

Cycles 1-6 in the transition sequence given in Table II were obtained by analyzing a large number of different shuffling permutations at each cycle, then choosing the one that would satisfy the goals above as well as result in a feed burnup distribution that most resembled the equilibrium cycle burnup distribution. To limit the number of possible permutations for these cycles, the order of the starter fuel is always arranged to have the lowest burnup starter fuel toward the center, and the order of the feed fuel is always arranged with the highest burnup feed zones toward the center. The only thing that is changed is the relative positions of the feed and starter fuel. Even with this constraint, there are still a large number of possible permutations to analyze, so deterministic REBUS calculations were used to evaluate them.

The permutation selected for a given cycle was the one that would maximize the value of the evaluation function given in Equation 2 while having a $k$-effective larger than a specified cutoff value (1.015 in the REBUS model).
\[ EQM = \sum_i P_i^* (BU_{eq,i} - BU_i) \] (25)

\( EQM \) stands for Equilibrium Matching function, \( P_i \) is the power in material \( i \), \( BU_i \) is the burnup in material \( i \), and \( BU_{eq,i} \) is the equilibrium cycle in material \( i \). In Equation 25, the material indices \( i \) do not correspond to the physical locations of the zones, but instead to the feed materials sorted in order of burnup; e.g., \( BU_2 \) and \( BU_{eq,2} \) are the burnups in the second most burned feed material and the second most burned feed materials in the equilibrium cycle. The EQM is maximized by preferentially increasing feed power in materials which have burnups far from their equilibrium cycle values. Variations of the EQM can be formed by modifying the exponent of the parenthetical term in Equation 25, from zero (which would cause EQM to be maximized by maximizing total feed power) to a large number (which would maximize power in the material with the largest burnup to make up). Instead of using burnup as a criterion, other parameters such as material \( k \)-infinity can be used to recreate the equilibrium cycle.

Once the permutation for a given cycle is determined according to the criteria above, the length of the subsequent cycle is determined by matching the middle-of-cycle \( k \)-effective of the cycle with that of the equilibrium cycle (1.046 in REBUS). At cycles 8 and beyond, the equilibrium cycle shuffling sequence is used with the equilibrium-cycle cycle length of 900 days, with one exception. For cycle 10, the cycle length is reduced from 900 days to 613.6 days in order to prevent the burnup in material 7 (the material starting in zone 7) from exceeding 11.8%.

Once a transition sequence was determined using REBUS, the model was rerun using MCNPX/Cinder. Results from REBUS were found to agree well with those from MCNPX. Flux and power distributions were the same for the two models, while REBUS calculated \( k \)-effectives roughly 0.5% higher than in MCNPX, due to the differences in cross section libraries used. The reactivity evolution computed by REBUS and MCNPX of the Table II shuffling scheme is given in Figure 7. In Figure 7, the equilibrium-cycle reactivity results given in Table I can be seen for the cycles occurring after about 12000 days. As seen in the REBUS results, the length of the first 7 cycles was chosen to yield the same middle-of-cycle \( k \)-effectives as the equilibrium cycle. Overall, the beginning-of-cycle and end-
of-cycle $k$-effectives deviate by less than 1% from their equilibrium cycle values; this variation can be reduced in more realistic systems which have more degrees of freedom for arranging feed and startup fuel.

The burnup for different fuel zones after 30 cycles for this transition case are given in Figure 8 (results are from the MCNPX model). Material numbers one through twenty seven have been discharged, and materials 28 and higher have assumed the equilibrium cycle burnup distribution. This burnup distribution does a good job of satisfying goals 3 and 4. The peak feed discharge burnup is 11.8%, only slightly above the equilibrium cycle value of 11.6%. Meanwhile, the peak starter discharge burnup is 12.1%, very close to the average value of 12.0%.

III.D. Comparison Between Transition Model and Predicted Results

There are two contributions to the $\Delta N_{adj}$ of a system: first there is contribution or deduction from cycles in which the $\bar{k}_{fuel}$ deviates from $\bar{k}_{eq}$, as given on the right side of Equation 24. This is referred to as the contribution from “reactivity deviations,” because it depends on how much the uncontrolled $k$-effective deviates from the equilibrium cycle average value. Second, fuel discharged from a system with a non-zero $\Delta N_{adj}$ leaves a $\Delta N_{adj}$ contribution within the system, which are the second and third terms on the left side of Equation 24. The contributions due to reactivity deviations are plotted in Figure 9. When cycle reactivity is high (e.g. cycle 9), more neutrons are lost to control, so the system $\Delta N_{adj}$ increases. Conversely, when cycle reactivity is low (e.g. cycle 11), system $\Delta N_{adj}$ decreases. Once the equilibrium cycle is established, $\bar{k}_{fuel}$ equals $\bar{k}_{eq}$ (with some statistical scatter), causing the $\Delta N_{adj}$ contribution from reactivity deviations to stop accumulating. The total contribution to $\Delta N_{adj}$ due to reactivity deviations is approximately $-2.7E-04 \text{ mol/cm}^2$, which is less than 0.5% of the total neutron cost of the equilibrium cycle, which was calculated earlier to be $-6.20E-02 \text{ mol/cm}^2$. This low value is a result of this transition sequence having an average $k_{fuel}$ quite close to that of the target equilibrium cycle.
The contributions to $\Delta N_{adj}$ from fuel depletion are summarized in Figure 10, which also shows the predicted values from the infinite-medium approximation and equilibrium cycle. Figure 10 shows that the starter fuel yields slightly fewer excess neutrons than in the infinite medium prediction. This is a result of the presence of nearby feed fuel, which softens the neutron spectrum. Meanwhile, transition feed fuel that is bred in the harder spectrum of the starter-fuel region ends up being discharged with a small positive adjusted neutron excess, rather than zero as in the equilibrium cycle. These two errors approximately cancel, which is a result of the spectral mixing between the two fuels in the transition model. The total adjusted neutron excess from the starter fuel is $5.7\times10^{-2}$ mol/cm$^2$ and $4.5\times10^{-3}$ mol/cm$^2$ from the intermediate feed fuel, leaving $-6.16\times10^{-2}$ mol/cm$^2$ behind in the equilibrium-cycle feed fuel. Adding the contribution from reactivity deviations gives a total of $-6.19\times10^{-2}$ mol/cm$^2$ neutrons to build the equilibrium cycle, very close to the measured value of $-6.20\times10^{-2}$ mol/cm$^2$.

The predictions for $\Delta N_{adj}$ from the equilibrium cycle for the feed and the infinite-medium depletion for the starter fuel compare well to the actual $\Delta N_{adj}$ taken from the transition model. The greater $\Delta N_{adj}$ from the feed due to a harder spectrum in the transition model is offset by the lower $\Delta N_{adj}$ in the starter fuel due to a softer spectrum. The predicted amount of starter fuel is remarkably accurate: the startup model required 20cm of 15% enriched starter fuel to be burned to an average of 12.0%, while the infinite-medium depletion predicted that the starter fuel needed to be burned to 12.3%, a difference of just three percent. This example shows that it is possible to make an accurate estimate of the starting fissile requirement for a B&B equilibrium cycle without explicitly determining a transition shuffling sequence. The ability to make such an estimate is important, because as this example shows, determining a transition shuffling sequence even for a simple system can be challenging and computationally expensive. More realistic systems with hundreds of fuel elements and additional constraints would be more challenging to develop transition sequences for.
IV. COMPARING DIFFERENT STARTER FUELS

One question that can be answered using the neutron excess concept is what composition of starter material minimizes the amount of fissile material needed for initiating a given equilibrium cycle, for example: if there is an optimum enrichment to use. A B&B equilibrium cycle carries with it a fixed neutron excess cost, so one only has to compare the neutron excess per unit of fissile material for different enrichments. The reactivity-adjusted neutron excess \( k_{eq} = 1.03 \) of different enrichments of the simplified core composition are shown in Figure 11 as a function of Displacements Per Atom (DPA) evaluated using DPA cross sections for HT9 stainless steel, taken from IRDF-2002 [8]. DPA is a measure of neutron-induced damage in a material, and is presently a limiting constraint in the design of B&B reactors. HT9 has been used as a structural material in fast reactors, and its composition is approximated as 87.5% iron, 12% chromium, and 0.5% nickel by weight for the purposes of calculating DPA cross sections. DPA values iron or other stainless steels would be very similar to the results given.

Results are obtained from an infinite-medium depletion approximation. From the figure, it is clear that higher enriched materials supply more neutrons at a given DPA. At high DPA, the lines become parallel as the U-235 is depleted. Figure 12 shows the specific neutron excess (i.e. the adjusted neutron excess divided by the amount of fissile material) plotted as a function of DPA. All the specific neutron excess vs. DPA curves cross at the same point at roughly 260 DPA. This behavior is not a coincidence. First, the neutron spectrum is similar in the all cases because of the same material fractions in each composition (the lower enrichment cases will have somewhat softer spectra). Second, one can imagine each composition to be a linear combination of two compositions: the same core composition with solely U-238 as its fuel, and a fictitious composition consisting of some concentration of U-235 and a negative concentration of U-238. At 260 DPA, the neutron excess contribution from the first composition is zero, while the contribution from the second is exactly proportional to the amount of U-235 present.

The coincident point in Figure 12 happens to occur at the discharge DPA of the equilibrium cycle, since that point is roughly where depleted uranium just manages to have a positive neutron excess. If the
equilibrium cycle discharge DPA is taken as a DPA limit, then it makes no difference from a fissile material minimization standpoint what enrichment one chooses as starter fuel. Of course, there are other considerations besides neutron excess to take into account. For example, higher enrichment fuel will encounter higher burnup for a given fluence and may result in unwanted fuel clad mechanical interaction. Higher enrichment fuel would also occupy less volume and generate less power for a given power density limit. Lower enrichments would be more efficient if they’re burned to a higher DPA or reused, although too low an enrichment may not be able to establish initial criticality. Ultimately, the interchangeability of different enrichments lends a tremendous amount of flexibility when it comes to configuring the starter fuel for a minimum burnup B&B reactor.
V. CONCLUSIONS

A minimum-burnup breed-and-burn reactor represents a unique type of reactor that minimizes neutron losses to leakage and control. For such systems, it is possible to formulate an expression for uncontrolled $k$-effective completely in terms of material depletion properties, by using the newly developed neutron excess concept. This allows one to connect the depletion properties of the starter fuel to the depletion properties of the fuel present in a desired equilibrium cycle. Because of the very hard spectrum present in a B&B reactor, the depletion behavior of starter fuel can be accurately estimated using an infinite-medium depletion approximation. This allows one to estimate how much of a particular type of starter fuel is required to launch a specified equilibrium cycle, without needing to explicitly model a transition fuel shuffling sequence. Performing such an estimate for an example one-dimensional B&B equilibrium cycle yielded a prediction that agreed within 3% to an explicitly modeled transition to the equilibrium cycle. Previous results [5] have shown that the depletion histories in 1D models accurately match those from corresponding 3D models, so this result would also apply to realistic three dimensional reactor configurations.

In addition to allowing one to estimate starter fuel quantities, the neutron excess concept can also be applied for several other purposes. First, it allows one to compare the “cost” of various equilibrium cycle states in terms of the neutron excess contained within them, which is directly proportional to the amount of starter fuel needed. It also allows one to compare the neutron-excess “worth” of different types of starter fuel, such as different enrichments of uranium and different actinide compositions, or different fuel, structure, and coolant combinations. Performing such a comparison for different enrichment fuel showed that higher enrichments yielded more neutron excess per unit fissile below a breakeven DPA value, while above this DPA value lower enrichments were better. At the breakeven DPA value (which corresponds to the discharge DPA of a minimum-burnup depleted uranium B&B reactor), the choice of enrichment does not matter from a neutron-excess perspective. Finally, the neutron excess concept also allows one to evaluate the effect of reactivity deviations from an equilibrium cycle value, for example by
determining how much extra starter material would be required to allow an extra 1% uncontrolled reactivity over a one year period.

Future work will build on these results to calculate the reactor doubling time of a fleet of B&B reactors, in which the discharged feed fuel from one generation of reactors is used to start up a subsequent generation, without undergoing chemical separation of actinides. Also, a survey of different core compositions (fuel, structure, and coolant combinations) will be performed to determine their minimum DPA and burnup and corresponding doubling times.
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Table I. Reactivity characteristics of selected equilibrium cycle

|                          |       |
|--------------------------|-------|
| BOEC $k$-effective       | 1.014 |
| MOEC $k$-effective       | 1.039 |
| EOEC $k$-effective       | 1.060 |
| Cycle reactivity swing ($\Delta k$-effective) | 0.047 |
| $k_{eq}$                | 1.0375 |
Table II. Transition model shuffling sequence (starter fuel is highlighted)

| Cycle number | Cycle Length (days) | Cycle fuel permutation – position from center of core (only inner 20 zones shown out of 50) |
|--------------|---------------------|------------------------------------------------------------------------------------------|
| 0            | 0                   | 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20                                     |
| 1            | 1445.1              | 1 5 2 3 6 7 4 8 9 10 11 12 13 14 15 16 17 18 19 20                                   |
| 2            | 977.7               | 5 4 6 3 7 2 1 8 9 10 11 12 13 14 15 16 17 18 19 20                                 |
| 3            | 1053                | 5 4 6 7 3 8 2 9 1 10 11 12 13 14 15 16 17 18 19 20                                |
| 4            | 1065.9              | 5 4 6 7 8 1 9 10 11 2 3 12 13 14 15 16 17 18 19 20                               |
| 5            | 1085.7              | 5 6 7 2 8 9 10 11 3 12 13 1 4 14 15 16 17 18 19 20                             |
| 6            | 1121.2              | 5 6 7 8 9 10 1 11 12 13 14 15 16 3 4 17 2 18 19 20                             |
| 7            | 813.8               | 9 8 7 6 5 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24                         |
| 8            | 900                 | 12 11 10 9 8 7 6 5 13 14 15 16 17 18 19 20 21 22 23 24                         |
| 9            | 900                 | 13 12 11 10 9 8 7 6 14 15 16 17 18 19 20 21 22 23 24                         |
| 10           | 613.6               | 14 13 12 11 10 9 8 7 15 16 17 18 19 20 21 22 23 24                          |
| 11           | 900                 | 15 14 13 12 11 10 9 8 16 17 18 19 20 21 22 23 24                          |
| 12           | 900                 | 16 15 14 13 12 11 10 9 17 18 19 20 21 22 23 24                          |
Figure 1. Schematic neutron excess vs. fluence curve for B&B reactor feed fuel
Figure 2. Equilibrium cycle burnup distributions from 1D slab model
Figure 3. Equilibrium cycle power distributions from 1D slab model
Figure 4. Neutron excess of equilibrium cycle feed fuel from 1D slab model
Figure 5. Neutron excess contained in equilibrium cycle from 1D slab model
Figure 6. Neutron excess of 15% enriched starter fuel from infinite medium (0D) model
Figure 7. Uncontrolled $k$-effective evolution of transition model
Figure 8. Fuel burnup after 30 cycles from transition model
Figure 9. Reactivity-deviation contribution to adjusted neutron excess from transition model
Figure 10. Fuel depletion contribution to adjusted neutron excess from transition model
Figure 11. Adjusted neutron excess vs. DPA for different enrichments \( (k_{eq} = 1.03) \) (0D approximation)
Figure 12. Specific neutron excess vs. DPA for different enrichments ($k_{eq} = 1.03$) (0D approximation)
Figure Captions:

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