

Automated Design and Optimization of Pebble-Bed Reactor Cores

H. D. Gougar,* A. M. Ougouag, and W. K. Terry

*Idaho National Laboratory, P.O. Box 1625
Idaho Falls, Idaho 83415-3870*

and

K. N. Ivanov

*The Pennsylvania State University, 0230 Reber Building
University Park, Pennsylvania 16802-1294*

Received December 18, 2008

Accepted November 1, 2009

Abstract—*This paper presents a conceptual design approach for high-temperature gas-cooled reactors using recirculating pebble bed cores. The method employs PEBBED, a reactor physics code specifically designed to solve for the asymptotic burnup state of pebble bed reactors in conjunction with a genetic algorithm to obtain a core with acceptable properties. The uniqueness of the asymptotic core state and the small number of independent parameters that define it suggest that core geometry and fuel cycle can be efficiently optimized toward a specified objective. A novel representation of the distribution of pebbles enables efficient coupling of the burnup and neutron diffusion solvers. Complex pebble recirculation schemes can be expressed in terms of a few parameters that are amenable to manipulation using modern optimization techniques. The user chooses the type and range of core physics parameters that represent the design space. A set of traits, each with acceptable and preferred values expressed by a simple fitness function, is used to evaluate the candidate reactor cores. The stochastic search algorithm automatically drives the generation of core parameters toward the optimal core as defined by the user. For this study, the design of two pebble bed high-temperature reactor concepts subjected to demanding physical constraints demonstrated the technique's efficacy.*

I. INTRODUCTION TO THE PEBBLE BED REACTOR DESIGN PROBLEM

I.A. Motivation and Context

High-temperature reactors (HTRs) based upon the particle fuel concept enjoyed a limited period of research and development in the latter half of the 20th century with test reactors and power stations built in Germany and the United States.¹ Various political and economic factors forced the decline and eventual cessation of industrial investment in the HTR in the late 1980s (Ref. 2), but by that time, the technology had been demonstrated.

Concurrently, the light water reactor (LWR) enjoyed similar commercial interest along with a significant investment in naval nuclear propulsion that continues to this day. While the basic technology has not changed much in decades, the LWR has benefited from advances in fuels, materials, and core design techniques that have kept nuclear power competitive with inexpensive coal for baseload electricity generation in spite of the much higher capital cost.

The decline in the discovery of new and politically stable oil reserves along with concerns about their environmental effects has led to historically unprecedented prices for fossil fuels.

This has energized interest in fission as a source of heat for industrial processes, particularly in the production of transportation fuel.^{3,4} However, the temperatures

*E-mail: Hans.Gougar@inl.gov

required for many of these applications are generally far above the outlet temperature of LWR coolant but are well within the range of the HTR. Thus, government and industrial investment in the HTR is returning. Advocates of modular HTRs can also tout passive safety features that can reduce capital costs and instill greater public confidence. The lower output of a single modular HTR may be a better fit for process heat applications and the electricity markets of developing countries.⁴

I.B. Relevant Characteristics of the Pebble Bed Reactor Core

The concept of a nuclear reactor comprising spherical fuel elements was proposed by Farrington Daniels in 1945 (U.S. Patent 2,809,931). In the late 1950s in Germany, Schulten proposed a power reactor core composed of a bed of spherical fuel elements consisting of fissile particles embedded in a graphite matrix.⁵ The advantages of the robust fuel and simple core design prompted significant investment in Germany and plans for extensive deployment of the pebble bed reactor (PBR). The concept of a modular HTR was introduced in the 1980s (Refs. 6 and 7). This HTR was a PBR, but a modular prismatic core was promoted by General Atomics.⁸ Variants of these concepts have been investigated more recently in the United States,^{9,10} Japan,¹¹ China,¹² and Europe.¹³ In the modular concept, smaller power units [200 to 600 MW(thermal)] can be clustered to match local power demands and added to accommodate growth projections. Modular units also rely more heavily on standardization, factory construction, and passive safety systems to keep capital costs down. Small HTRs have even been proposed for ship propulsion.^{14–16}

The modular pebble bed HTR core possesses a number of features that distinguish it from LWRs. The most significant of these include the geometry of the fuel (spherical); the graphite moderator; and the fact that, in most designs, this fuel is in motion during operation. This last characteristic also distinguishes the PBR from its HTR cousin, the prismatic or block reactor. The ability of the modular HTR (prismatic or pebble) to withstand a complete loss of coolant flow is a result of a combination of fuel morphology and core geometry. At the heart of the design of all HTRs is the tri-isotropic (TRISO) particle. Tiny kernels of uranium dioxide (UO_2), uranium carbide (UC_2), thorium dioxide (ThO_2), or a mixture thereof are coated with layers of pyrolytic carbon and silicon carbide. These particles are embedded in a graphite matrix to form spherical or cylindrical fuel elements that are able to tolerate relatively high temperatures (up to $\sim 2000^\circ\text{C}$) for extended periods of time without disintegrating and releasing significant amounts of fission products.¹⁷ The graphite matrix serves as a moderator, but it also possesses thermal characteristics that facilitate the removal of heat from the core by gas

convection during operation and by conduction and radiation during a loss-of-coolant event. This passive safety feature was demonstrated repeatedly in the Arbeitsgemeinschaft Versuchsreaktor (AVR), the German pebble bed experimental reactor that ran for >20 yr (Ref. 18). In the event of a core thermal excursion, the strong negative temperature coefficient stops the fission reaction without the help of control rods, which are inserted only to keep the core subcritical after cooldown. The decay heat is transmitted away from the core and into the surrounding heat sink at a sufficiently high rate to prevent the fuel from reaching a failure temperature.

This can happen when the core is designed with passive safety in mind. The modern HTR has a very high aspect ratio (height/diameter >3) that keeps the overall power density low (typically 3 to 4 W/cm^3) while providing a very short heat transfer path out of the core. (The high aspect ratio also leads to an elevated rate of neutron leakage in the radial direction, a feature that is also exploited for control purposes. In modular PBRs, the control rods are located only in the graphite reflectors, not in the core itself.) Thus, a properly designed PBR core represents a balance of core geometry, thermal power, and fuel design that results in a power plant that is essentially immune to core disassembly induced by a loss of coolant. Historically, this balance was achieved by the application of engineering expertise and confirmatory calculations. Tools that automate even part of the design process had yet to be developed.

I.C. High-Temperature Reactor Core Analysis Tools

Light water reactor cores have been optimized using a variety of techniques developed over decades and applied to thermal-hydraulic analysis, instrumentation and control, water chemistry, and core physics. HTR technology may also benefit from these advances and techniques if the differences in core types are taken into account. Indeed, a number of countries support HTR methods development and evaluation,¹⁹ but significant time and resources will have to be expended before the HTR reaches the level of technical maturity found in the LWR. Furthermore, the fundamental differences in these reactor concepts may prevent direct application of some techniques without considerable modification.

One such example, and the focus of this work, is in the area of core design of and fuel management in recirculating PBRs. The pebble bed HTR differs from the LWR in a number of ways, the most obvious of which is the geometry of the fuel (spherical) and the fact that this fuel is in motion during operation. The graphite moderator yields a longer mean free path for neutrons and stronger coupling between adjacent regions of the core. The helium coolant is essentially transparent to neutrons so that there is no void reactivity feedback. LWR burnup and fuel management tools are simply not designed to

address the physics of these systems, particularly with regard to the movement of fuel. The most sophisticated LWR reload design tools are therefore useless for this application. On the other hand, some advanced optimization techniques successfully demonstrated on LWR cores can be applied to the PBR burnup problem if that problem is properly posed.

There are, of course, core analysis and fuel management codes specifically designed for the recirculating PBR. The most widely used and mature tool is the Very Superior Old Programs (VSOP) code²⁰ developed at the Jülich Research Center for the German HTR program. The code has been updated and improved for the design and licensing of the South African Pebble Bed Modular Reactor²¹ (PBMR). VSOP is an integration of a number of legacy core analysis tools such as CITATION (neutron diffusion) and THERMIX (heat transfer and gas dynamics). Burnup calculations are enabled by a stepwise time-dependent coupling of the diffusion and linear depletion equations using a stepwise pebble flow management scheme. Pebbles of different types and burnup states are tracked in batches that travel axially and radially through the core along prescribed flow lines. Pebbles that attain a specified burnup level are discharged from the core and replaced with fresh pebbles.

If the discharge burnup level, fresh pebble composition and feed rate, circulation pattern, and power level remain unchanged, the core flux and burnup distributions will approach an asymptotic or “equilibrium” state. Theoretically, the so-called “running-in” period lasts from 6 months to 3 yr, after which the core would remain in this equilibrium state for the remainder of operation unless full-core offload is required for maintenance or repair. VSOP can simulate the running-in period along with the subsequent equilibrium core power and temperature conditions.

A small number of other codes have been developed with this functionality in mind. The PANTHERMIX code, developed at the research consortium NRG in the Netherlands,²² is also an integration of established core analysis tools that were originally designed for other core types but were recently adapted for PBR analysis with the adoption of a pebble flow model. The PANTHERMIX scheme uses a somewhat more sophisticated model for shifting batches of pebbles that accounts for the numerical diffusion in the shift calculations arising from the variation in pebble speed in different flow zones. The ANSWERS code²³ recently built on the WIMS platform also uses the basic batch tracking and mixing approach found in VSOP. These code systems all feature loosely coupled diffusion, depletion, and spectrum modules that can track the state of the core from fresh fuel loading to the attainment of the equilibrium burnup profile.

Recently, Boer et al. developed a code to optimize a recirculating pebble bed fuel cycle to minimize peak power density with the ultimate goal of lowering the peak depressurized loss-of-flow condition (DLOFC) fuel

temperature.²⁴ This approach exploits a heuristic method to select the radial placement of fuel pebbles on successive passes. Using the Dalton diffusion solver and THERMIX-DIREKT for gas dynamics and heat transfer, this code package was used successfully to reduce the power peaking and peak accident fuel temperature in the PBMR-400, a 400-MW(thermal) PBR under development in South Africa.²⁵ This technique, however, is applicable to PBR designs that employ a fuel-loading mechanism that allows the placement of pebbles into specified radial zones, a capability not currently possessed by the PBMR-400 or other concepts under development. Like PEBBED, however, the code does show how modern optimization techniques can be applied to the PBR fuel management problem.

While all of these codes can address the fuel management problem for a given PBR design, none of them are particularly well suited for extensive parametric studies and optimization of core geometry with or without multiple pebble types. The specification of the reloading and mixing of pebbles of various types and burnup levels and from different flow channels is simply too cumbersome for parametric studies involving hundreds of small variations in core or fuel parameters. Modern stochastic optimization techniques, successfully applied to the LWR fuel and burnable poison loading problems over the past 15 yr, in which hundreds or even thousands of potential cores are evaluated, cannot practically be used in conjunction with existing PBR analysis codes.

The PEBBED code,²⁶ however, was created specifically with this sort of analysis and optimization capability in mind. Although in its current form, PEBBED can analyze only the initial and equilibrium core states (not the running-in period), it exploits a different representation of pebble flow and mixing that is amenable to a variety of optimization techniques, including stochastic. One such technique, the so-called genetic algorithm, has been successfully adapted for use with the code as was demonstrated in a 2004 design study for the U.S. Department of Energy’s (DOE’s) Next Generation Nuclear Plant (NGNP) project.²⁷ If the modular PBR is to be extensively deployed, such a capability can yield significant savings in capital and operating costs. Results from design calculations of two proposed PBR concepts are described in this paper.

I.D. Design Principles

As mentioned previously, designing a passively safe modular HTR involves finding that balance of core geometry and fuel composition that yields a core that burns fuel efficiently but does not exceed some prescribed accident temperature (usually 1600°C). Often, this has meant starting with the fuel. The heavy metal loading and enrichment of the pebble are chosen to yield an acceptable temperature reactivity coefficient. The core dimensions are chosen based upon pressure vessel size limitations,

predicted accident temperature, and desired thermal power output. Particularly in the case of the modular PBR, the core diameter may also be limited by the reactivity worth of the control rods and secondary shutdown elements that are generally restricted to the reflector. The inlet and outlet temperatures of the coolant, functions of material limits, and plant power requirements will also affect the operating and accident fuel temperatures. Altogether, such factors have generally limited PBR thermal output to ~ 500 MW(thermal). PBRs with power output >250 MW(thermal) would probably require a central reflecting column that acts as a temporary heat sink. The inner reflector also reduces the width of the fuel annulus to facilitate removal of decay heat.

With its stationary fuel, the prismatic HTR core permits control rods to be inserted directly into well-defined channels in the core, thus allowing higher thermal power output.²⁸ The size is still limited by the need to remove decay heat quickly in an accident and by the allowed pressure vessel dimensions.

Liem outlined such an approach to the design of the modular HTR (Ref. 29). A fuel design is first chosen along with the specified burnup limit as determined by the fuel qualification program and heavy metal loading. Core dimensions are chosen to limit the average power density to some safe value (~ 3 W/cm³) within a proposed pressure vessel. A loss-of-coolant accident is simulated to predict the peak fuel temperature. The core thermal power is adjusted by trial and error to obtain a peak accident temperature as close as possible to, but not exceeding, the 1600°C limit plus some suitable margin.

Alternatively, a desired thermal output and pressure vessel dimensions are prescribed. Fuel enrichment and reflector dimensions are then varied until a satisfactory peak accident temperature is achieved. Such an approach was used for the PBMR-400 (Ref. 25).

These approaches do not guarantee an optimal core design, just one that satisfies plant technical and economic requirements. Given the experience with LWR design and fuel management advances over the decades, it is safe to presume that HTRs can achieve greater economic viability with the development and application of modern optimization methods.

II. THEORY: EQUILIBRIUM CYCLE ANALYSIS OF ARBITRARY FUEL MANAGEMENT SCHEMES

II.A. Capturing the Relevant Physics

PEBBED solves the neutron diffusion equation in one, two, or three dimensions. Cartesian or cylindrical diffusion models can be solved, but because PEBBED was designed with PBRs in mind, the burnup and thermal-fluid solvers can be used only in cylindrical geometry. A standard finite-difference algorithm is employed for the

neutron diffusion module with user-specified boundary conditions. A novel analytic nodal solver^{30,31} has been implemented as an alternative in one or two dimensions (*R-Z*). The three-dimensional nodal solver is currently under development.

The temperature and burnup variations over the core of an HTR result in commensurate variation in absorption and scattering cross sections. For this reason, accurate results cannot be obtained without a reasonable determination of local material temperatures. PEBBED contains a dedicated steady-state convection module that generates local helium and pebble temperature maps. Although computationally quick, it is a one-dimensional solver that assumes that radial coolant flow is negligible. For improved accuracy and flexibility, the THERMIX-KONVEK module used in VSOP 1994 was coupled to PEBBED. THERMIX-KONVEK solves the heat transfer and gas dynamics equations in two dimensions (*R-Z*) and contains many material and heat transfer correlations appropriate for PBR analysis. Work is under way at Idaho National Laboratory (INL) to couple PEBBED to RELAP5 (Ref. 32) as an alternative to THERMIX and to simulate broader system behavior.

Few-group cross sections are generated using COMBINE (Ref. 33). COMBINE-7 is an INL code that solves the one-dimensional B-1 or B-3 approximations to the multigroup neutron transport equation for a unit cell with groupwise buckling terms to account for cell leakage. COMBINE-7 uses ENDF/B-VII data libraries processed with NJOY99 (Ref. 34) to solve for the flux over the entire energy range (2×10^7 to 1×10^{-5} eV). This avoids the limitation of many legacy unit cell spectrum codes that have separate thermal and fast spectrum modules that are unable to treat upscattering and low-energy resonances simultaneously. The spectrum is computed in 167 groups and collapsed to a few specified by the user. COMBINE-7 uses the Bondarenko method for treatment of the unresolved resonance region and either the Bondarenko or Nordheim numerical method for resolved resonances. The double heterogeneity of the fuel is addressed using separate Dancoff factors for the pebbles and TRISO particles. PEBBED exploits the rigorous method of computing Dancoff factors for randomly distributed pebbles and particles developed by Kloosterman and Ougouag and implemented in the PEBDAN code.³⁵ Although the cell homogenization algorithm in COMBINE-7 does not preserve the interpebble leakage rates, the correction developed by Lieberoth and Stojadinović is applied to adjust the diffusion coefficients.³⁶ Similarly, diffusion coefficients for the gas plenum between the top of the core and the top reflector can be computed using Gerwin and Scherer's method.³⁷

Because the PBR core does not contain well-defined assemblies, the user must (somewhat arbitrarily) divide the neutronics model into "spectral zones." For each zone, a unit cell COMBINE-7 model is executed, and cross sections are generated. Recently, a collaborative effort

between INL, Pebble Bed Modular Reactor (Pty) Limited (PBMR Pty), and the Pennsylvania State University resulted in a rigorous method for partitioning the core into these spectral zones in a way that maximizes overall accuracy.³⁸

Each spectral zone is divided into one or more nodes, the collection of which constitutes the mesh over which the diffusion and depletion equations are solved. Mesh sizes of 5 to 10 cm within the core are sufficient to achieve spatial convergence, a consequence of the long mean free path of neutrons in graphite. Spatial refinement is performed as part of model construction and testing.

The diffusion, spectrum, and thermal-fluid modules are solved in an iterative fashion until a final, internally consistent solution is obtained. When solving for the equilibrium core, a depletion module is also called for (see Fig. 1). The convergence criteria can be set by the user, but a value of no more than 10^{-6} for the eigenvalue and 10^{-4} for the local fission source are usually adequate to achieve iterative convergence. If depletion is performed, a criterion of 10^{-4} is used on the local burnup profile and 0.001 for the discharge burnup.

An extreme depressurized loss-of-coolant accident, also referred to as a DLOFC or depressurized conduction cooldown, can be simulated relatively quickly by ignoring the initial blowdown and any other effects of gas in the vessel. It becomes a time-dependent heat trans-

fer problem with the decay heat generated by the fuel, which has a known time dependence, as the volumetric heat source. The spatial distribution of the decay heat source is assumed to be constant and that of the steady-state diffusion solution (a conservative assumption). If a quick approximation is desired, PEBBED possesses a transient conduction-radiation solver that predicts the peak fuel temperature by assuming that decay heat is transferred out of the core in the radial direction and that the peak temperature occurs at the axial location of the peak power density during steady-state operation. For greater accuracy, THERMIX can solve the same conduction-radiation problem in two dimensions.

Such an event would have to be triggered by a massive failure of the coaxial coolant pipe attached to the vessel and, in all likelihood, is well beyond the design basis of any HTR currently on the drawing boards. The bounding nature of this transient and the relative ease with which it can be simulated, however, make it a common scenario for evaluating the passive heat removal capability of an HTR concept.

The coupling of the diffusion and depletion equations that takes into account the movement of the pebbles is central to the PEBBED algorithm. It is discussed in detail in Sec. II.C.

II.B. Physics Captured Inadequately or Not At All (Currently)

PEBBED is still under development and as of yet does not adequately capture some of the physics of the PBR. The following features of the PBR are subjects of continued methods and code development at INL:

1. Transport effects (phenomena not adequately captured by diffusion theory) are observed near the core periphery because of the sudden change in material composition and the presence of strong absorbers (control rods). In collaboration with the Georgia Institute of Technology, INL is developing new methods of capturing the transport phenomena associated with these core features.³⁹

2. PEBBED currently assumes a uniform packing fraction of pebbles in the core although the variable nature of sphere packing in a pebble bed has been documented. This assumption does not appear to be a cause of significant errors.⁴⁰ The PEBBED code is being modified to allow for radially varying packing density.

3. PEBBED can solve the diffusion equation in three dimensions so that the neutronic effects of control rods can be captured to first order. The THERMIX-KONVEK solver coupled to PEBBED is limited to the *R-Z* plane, and thus, azimuthal temperature variability is neglected. The fuel-loading algorithm assumes that pebbles emerging from different azimuthal zones are mixed upon re-entry. This is appropriate for all PBR concepts proposed to date. The algorithm can be generalized to account for

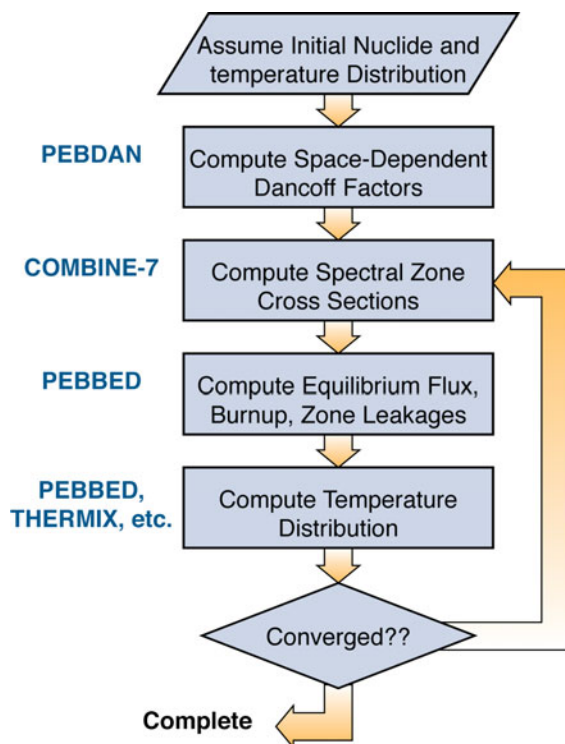


Fig. 1. High-level iterative scheme for equilibrium cycle analysis.

asymmetric azimuthal fuel loading if desired, but this is not anticipated.

4. PEBBED assumes that the pebble bed is a square cylinder in shape even though the pebbles form a conical shape under the loading chute(s) and just above the discharge chutes. The narrow discharge chutes in particular force radial motion by the pebbles near the bottom of the core. PEBBED currently assumes that all pebble motion is strictly axial. The method of coupling pebble motion to burnup, described below, is applicable to the general pebble motion problem.

The lack of treatment of these effects does reduce the accuracy of the results and should be addressed as part of a complete methods development effort. It does not, however, detract from the efficacy of the method described in Sec. II.C.

II.C. Coupling Pebble Flow to Burnup: The Recirculation Matrix

The key to applying high-performance optimization tools to the PBR core design problem is in finding an efficient mathematical representation of pebble flow. With such a representation, the solution space of even sophisticated fuel management schemes can be sampled and explored with the manipulation of a few well-defined parameters. The so-called recirculation matrix, introduced by the authors in an earlier work,⁴¹ is developed further in this section.

II.C.1. Solution to the Equilibrium Cycle Core

For simplicity and without loss of generality, assume that the flow direction of pebbles is strictly axial but that the pebble velocity can vary in the radial direction. The continuity equation of the atom density N of the k 'th nuclide in a reactor core is thus given by Eq. (1):

$$\begin{aligned} & \frac{\partial N_k(r, z, t)}{\partial t} + \frac{\partial N_k(r, z, t)}{\partial z} v_z(r, z) \\ &= \phi(r, z, t) \sum_{i=1}^m N_i(r, z, t) \sigma_{fi} y_{ik} \\ &+ \phi(r, z, t) \sum_{s=r}^q N_s(r, z, t) \sigma_{asi} \gamma_{sk} \\ &+ \sum_{j=n}^p N_j(r, z, t) \lambda_j \alpha_{jk} - \lambda_k N_k(r, z, t) \\ &- \phi(\vec{r}, t) N_k(r, z, t) \sigma_{ak} . \end{aligned} \quad (1)$$

The terms on the right side of Eq. (1) correspond to the positive contributions from the fission yield of (fissionable) nuclides $i = 1 \dots m$, neutron capture in nuclides $s = r \dots q$, radioactive decay in nuclides $j = n \dots p$,

and negative contributions from decay and neutron capture, respectively. In stationary (batch loaded) cores, $v_z(r, z) = 0$, and the second term on the left vanishes. This is the basic equation solved by depletion codes such as ORIGEN and CINDER for LWR and prismatic HTR analysis.

This is also the equation solved in VSOP and PANTHERMIX, but in a stepwise fashion. A batch of fuel residing in a specified local region of the core is burned for a period corresponding to the transit time of pebbles passing through the volume. The depleted batch is moved to the next volume in the flow stream with the depleted number densities used as the initial concentrations for the next time step. Between the steps, the flux profile is updated with a call to the diffusion module.

PEBBED converges directly upon the asymptotic (equilibrium) core and thus assumes that the first term on the left vanishes to yield Eq. (2):

$$\begin{aligned} & \frac{\partial N_k(r, z, t)}{\partial z} v_z(r, z) = \phi(r, z, t) \sum_{i=1}^m N_i(r, z, t) \sigma_{fi} y_{ik} \\ &+ \phi(r, z, t) \sum_{s=r}^q N_s(r, z, t) \sigma_{asi} \gamma_{sk} \\ &+ \sum_{j=n}^p N_j(r, z, t) \lambda_j \alpha_{jk} \\ &- \lambda_k N_k(r, z, t) \\ &- \phi(\vec{r}, t) N_k(r, z, t) \sigma_{ak} . \end{aligned} \quad (2)$$

The final solution to Eq. (2), the static nuclide distribution in the core, is obtained by solving it and the diffusion equation iteratively until burnup convergence is achieved. The thermal-fluid and spectrum equations are also solved in this loop to yield a fully consistent core solution.

Solving Eq. (2) requires an axial boundary condition corresponding to the initial condition required of the solution to the time-dependent depletion equation. In a so-called "once through then out" (OTTO) core in which pebbles pass through the vessel once before final discharge, the upper ($z = 0$) boundary condition is simply the set of fresh fuel nuclide densities in the pebble. The nuclide densities at each subsequent axial node boundary descending through the core are obtained by solving Eq. (2) using the local flux and the densities from the preceding mesh boundary. The core thermal power, height, and downward velocity $v_z(r, z)$ determine the burnup accrued by a pebble during its transit through the core.

The top axial boundary condition $N(r, z = 0)$ is not so obvious for PBRs in which partially burned pebbles are removed from the bottom ($z = H$) and dropped back onto the top of the pebble bed along with fresh pebbles. For simple systems in which pebbles are dropped randomly into the core and recirculated for a total of M

passes before final discharge, the top (or entry plane) nuclide density is simply the average of the fresh fuel density (oN) and the densities of the pebbles at the bottom (or exit plane) after passes 1 through $M - 1$:

$$N(z = 0) = \frac{{}^oN + \sum_{m=1}^{M-1} {}^mN(z = H)}{M} . \quad (3)$$

Equation (3) is fairly straightforward to compute and enables the burnup analysis of simple PBR cores such as the HTR Modul 200 in which there is only one pebble type and one central loading tube. Such a calculation was invoked in the original method developed by Terry et al.²⁶

II.C.2. Development of a General Axial Boundary Condition

The general situation in which there may be multiple pebble types and radially distributed loading tubes is more complex but, as will be shown here, for all cases of practical interest is actually quite tractable and can be expressed in terms of a few known parameters.

Consider the case in which the pebble bed consists of J radial flow channels (see Fig. 2 with $J = 4$), each with a known axial speed and cross-sectional area, and therefore a known volumetric flow rate (e.g., cubic centimeters of pebbles per day) given by f_i .

If the total flow rate of the core is F , then

$$\sum_{i=1}^J f_i = F . \quad (4)$$

The fraction of the total core pebble flow that flows through channel i is expressed as the flow partition coefficient:

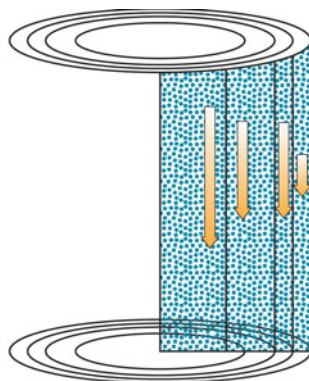


Fig. 2. Pebble bed divided into four flow channels. The arrows indicate the magnitude of the flow rate.

$$\alpha_i = \frac{f_i}{F} . \quad (5)$$

Assume a complex core composed of P types of pebbles. Different pebble types may include driver pebbles with 10% low-enriched uranium (LEU), burner pebbles with plutonium derived from weapons stockpiles, graphite pebbles with no fuel, etc. Pebble types may also have the same initial composition, but they differ in their trajectory through the core. A burnup policy is imposed that requires pebbles of type $p = 1$ to pass through the core an average of 1M times, pebbles of type $p = 2$ to pass through the core 2M times, and so on as determined by the desired burnup.

The flow in the core is partitioned first by radial channel, then by pebble type, and then by pass number as follows. Denote the fraction of the flow in channel i composed of pebbles of type p as f_i^p such that

$$\sum_{p=1}^P f_i^p = f_i \text{ (the total flow rate of pebbles in channel } i \text{)} . \quad (6)$$

Partition f_i^p by passes (i.e., denote the fraction of pebbles of pebble type p in channel i that are on their m 'th pass as ${}^m f_i^p$) so that

$$\sum_{m=1}^M {}^m f_i^p = f_i^p \text{ (the total flow rate of pebbles of type } p \text{ in channel } i \text{)} . \quad (7)$$

At this point it is necessary to distinguish the volumetric nuclide density N , which may consist of contributions from a number of different pebble types at various burnup levels, from the homogenized number density of the flow of a specific pebble type, which is denoted as \hat{N} . The flow rate ${}^m \dot{n}_i^p$ (e.g., atoms per second) of pebbles of type p in channel i on their m 'th pass is related to the homogenized nuclide density (e.g., atoms per cubic centimeter) in pebbles of the same type, in the same channel, and on the same pass, by

$$\begin{aligned} {}^m \dot{n}_i^p &= {}^m \hat{N}_i^p \cdot f_i \cdot \frac{f_i^p}{f_i} \cdot \frac{{}^m f_i^p}{f_i^p} \\ &= {}^m \hat{N}_i^p \cdot f_i \cdot \alpha_i^p \cdot {}^m \alpha_i^p . \end{aligned} \quad (8)$$

Here are two more partition coefficients introduced and defined as follows:

$$\alpha_i^p = \frac{f_i^p}{f_i} \text{ (type coefficient)} , \quad (9)$$

equal to the fraction of pebbles in channel i that are of type p , and

$${}^m \alpha_i^p = \frac{{}^m f_i^p}{f_i^p} \text{ (pass coefficient)} , \quad (10)$$

equal to the fraction of pebbles of type p in channel i that are on their m 'th pass.

To obtain the total flow of a nuclide into channel i , sum over M passes and P types:

$$\sum_{p=1}^P \sum_{m=1}^M m \dot{n}_i^p = \dot{n}_i = N_i f_i . \quad (11)$$

Substitute Eq. (8) into Eq. (11) to obtain an expression for the total flow rate of the nuclide in terms of the contributions from all pebbles and passes:

$$\dot{n}_i = \sum_{p=1}^P \sum_{m=1}^M m \dot{n}_i^p = \sum_{p=1}^P \sum_{m=1}^M m \hat{N}_i^p f_i \cdot \alpha_i^p \cdot \alpha_i^p . \quad (12)$$

The flow of a nuclide into channel i is composed of contributions from the channel exit plane flows (except for the last pass), denoted here by ${}^m \hat{n}_j^p$, and the injection of the nuclide in fresh pebbles, ${}^1 n_i^p = {}^1 \hat{N}_i^p {}^1 f_i^p$. Partially burned pebbles dropping out of channel j will be distributed over all channels depending on the recirculation policy, so they are defined as another partition coefficient

$${}^m \alpha_{i \leftarrow j}^p = \frac{{}^{m+1} f_{i \leftarrow j}^p}{m f_j^p} \text{ (transfer coefficient)} \quad (13)$$

as the fraction of pebbles on pass m , of type p , in channel j that are transferred to channel i at the entry plane for their $m + 1$ 'th pass. The flow rate of type p pebbles on their $m + 1$ 'th pass in channel i is thus the sum of contributions from the type p pebbles in all channels j having completed their m 'th pass:

$$\begin{aligned} {}^{m+1} \dot{n}_i^p &= \sum_{j=1}^J {}^m \hat{n}_j^p \cdot {}^m \alpha_{i \leftarrow j}^p \\ &= \sum_{j=1}^J ({}^m \hat{N}_j^p \cdot f_j \cdot \alpha_j^p \cdot \alpha_j^p) {}^m \alpha_{i \leftarrow j}^p . \end{aligned} \quad (14)$$

Now sum this over all passes m except for the last pass, add the fresh flow contribution ${}^1 n_i^p$, and sum over all pebble types p to get the total flow of the nuclide into the channel:

$$\sum_{p=1}^P \sum_{m=1}^M m \dot{n}_i^p = \sum_{p=1}^P \left\{ {}^1 \dot{n}_i^p + \sum_{j=1}^J \sum_{m=1}^{M-1} {}^m \hat{N}_j^p \cdot f_j \cdot \alpha_j^p \cdot \alpha_j^p \cdot {}^m \alpha_{i \leftarrow j}^p \right\} . \quad (15)$$

Using Eq. (11) and dividing by f_i , this becomes

$$N_i = \frac{1}{f_i} \sum_{p=1}^P \left\{ {}^1 \hat{N}_i^p {}^1 f_i^p + \sum_{j=1}^J \sum_{m=1}^{M-1} {}^m \hat{N}_j^p \cdot f_j \cdot \alpha_j^p \cdot \alpha_j^p \cdot {}^m \alpha_{i \leftarrow j}^p \right\} . \quad (16)$$

The denominator can be brought inside the sums, and noting that

$${}^1 f_i^p = {}^1 \alpha_i^p \cdot \alpha_i^p \cdot f_i , \quad (17)$$

then

$$N_i = \sum_{p=1}^P \left\{ \frac{{}^1 \hat{N}_i^p f_i {}^1 \alpha_i^p \alpha_i^p}{f_i} + \sum_{j=1}^J \sum_{m=1}^{M-1} {}^m \hat{N}_j^p \cdot \frac{f_j}{f_i} \cdot \alpha_j^p \cdot \alpha_j^p \cdot {}^m \alpha_{i \leftarrow j}^p \right\} . \quad (18)$$

Finally, given that

$$\frac{f_j}{f_i} = \frac{\frac{f_j}{F}}{\frac{f_i}{F}} = \frac{\alpha_j}{\alpha_i} , \quad (19)$$

one can write

$$N_i = \sum_{p=1}^P \left\{ {}^1 \hat{N}_i^p \cdot {}^1 \alpha_i^p \cdot \alpha_i^p + \sum_{j=1}^J \sum_{m=1}^{M-1} {}^m \hat{N}_j^p \cdot \frac{\alpha_j \cdot \alpha_j^p \cdot \alpha_j^p \cdot {}^m \alpha_{i \leftarrow j}^p}{\alpha_i} \right\} . \quad (20)$$

Evaluating Eq. (20) yields the nuclide concentration at the entry plane for each channel and thus provides the axial boundary condition required to solve Eq. (2). The exit plane pebble densities at the end of the first pass are obtained by depleting the fresh compositions for each pebble type through each channel given an assumed asymptotic

flux profile. Channel-specific weighted averages of the exit plane densities then become the initial densities for the next pass. The computation is repeated up to the specified number of passes for each pebble type.

The partition coefficients, α_j , α_j^p , ${}^m\alpha_j^p$, and ${}^m\alpha_{i\leftarrow j}^p$, are functions of the core geometry and the pebble loading and recirculation policy. The fraction of total core flow in channel j (α_j) is obtained from the radial boundaries of the channel and the velocity profile (given as input). The pebble type fraction per zone (α_j^p) and the transfer coefficient (${}^m\alpha_{i\leftarrow j}^p$) are both functions of the pebble loading mechanism. These may be considered to have user-specified values in that they can be altered either in the core design process or, if the design allows, during operation. The remaining coefficient, the fraction of pebbles of type p on pass m (${}^m\alpha_j^p$), is now shown to be a function of the other coefficients.

The flow of pebbles of type p that are on their m 'th pass and in channel j is a fraction of the total flow as given by

$$\begin{aligned} {}^m\hat{f}_i^p &= \hat{F} \cdot \frac{\hat{f}_i}{\hat{F}} \cdot \frac{\hat{f}_i^p}{\hat{f}_i} \cdot \frac{{}^m\hat{f}_i^p}{\hat{f}_i^p} \\ &= \hat{F} \cdot \alpha_i \cdot \alpha_i^p \cdot {}^m\alpha_i^p, \end{aligned} \quad (21)$$

where

\hat{f} = pebble flow rate (e.g., pebbles per second) rather than the volumetric flow rate

\hat{F} = total core pebble flow rate.

The two rates are related by the homogenized number density of the pebble and surrounding void.

This flow rate can also be evaluated from that of pebbles completing the $m - 1$ 'th pass:

$${}^m\hat{f}_i^p = \sum_{j=1}^J \hat{F} \cdot \alpha_j \cdot \alpha_j^p \cdot {}^{m-1}\alpha_j^p \cdot {}^{m-1}\alpha_{i\leftarrow j}^p. \quad (22)$$

Equating Eqs. (21) and (22) and eliminating the total core flow rate yield

$$\alpha_i \cdot \alpha_i^p \cdot {}^m\alpha_i^p = \sum_{j=1}^J \alpha_j \cdot \alpha_j^p \cdot {}^{m-1}\alpha_j^p \cdot {}^{m-1}\alpha_{i\leftarrow j}^p. \quad (23)$$

Solve for ${}^m\alpha_j^p$ to obtain

$${}^m\alpha_j^p = \frac{\sum_{j=1}^J \alpha_j \cdot \alpha_j^p \cdot {}^{m-1}\alpha_{i\leftarrow j}^p}{\alpha_i \cdot \alpha_i^p}. \quad (24)$$

This indicates that each pass-type partition coefficient ${}^m\alpha_j^p$ is a function of ${}^{m-1}\alpha_j^p$ ($j = 1 \dots J$). Equation (24) is valid for $m > 1$ (i.e., all recirculated pebbles). To obtain a fully determined set of linear equations, one more linear relation among these coefficients is needed.

This expression is obtained from the fact that, by definition, the sum of ${}^m\alpha_j^p$ over all passes is unity:

$$\sum_{m=1}^M {}^m\alpha_j^p = 1 \quad \text{for all } j, p. \quad (25)$$

The system of equations is more obvious if one substitutes the following into Eq. (24). Let

$${}^{m-1}K_{ij}^p = \frac{\alpha_j \cdot \alpha_j^p \cdot {}^{m-1}\alpha_{i\leftarrow j}^p}{\alpha_i \cdot \alpha_i^p} \quad (26)$$

so that

$${}^m\alpha_i^p = \sum_{j=1}^J {}^{m-1}K_{ij}^p \cdot {}^{m-1}\alpha_j^p. \quad (27)$$

Or, cast as a linear equation with constant coefficients

$$\begin{aligned} {}^m\alpha_i^p - {}^{m-1}K_{i1}^p \cdot {}^{m-1}\alpha_1^p - {}^{m-1}K_{i2}^p \cdot {}^{m-1}\alpha_2^p \dots \\ - {}^{m-1}K_{iJ}^p \cdot {}^{m-1}\alpha_J^p = 0 \quad (m = 2, \dots, M). \end{aligned} \quad (28)$$

Equations (28) and (25) yield a fully determined set of linear equations of order $J \cdot {}^pM$ that can be solved, for each pebble type, using common matrix inversion routines.

The total number of passes M of each type is a function of the pebble flow rate f , thermal power P , heavy metal content m_{hm} of the fresh pebbles, and the burnup B_d to be attained before final discharge:

$$M = \text{int} \left(\frac{B_d m_{hm} f}{P} \right). \quad (29)$$

This value must be an integer as pebbles cannot be discharged from the interior of the core. The actual burnup accrued after M passes will most certainly differ from the desired value. In PEBBED, therefore, another iterative loop is implemented with the total flow rate and total number of passes adjusted until the desired and computed burnup values match within a defined tolerance for the predominant or user-specified fuel type.

II.D. Limits of Validity of the Continuous Pebble Flow Assumption

An underlying assumption of the pebble flow formulation described in Sec. II.C is that pebble (and thus nuclide) flow is continuous and infinitely divisible. This is of course invalid in the limit of very low flow rates, as pebbles are discrete and indivisible. An overall core flow rate of, for example, 5000 pebbles/day equates to dropping a single pebble into the core every ~ 17 s. If the core is divided into five flow channels, any one flow channel may receive a fresh pebble only once every 3 or 4 min rather than a continuous trickle of fresh fuel, as implied in the algorithm. Within a volume of a few liters,

there is no homogeneous mixture of all different types and burnup levels of pebbles. Rather, a few pebbles of a certain type and burnup level are present, and those of other types and burnups are not present at all. The pass partition coefficient [Eq. (10)] is really a measure of the probability of finding a pebble of type p on its m 'th pass in that volume. As the size or number of volumes sampled increases, or as the frequency at which a given volume is sampled increases, the average distribution of pebbles will approach the value predicted by the continuous flow model.

The continuous flow assumption is assumed to be reasonable for the modular PBR cores under consideration. The ratio of the core volume to the effective pebble volume (450 000:1 in the case of the PBMR-400) is large enough to smooth out the effects of local heterogeneity. The total residence time of a single pebble (~ 2.5 yr for the PBMR-400) is long compared to the time between consecutive pebble injections, so that the actual (discretized) nuclide injection rate approaches the continuous limit. Nonetheless, the results of any core analysis or optimization in which very small flow rates for a given type or burnup are computed should be interpreted with caution. The actual burnup or power density within a small control volume of the core may differ considerably from the value computed with codes such as PEBBED. The stochastic nature of fuel loading in the PBR means that there is a finite probability of "hotspot" formation in which two or more fresh pebbles will be collocated in a region of elevated thermal flux. For fission product release during an accident, the consequences of such clumping increase with the number of fresh pebbles in the clump. Fortunately, the probability that a clump will form decreases dramatically with this number. Investigations of this scenario have been performed and documented by PBMR Pty and INL (Refs. 42 and 43), but further study is planned.

Using examples from literature, Sec. III describes how partition coefficients can be obtained for two types of PBRs. It shows how to compute the partition coefficients for various pebble-loading schemes directly from a few-core geometry and pebble flow parameters. This facilitates the use of a wide variety of optimization techniques for pebble bed fuel management and core design, one of which has been implemented and is described in Sec. IV.

III. APPLICATION TO DIFFERENT FUEL MANAGEMENT SCHEMES

III.A. A Simple Core (Single Type, Burnup Independent)

III.A.1. The Mathematical Model

The simplest type of pebble recirculation scheme is exploited in the HTR Modul. There is only one pebble

type, and single, centrally located fuel loading and discharge chutes allow for no radial "zoning" of pebbles. The flow rate and discharge burnup were chosen such that each pebble passes through the core an average of 15 times.

The number of flow channels J is set by the user to resolve the potential burnup variation in the radial direction that results from changes in the radial flux and pebble flow rates, particularly near the core reflector boundaries. In PEBBED, this number is limited only by the number of nodes in the radial direction inside the core region that are defined for the solution of the neutron diffusion equation. Five channels are typically used with the mesh boundaries chosen to yield approximately the same flow fraction per channel (i.e., $\alpha_j \approx 0.2$).

Because there is only one pebble type, then $\alpha_j^p = 1$ for all j ($P = 1$). Finally, with only a single loading tube, partially burned pebbles exiting the core will be probabilistically distributed among channels at the entry plane according to their individual flow rates:

$${}^m\alpha_{i \leftarrow j}^p = \alpha_j \quad (30)$$

The pass partition coefficients ${}^m\alpha_j^p$ can be obtained by solving the linear system described in Sec. II.C. With this simple recirculation system, however, all burnup levels must be equally represented in each channel (i.e., ${}^m\alpha_j^p = \frac{1}{15}$, for all j and m).

III.A.2. Results of Equilibrium Core Analysis

PEBBED results for this system are shown below. Figure 3 shows the core model with dimensions of the major components in the neutronic and thermal-hydraulic model. The bottom and top pebble codes have been flattened so that the core height corresponds to the mean value of 960 cm with a 40-cm gas plenum above it. The entire core is surrounded by a mostly solid graphite reflector except for the bottom reflector, which is porous to allow the coolant to exit. A control rod penetrates the radial reflector to a depth of 150 cm below the top of the pebble bed. In this R - Z model, the control rod is modeled as a "gray curtain" surrounding the core.

The pebbles each contain ~ 7 g of uranium enriched to 7.8% ^{235}U . They were designed to be discharged with an average burnup of 80 GWd/kg HM, which, with an axial flow rate of ~ 15 cm/day, means that each pebble passes through the core 15 times before final discharge.

Figure 4 is a contour map of the local power density in watts per cubic centimeter. A peak power density of 6.3 W/cm³ occurs at the center of the core ~ 390 cm below the top. The THERMIX-KONVEK module computes a peak operating temperature of 830°C and a peak accident temperature (after a depressurized loss-of-coolant flow) of 1601°C. PEBBED predicts a core

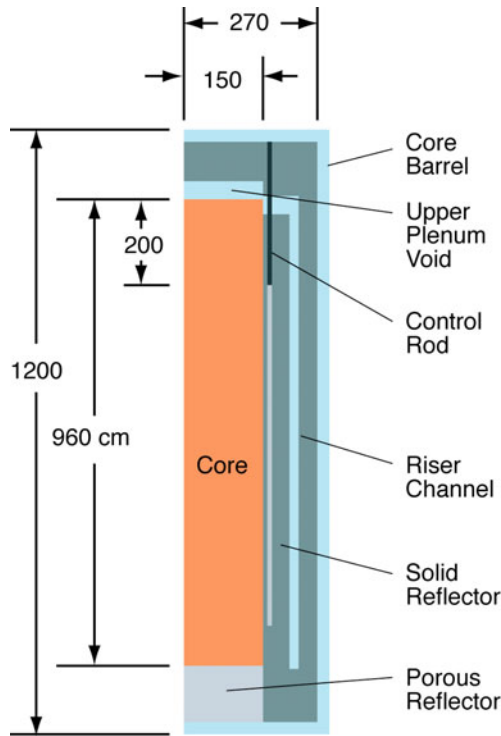


Fig. 3. One-type, one-zone recirculation pattern.

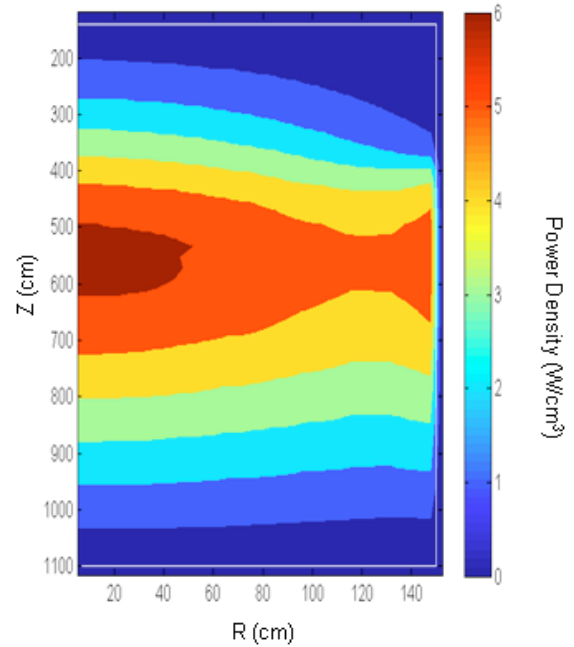


Fig. 4. Local power density in the HTR Modul equilibrium core. The origin corresponds to the top center of the pebble bed.

eigenvalue of 1.043. This value would drop considerably with the inclusion of more fission products (only xenon and samarium were included in this model), but there seems to be considerable excess reactivity margin that would allow the use of lower enrichment or higher discharge burnup.

*III.B. A Core with Two Radial Zones
(Two Types, Burnup Independent)*

An early version of the reactor being developed in South Africa featured an inner reflector composed of graphite pebbles that circulated along with the fuel pebbles. This so-called dynamic inner reflector would be replenished via the central fuel-loading tube. The fuel pebbles would be dropped into the annulus via three loading tubes arranged some distance from the core centerline (see Fig. 5).

The core was designed to use about 332 000 fuel pebbles in the active core. Each would contain 9 g of uranium dioxide enriched to 8% and would be burned to 80 GWd/kg HM over ten passes.

Although no longer under consideration by PBMR Pty, this concept has some attractive features, including the lack of the need to replace inner reflector blocks at periodic intervals.

The stochastic loading of pebbles and the small amount of radial motion that occurs while the pebbles

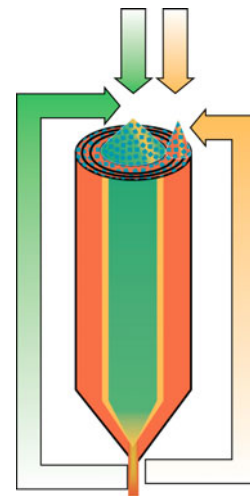


Fig. 5. Loading pattern with two radial zones and pebble types.

move through the core result in some mixing of the graphite and fuel pebbles. Computer simulations⁴⁴ suggest that this mixing would occur over a 30-cm-wide band centered ~87 cm from the core centerline. Within this “mixing channel” the average ratio of graphite to fuel pebbles would be about 1:1, but the local ratio would vary smoothly from all graphite to all fuel with increasing distance from the centerline.

III.B.1. The Mathematical Model

In a model developed for VSOP, the boundary between the inner graphite column and the outer fuel annulus lies about halfway through the second pebble flow channel, and thus, this channel contains both graphite and fuel. The location of this boundary is determined by the relative flow rates of pebbles loaded into these two major core zones. Channel boundaries are chosen so that the second channel is the only one that contains both fuel and graphite pebbles. The inner channel (1) contains only graphite, and the outer channels (3, 4, and 5) contain only fuel. The type partition coefficients α_j^p are computed from the user-supplied parameter that specifies the fraction of total pebble flow that is loaded into the outer zone. This parameter is defined in Eq. (31):

$$\alpha_o = \frac{\hat{f}_o}{\hat{F}} . \quad (31)$$

For the PBMR, this value is about 0.75, which means that 75% of the total pebble flow in the core is loaded via the outer fuel-loading chutes. The remaining 25% of pebbles is loaded through the central loading chute. Radiation instrumentation installed below the discharge chute would enable the graphite pebbles to be separated from the fuel pebbles. Graphite pebbles are thus directed to the central loading tube while the fuel pebbles are directed to the peripheral chutes (or discarded if damaged or fully spent). The resulting pebble flow distribution in the core is depicted in Fig. 6.

The points in Fig. 6 represent the pebble centers, the locations of which were generated using the pebble placement algorithm in PEBDAN (Ref. 45). The lighter points

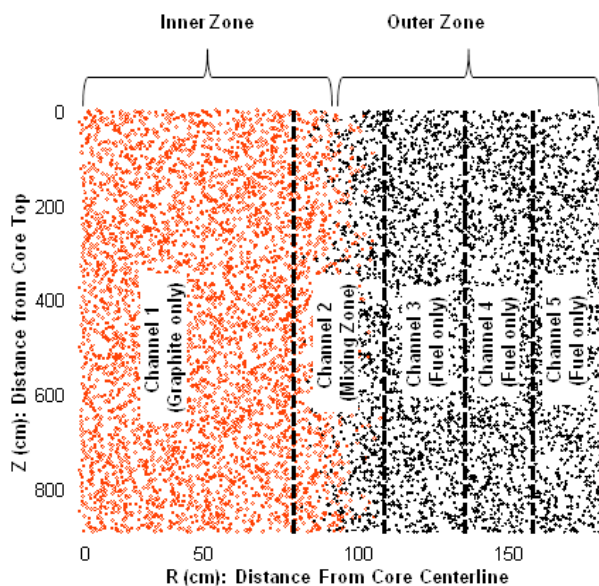


Fig. 6. Pebble distribution in PBMR-268 core.

are graphite pebble centers while the darker points correspond to fuel. This method generates a large and randomly placed collection of points within a vessel and then removes a subset of these points that can physically represent nonoverlapping pebbles. The technique does not fully capture the packing geometry of a drop-in loaded pebble bed, including the loading and discharge cones, but it does reproduce the statistical and deterministic variations in packing fraction. As mentioned in Sec. II.B, PEBBED is not currently structured to model the discharge and loading cones, so these deficiencies in PEBDAN do not contribute significantly to any error in the final result. Assuming that the flux is low in the cone regions, the error introduced by this simplification is considered small enough as to not invalidate the analytical results.

The type coefficients are computed from α_o and the flow coefficients using, for fuel ($p = 1$), Eq. (32):

$$\alpha_j^p = \begin{cases} 1 & \text{for } \frac{\alpha_o - \sum_{i=1}^j \alpha_i}{\alpha_j} > 1 \\ \max\left(0, \frac{\alpha_o - \sum_{i=1}^j \alpha_i}{\alpha_j}\right) & \text{for } \frac{\alpha_o - \sum_{i=1}^j \alpha_i}{\alpha_j} \leq 1 \end{cases} . \quad (32)$$

The complement of these values yields the type coefficients for graphite pebbles ($p = 2$), Eq. (33):

$$\alpha_j^2 = 1 - \alpha_j^1 . \quad (33)$$

The transfer coefficients ${}^m\alpha_{i \leftarrow j}^p$ are type dependent. Graphite pebbles are directed to the inner zone (channels 1 and 2) while fuel pebbles are directed to the outer zone (channels 2 through 5).

The transfer partition coefficients can be computed from

$${}^m\alpha_{i \leftarrow j}^p = \frac{\alpha_i^p \alpha_j}{\sum_{n=1}^p \alpha_n^p \alpha_n} \quad \text{for all } m . \quad (34)$$

The numerator is the fraction of total core pebble flow that occurs in channel i and consists of type p . The summation in the denominator is the fraction of the total core pebble flow in all channels that consists of type p . For $p = 1$ (fuel), the summation in the denominator is just α_o . For graphite pebbles, the summation equals $1 - \alpha_o$.

These relations are coded into PEBBED and can be invoked by flagging a two-zone, burnup-independent recirculation option in the input. The user needs only to supply the radial velocity distribution and channel radii, total core flow rate, target discharge burnup, and fraction

TABLE I
Partitioned Pebble Flow (Pebbles per Hour) in the PBMR-268

Pass	Channel				
	1	2	3	4	5
Partition of Fuel Pebbles by Channel and Pass Number					
1	0	2.19	4.62	4.41	4.48
2	0	2.19	4.62	4.41	4.48
3	0	2.19	4.62	4.41	4.48
4	0	2.19	4.62	4.41	4.48
5	0	2.19	4.62	4.41	4.48
6	0	2.19	4.62	4.41	4.48
7	0	2.19	4.62	4.41	4.48
8	0	2.19	4.62	4.41	4.48
9	0	2.19	4.62	4.41	4.48
10	0	2.19	4.62	4.41	4.48
All passes	0	21.9	46.2	44.1	44.8
Partition of Graphite Pebbles by Channel and Pass Number					
1	41.29	18.88	0	0	0

of core flow in the outer zone α_o . The code computes the remaining partition coefficients from these parameters.

As in the HTR Modul, the radial distribution of pebbles at the entry plane is not burnup dependent, and thus, all burnup stages are equally represented at each location in the fueled channels (i.e., ${}^m\alpha_i^1 = \frac{1}{10}$ for all passes m). The graphite pebbles are similarly distributed by pass, but since no burnup is accrued in these pebbles, they can be circulated using an OTTO policy without affecting the neutronic solution. The partitioned pebble flow data,

based upon an overall core pebble flow rate of 6751 pebbles/day, are shown in Table I.

III.B.2. Results of Equilibrium Core Analysis

Portions of the PEBBED results are illustrated in the contour plots of Fig. 7. The boundaries of the pebble bed are denoted by the thin white line. The fast flux (1.7×10^7 to 1.1×10^5 eV) peaks at 6.0×10^{13} n/cm²·s inside the core while the thermal flux (1.86 to 10^{-5} eV) reaches

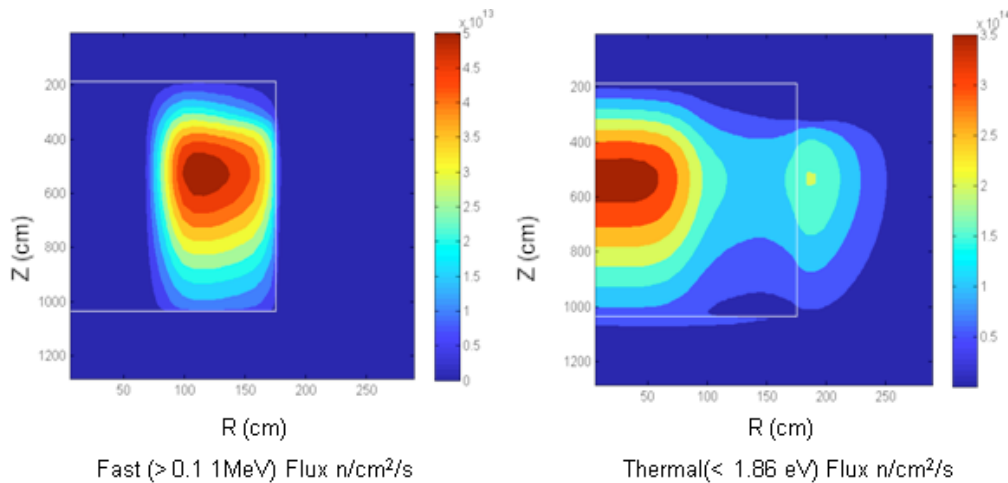


Fig. 7. Thermal and fast flux in the PBMR-268 equilibrium core.

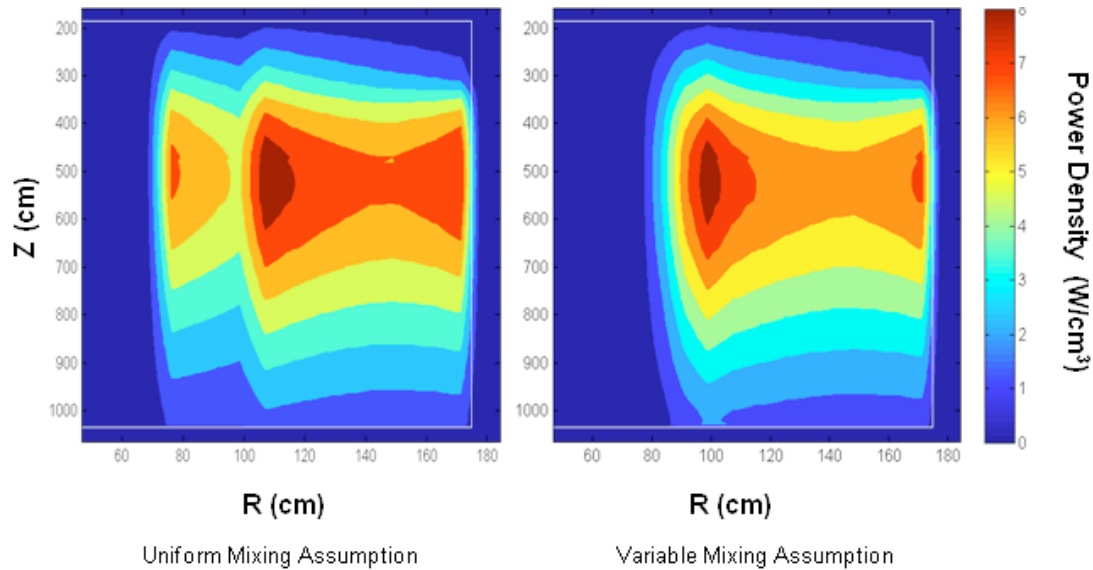


Fig. 8. Power density maps of PBMR-268 core assuming different pebble mixing profiles in the mixing zone.

a maximum of 3.7×10^{14} n/cm²·s inside the inner reflector. PEBBED computes an equilibrium core multiplication factor of 1.0090. The point of maximum power density is located 99 cm from the core axis (in the mixing zone) and 335 cm from the top of the pebble bed. The peak DLOFC temperature computed by THERMIX-KONVEK is 1559°C and occurs ~62 h after shutdown.

As stated previously, the distribution of pebbles in the mixing channel is not uniform with regard to type but rather varies smoothly from all graphite to all fuel moving outward from the centerline. PEBBED assumes a half-sinusoid shape, varying the number densities smoothly from the inner zone composition to the outer zone composition. Other codes assume a uniform average composition across the mixing zone even though it may be divided into multiple diffusion nodes. For comparison, the power densities were computed using both assumptions and compared in Fig. 8. The uniform mix-

ing assumption yields a second peak in power density in the mixing zone resulting from the rise in the thermal flux in this region. With a smoothly varying transition from fuel to graphite pebbles, the increasing thermal flux is offset by the decreasing fuel density, and this second peak disappears.

Other core parameters are compared in Table II. The uniform mixing assumption appears to err on the conservative side with regard to the maximum accident fuel temperature, but it may underestimate the maximum steady-state fuel temperature. Firm conclusions should be drawn only after studies are performed with more refined neutronics and thermal-fluid models.

III.B.3. Pebble Recirculation and Isotopic Variability

The nature of fuel management in a stochastically loaded, recirculating PBR means that the exposure history

TABLE II
Effect of Different Pebble Mixing Assumptions on Core Parameters

Core Parameter	Uniform Distribution	Sinusoidal Distribution
k_{eff}	1.0068	0.9960
Peak fuel temperature: steady state (°C)	1016	1034
Peak fuel temperature: DLOFC (°C)	1636	1612
Peak pebble power (W)	2330	2400
Axial location of power density peak (cm from top)	235	235
Radial location of power density peak (cm from centerline)	109	95
Time after shutdown at which peak occurs (h)	57.2	58.5

of a specific pebble can only be approximately computed. Most of the variability occurs when the pebble is dropped onto the top of the bed. The final azimuthal and radial location cannot be predicted for a given pebble. Because the number of pebbles in the core is large, however, a predictable distribution of pebbles over the bed surface (entry plane) can be computed. Given the steady-state flux profile assumption of the equilibrium core, the variability of exposure among pebbles can be computed using the machinery in PEBBED. The resulting information can be useful for core monitoring, nonproliferation, and source term analysis.

The calculation is relatively straightforward. For simplicity, one can assume that azimuthal variations in flux are minimal and that the burnup accrued by a pebble is a function of its radial distance from the core centerline. The spatial discretization of the core into a small number of radial channels implies that a given pebble has a finite number of trajectories it can follow during its life in the core. For example, in the two-zone PBMR model analyzed in Sec. III.B, there are five radial pebble flow channels into which fuel pebbles can drop into the outer four (see Fig. 6). Thus, there are four possible burnup pathways for a pebble on its first pass. Because each pebble is recirculated about ten times through the core before discharge, the number of possible life trajectories of the pebble is 4^{10} or 1048576. After the equilibrium core calculation is completed, the flux profile is used in a burnup analysis of each of these trajectories. Following all 1048576 trajectories takes ~ 2 weeks on a single processor, so this is not a default option in PEBBED. Nonetheless, it is not prohibitively expensive as part of an overall core analysis campaign.

Figure 9 shows the distribution of burnup in pebbles discharged from the 268-MW(thermal) PBMR core. The

average discharge burnup is ~ 81 GWd/kg HM. The lowest discharge burnup is 76.6 GWd/kg HM, which is accrued by the 0.0011% of pebbles that passes through channel 3 (middle of the core annulus) for the first six passes and through channel 4 for the remaining four passes. The highest discharge burnup is 87.8 GWd/kg HM, which is accrued by the 0.042% of pebbles that passes through the sequence 2,2,4,2,2,4,2,5,4,2 for their ten passes through the core. Channel 2 is close to the inner reflector and contains a mixture of fuel and graphite pebbles, so the neutron spectrum is highly thermalized. Channels 3 and 4 are in the middle of the core annulus and thus possess a harder spectrum. The trajectory sequence for this high-burnup pebble reveals the complex interplay between the burning and breeding of fissile isotopes in PBR fuel.

The distribution of concentrations in discharged pebbles of specific nuclides is also interesting to study. Plutonium isotopes are created when ^{238}U captures a neutron. The concentration of ^{238}U changes by a small fraction over the life of the pebble in the core, but the concentration of intermediate capture products can vary significantly depending on local spectral conditions. Figure 10 shows the variation in the mass of two plutonium isotopes in discharged pebbles. Plutonium-239 appears to be particularly sensitive to the exposure history of the pebble and exhibits a broad and irregular range of mass while its capture product ^{240}Pu has a narrower and more normal distribution of mass among discharged pebbles. This variability presents a challenge for safeguards and spent-fuel management, but it can be managed if the distribution can be predicted with a code like PEBBED.

Figure 11 shows the variability in discharged pebbles of two fission products of interest: ^{109}Ag and ^{137}Cs . Silver is of interest because of its tendency to migrate

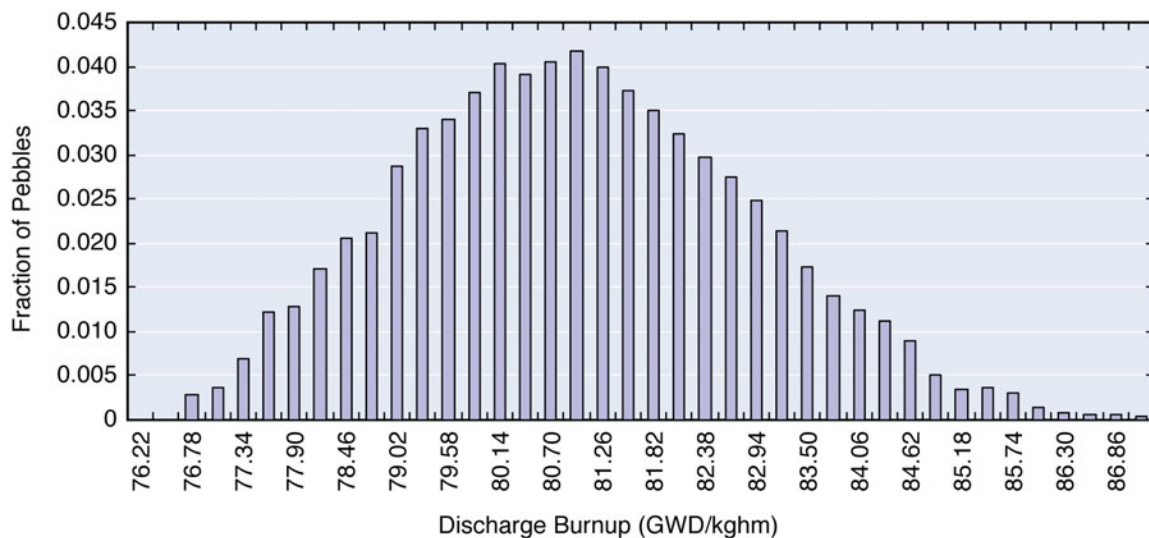


Fig. 9. Distribution of burnup in discharged pebbles: 268-MW(thermal) PBMR.

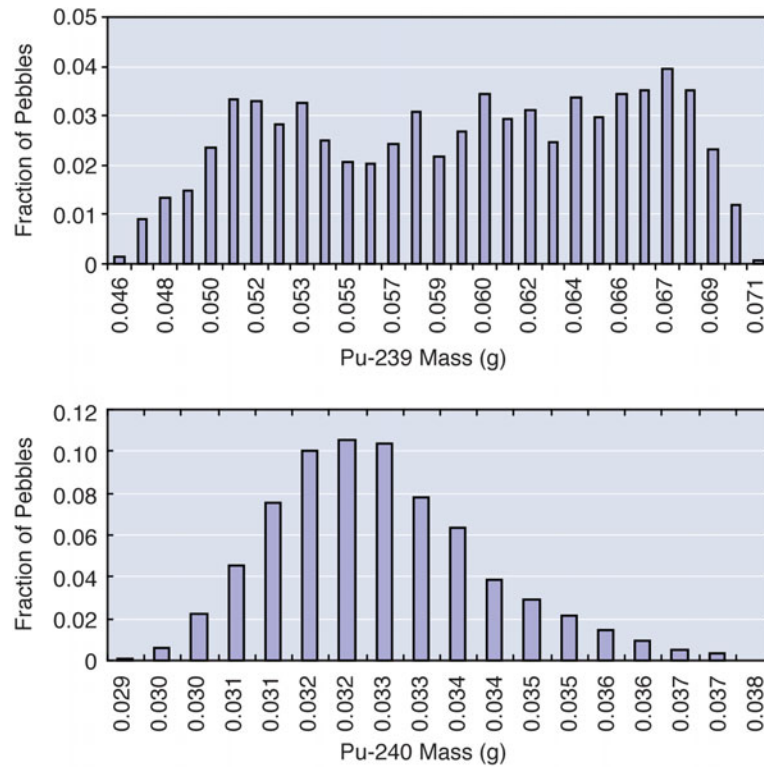


Fig. 10. Distribution of ²³⁹Pu and ²⁴⁰Pu mass in discharged pebbles: 268-MW(thermal) PBMR.

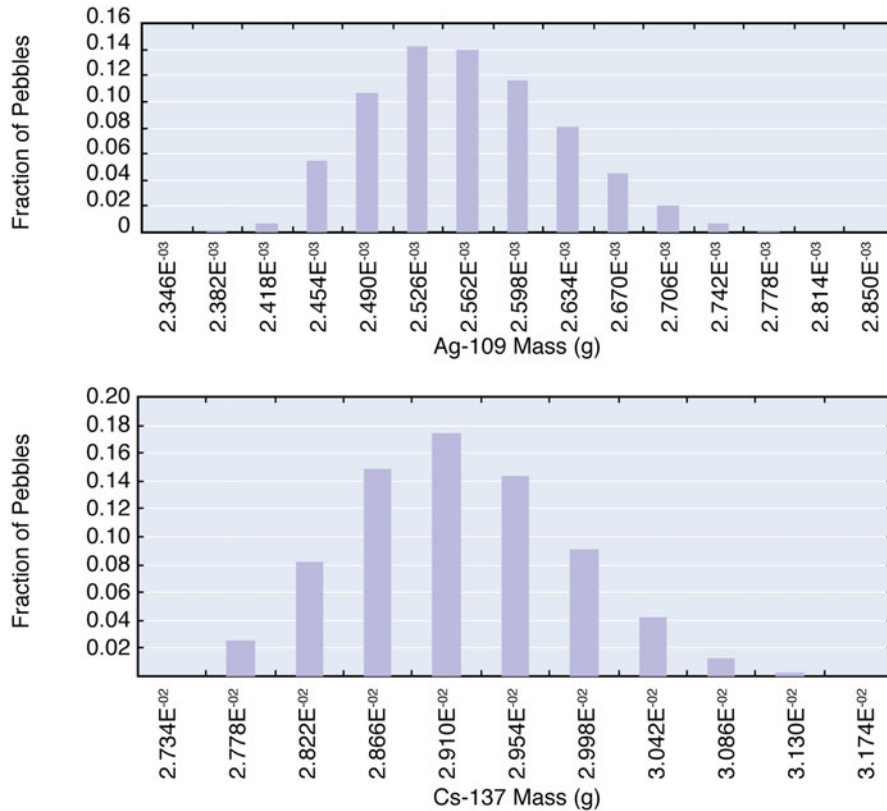


Fig. 11. Distribution of ¹⁰⁹Ag and ¹³⁷Cs mass in discharged pebbles: 268-MW(thermal) PBMR.

quickly through the TRISO barriers and enter the primary coolant stream. Uncertainties in source term analyses can be characterized more thoroughly with a priori knowledge of the inherent variability in fission product concentrations. Likewise, ^{137}Cs has been proposed for some burnup monitoring systems because of the strong correlation between pebble burnup and the strength of the gamma signal emitted by this species.⁴⁶ Knowing the distribution in the ^{137}Cs content would allow for faster and more accurate pebble burnup measurements during power operation.

IV. DESIGN APPLICATIONS

IV.A. Genetic Algorithm Optimization

IV.A.1. A Brief Introduction

Genetic algorithms have been used for a variety of optimization applications, including LWR fuel cycle optimization. A genetic algorithm is a stochastic search method in which a large number (a population) of individual cases are generated randomly to cover the design space. These individual cases are evaluated and ranked according to some prescribed fitness function. The least-fit individuals are discarded, but the attributes of the fittest members of the population are mixed (crossed) to generate a new population, some of the members of which may contain more desirable attributes. The process is repeated for a prescribed number of “generations.” Occasionally, the attributes (the genes) of one or more individuals are randomly altered (mutated) with the effect of increasing or decreasing the overall value of its fitness. This repeated process of selection, crossover, and mutation is modeled upon the biological process of evolution. Though computer simulations of biological evolution can be traced to the late 1950s (Ref. 47), the algorithm was first proposed as a method of optimization by Bremermann in the 1960s (Ref. 48). It was applied to engineering optimization problems by Rechenberg and Schwefel and subsequently shown by Holland to be applicable to a wider variety of problems.^{49–51}

In 1993, Poon and Parks first published results of an LWR core loading that was optimized using a genetic algorithm.⁵² Variations on the technique have been proposed ever since,^{53–56} and genetic algorithms are now an accepted technique for in-core fuel management. Other stochastic techniques, such as simulated annealing and Tabu search, have been developed with varying degrees of success and utility.

It is beyond the scope of this paper to review modern core optimization techniques, nor is it the objective of this work to show that a given genetic algorithm or even genetic algorithms as a whole are the preferred approach for PBR design. This paper does, however, show how the recirculating PBR core is amenable to such meth-

ods. Powerful mathematical and computational tools can thus be brought to bear on the problem of PBR core optimization.

IV.A.2. Implementation in PEBBED

IV.A.2.a. Multiobjective, Real-Valued Search Technique

The optimization algorithm implemented in PEBBED is a so-called real-coded genetic algorithm in which the independent variables being manipulated are coded as real numbers rather than the binary words often used.⁵⁷ The quantities being manipulated are continuous; there are no well-defined positions for assemblies or burnable poisons.

In real-coded genetic algorithms, population characteristics are stored as real variables rather than binary words. Crossover may result in the direct transposition of genes from the parents, but it also may result in a hybrid (i.e., a weighted average of the genes of the parents). A variety of “crossover operators” has been proposed and employed in different optimization routines. Crossover does not guarantee that the “offspring” solution will be superior, but it does focus the search algorithm on regions that have a higher concentration of favorable attributes. Selection ensures that the fittest individuals in each generation are used to produce the next generation. Mutation helps to prevent the algorithm from converging on a local, rather than the global, optimum.

Because of the ease of use and effectiveness, genetic algorithms have been the subject of much study and broad application. A full review of these efforts is beyond the scope of this paper and would not improve upon some definitive work already completed. Goldberg provides a comprehensive text on the theory and practice of genetic algorithms as well as a list of authors of many of the early developments in the field.⁵⁸

Poon and Parks investigated LWR optimization with different stochastic routines such as genetic algorithms and simulated annealing in the FORMOSA code.⁵² They observed that the genetic algorithm was superior in narrowing down the initial global search, but the simulated annealing algorithm converged on the local solution more quickly. This conclusion was consistent with the belief that genetic algorithms are efficient for locating the region in which a global solution resides but that other techniques are better for pinpointing the exact optimal point. This may also be true for PBR optimization, but so far it has not been investigated.

Initial work with genetic algorithms indicated the promise of the technique even though not all of these attempts yielded success. Parks extended the work to multiobjective optimization to simultaneously maximize the end-of-cycle boron concentration and discharge burnup while minimizing power peaking. Multiobjective optimization with genetic algorithms remains

an interesting field of study with at least one nuclear application in the design of PBRs. As implemented in PEBBED, the genetic algorithm may manipulate a number of variables to yield a core with the desired attributes. The resulting core may not be the global optimum (i.e., with different weights imposed on the various core attributes, the search may be driven toward a slightly different core that also achieves the design goal to a greater or lesser degree). Different optimization approaches may thus prove more effective in yielding an optimal design.

For PEBBED, the user may choose one or more core parameters to manipulate. These are the genes, which (currently) include core height; reflector thickness (inner and outer); core annulus width; enrichment; and, for two-zone cores only, the fraction of the core in the outer zone. The user also sets the upper and lower limits of each gene.

For simplicity, the fitness function is constructed using four-point, piecewise linear relations that specify how much each core attribute, or trait, contributes to the overall fitness of the core design. Chosen by the user, the traits and their relative weights are based upon an engineering judgment.

The total fitness specification is composed of the sum of the fitness contributions from the selected traits as determined in the PEBBED equilibrium core analysis. As currently implemented, the contributions are added, and the design with the highest overall fitness after the last generation is the one that best satisfies the objective. The problem can easily be recast as an error minimization by specifying target values for each of the traits and evaluating the difference between the target and computed values. The fittest individual would then be that which yields the lowest overall error residual with the user-specified weight for each selected trait. As implemented in these examples, the genetic algorithm cannot be guaranteed to produce the optimal solution for a given fitness function; however, it does produce a solution that satisfies the design requirements.

Once the gene ranges and trait fitness points are specified, the code generates the initial population by making appropriate modifications to a PEBBED base input; analyzes each core in the population; applies the selection, crossover, and mutation operations; and generates a new population. This is repeated for the specified number of generations. This process requires a separate PEBBED run for each individual in the population in every generation—often hundreds of PEBBED runs for an optimization analysis. The genetic algorithm code automates the modification of PEBBED input for successive PEBBED runs. The efficiency of PEBBED's direct solution for the equilibrium state permits performing the required large number of PEBBED runs in a reasonable time.

PEBBED and COMBINE-7 were programmed in FORTRAN-90 to run on a single processor. THERMIX-

KONVEK was programmed in FORTRAN-77. COMBINE-7 offers either the relatively fast Bondarenko treatment of resolved resonances or the more accurate, but much slower, Nordheim integral treatment of resolved resonances. To balance speed and accuracy, the Nordheim treatment was chosen only for the major uranium and plutonium isotopes. Nonetheless, for a core model with over 20 spectral zones in the pebble bed, the COMBINE-7 spectrum calculations comprise the bulk of the total execution time of an equilibrium cycle analysis. On a single Intel processor, the execution time is ~ 100 min, so an optimization run with 30 individuals over 6 generations would take just under 2 weeks to complete. A considerable reduction in run time could be achieved with parallelization. The individual core analyses in a generation can be distributed among the available processors. Alternatively, the individual zone spectrum (COMBINE-7) runs could be divided among the processors. Neither scheme would require parallelization of the underlying solver algorithms, but the increase in processing time would scale very well with the number of processors up to either the number of spectral zones in the model or the number of individuals in a generation. Parallelization of PEBBED is a priority for the next phase of code development.

IV.B. Examples

Pebble bed cores with different pebble circulation techniques have been modeled and optimized using the aforementioned techniques. Two of the more familiar types are described here. A third type, in which fuel pebbles are loaded into the outer part of the core and circulated for a few passes before being transferred to an inner radial zone, has also been successfully modeled and will be the subject of a future paper. In each case, it is shown that somewhat complex pebble flow patterns can be expressed in terms of a few parameters that are part of the core and fuel design. Specifically, if one knows (a) the heavy metal loadings and burnup limits of the proposed pebbles, (b) the core geometry, and (c) the fuel-loading rate into the various regions of the core, then the fuel recirculation pattern is fully determined. This fact enables the application of both simple and sophisticated optimization methods that can achieve better design margins and fuel economy than those that can be obtained with other tools currently available. In this section, such an optimization capability will be demonstrated.

The following cases demonstrate the ability of the code and procedure presented above. Each case invokes variants of the following sets of models:

1. A two-dimensional (R - Z) neutron diffusion model (PEBBED) that includes the pebble bed core, graphite reflectors (radial and axial), a gas plenum above the core, and a gray curtain control rod partially inserted from above and into the side reflector near the core-reflector

boundary. The flux spectrum is solved in six groups, which has been found to be adequate for most HTR fuel management problems.⁵⁹

2. A two-dimensional (*R-Z*) thermal-fluid model (THERMIX-KONVEK) with helium entering an inlet plenum near the bottom of the core barrel, rising up between the outer reflector and core barrel, passing into the upper gas plenum, and then flowing down through the core and out. Roughly 5 to 10% of the overall coolant flow is assumed to bypass the core through the outer reflector. A stagnant helium gap separates the core barrel from the reactor pressure vessel (RPV), and a stagnant air gap separates the RPV from the ultimate heat sink, which is an isothermal boundary condition simulating a reactor cavity cooling system.

3. Unit cell transport models corresponding to each of a number of spectral zones into which the neutronics model is divided. A COMBINE-7 input file is created for each.

Base input decks are constructed to execute a core calculation to generate flux, power, temperature, and burnup profiles for the asymptotic (equilibrium) core. The result of this calculation provides the initial conditions for a DLOFC simulation in which it is assumed that fission power and forced cooling immediately cease.

From the user-supplied genetic algorithm specification, PEBBED randomly generates an initial population of core candidates that differ in core dimensions and enrichment. The base decks above are modified to match each of the individual candidates. The results of each core simulation are stored for subsequent processing by the algorithm.

IV.B.1. Low-Power HTR with Transportable Vessel

The first modular PBR design was the German HTR Modul, a 200- to 250-MW(thermal) power plant that produced 700°C helium to drive a steam cycle for electricity or process heat. Though rather small even by today's HTR standards, the RPV would still be a very large component requiring piecemeal fabrication. Forgings manufactured at designated steel works would be shipped to the site for welding, which is an expensive process.

The economics of large-scale deployment of HTRs may be improved if the RPVs could be manufactured in one piece and delivered to the site as just another part in the overall plant assembly. A limiting factor, however, is the transport of such a large piece. The largest train car, the so-called Schnabel car (U.S. Patent 3,788,237), can carry loads with a total width of no more than ~427 cm (14 ft) and a length of no more than 34.5 m. The width is a hard limit on the outside diameter of a pressure vessel's flange. The economics of baseload nuclear power plants have historically favored larger power

TABLE III

Gene Domain for the Small HTR Optimization

Gene	Range
Pebble bed radius (cm)	110 to 160
Outer reflector width (cm)	20 to 60
Height of active core (cm)	1000 to 1200
Uranium enrichment (%)	12 to 16

output [>600 MW(thermal)]. Those economics may shift to favor smaller units with the advent of factory fabrication and transport of pressure vessels.

The goal then is to design the largest (i.e., having the most thermal power) passively safe PBR core that can fit inside a pressure vessel with a maximum outer diameter of 427 cm.

The variables (genes) chosen to be manipulated and their limits are shown in Table III. The HTR Modul design calls for a pebble bed radius of 150 cm, a height of ~940 cm, and an enrichment of 7%. These values were used for the base case in the optimization. A reactor that can fit inside a smaller vessel will probably have a much smaller core radius and a higher enrichment to compensate for the increased radial leakage. The 8-cm-thick pressure vessel must also contain a carbon brick insulator (8 cm), core barrel (5 cm), and 5-cm gas channels between those three structures. These dimensions, the largest allowed pebble bed radius, and the widest allowed reflector width would together require an unacceptably large pressure vessel, but the ranges were allowed for flexibility in design. The neutronics model contains 2929 computational nodes and 42 spectral zones. The feed fuel pebbles each contain 7 g of LEU, the same as was proposed for the HTR Modul. The thermal-fluid model was designed for an outlet pressure of 70 bars and inlet and outlet coolant temperatures of 500 and 900°C, respectively, which is somewhat higher than the HTR Modul.

The desired traits were a maximum DLOFC fuel temperature of $<1585^{\circ}\text{C}$ and a maximum outer reflector radius of 163 cm to accommodate the carbon insulator, core barrel, riser channel, and pressure vessel. The thicknesses of these components were considered fixed but not optimized. A criticality search feature was employed to yield a core eigenvalue of 1.0 by iterating on the discharge burnup. The contributions of each trait to the overall fitness are shown in Fig. 12.

Note here that a PEBBED analysis is not required to compute the fitness contribution from the outer reflector radius. It can be computed directly from the core and reflector dimensions generated by the genetic algorithm. The peak DLOFC temperature, however, requires a full-coupled core computation.

It is not guaranteed that the severe size restrictions on the vessel would allow a core power of 200 MW as in

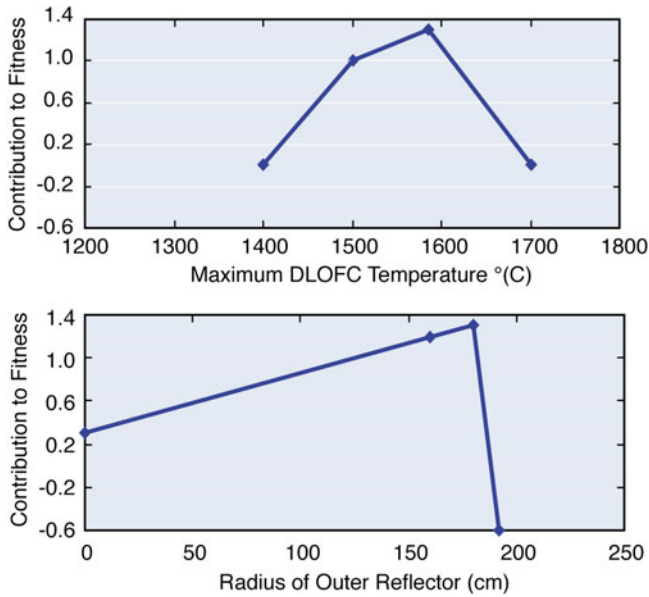


Fig. 12. Fitness function for the transportable HTR.

the HTR Modul. Nonetheless, this value was used in the initial attempt. Again, the simulation was allowed to run for six generations. In fact, the optimal core design was located after the first generation, and the subsequent mutations and crossbreeding produced no core with a higher fitness. The best individual obtained after this run possessed the traits shown in Table IV.

This core is good but not good enough. The peak DLOFC temperature slightly exceeds the design limit of 1600°C. Furthermore, the pressure vessel outer diameter is ~15 cm too large to fit onto the Schnabel car. Therefore, the core power was reduced to 175 MW(thermal), and the optimization was performed again. The resulting optimized core had the following characteristics, displayed in Table V.

This core is slightly narrower and taller but has all the desired features. Note the feed enrichment is over double that of the original HTR Modul. This is due in part to the elevated neutron leakage from the smaller

TABLE IV

Properties of Optimized 200-MW(thermal) PBR

Core height (cm)	1184
Core radius (cm)	136
Outer reflector width (cm)	42
Pressure vessel outer diameter (cm)	456
Core eigenvalue	1.026
Feed enrichment (%)	15.9
Maximum steady-state fuel temperature (°C)	936
Maximum DLOFC-state fuel temperature (°C)	1609

TABLE V

Properties of Optimized 175-MW(thermal) PBR

Core height (cm)	1195
Core radius (cm)	120
Outer reflector width (cm)	42
Pressure vessel outer diameter (cm)	426
Core eigenvalue	1.026
Feed enrichment (%)	15.6
Maximum steady-state fuel temperature (°C)	901
Maximum DLOFC-state fuel temperature (°C)	1580

core but is also due to the elevated burnup achieved in the pebbles. The discharge burnup computed by PEBBED is 121 MWd/kg HM, compared to 80 MWd/kg in the HTR Modul.

The economics of low-power reactors is dependent on many factors other than core design. The mere existence of a passively safe core with a high outlet temperature and a transportable pressure vessel does not imply that these will be rolling off the assembly line in the near future. Nonetheless, the minimum requirements of the reactor core have been met by the application of the PEBBED algorithm.

IV.B.2. A 600-MW(thermal) Pebble Bed VHTR

In 2003, the DOE began a program to develop a nuclear power plant with the primary purpose of the simultaneous production of electricity and hydrogen to serve industrial or transportation markets. An offspring of the Generation IV advanced reactor concepts, the NGNP will feature a very high-temperature gas-cooled reactor (VHTR) because of its passive safety features and the high outlet temperature needed for economic hydrogen production. The easily understood safety basis will permit substantially reduced emergency planning requirements and improved siting flexibility compared to current and advanced LWRs. The scope of the project includes development of a very high-temperature gas-cooled nuclear system, alternative hydrogen production technologies that can efficiently use the process heat from the nuclear system, and power conversion technologies that promise greater thermodynamic efficiency.⁹

As initially envisioned, the VHTR core would operate with an outlet temperature of ~1000°C, thereby placing considerable demands upon the structural materials in the reactor vessel and power conversion system. A power level of 600 MW(thermal) was specified in the reference concept because of previous work showing that a modular, passively safe, 600-MW(thermal) HTR could be constructed with known technology and infrastructure.⁶⁰ The General Atomics gas turbine–modular helium

reactor (GT-MHR) was designed for an outlet temperature of 850°C and would require some modification to accommodate the requested outlet coolant temperature. A reconfiguration of the coolant paths through the vessel indicated that this could be achieved.⁶¹

A passively safe 600-MW(thermal) pebble bed VHTR had no such precedent. Existing PBR concepts would operate at lower temperatures or powers or would rely upon active cooling measures in the event of a severe loss of coolant. The PEBBED code with its genetic algorithm was in the early stages of development and testing but was employed to see if such a large PBR could be designed.

IV.B.3. Pebble Bed VHTR Optimization

The initial effort was successful in demonstrating the efficacy of the PEBBED method.^{27,62} The code and model suffered from deficiencies that severely limited the validity of the results. First, the temperature profiles were generated using the simple one-dimensional heat transfer and fluid models written specifically for PEBBED to conduct rapid scoping studies. Second, the microscopic cross sections were generated using an earlier version of COMBINE and an average core temperature. These single-set cross sections were applied over the entire model. Later on, PEBBED was coupled to the THERMIX-KONVEK code for improved temperature analysis. Also, the ability to accept cross sections for different core spectral zones was added. The cross sections were computed off-line for the base optimization case and therefore were not updated for each new core geometry. This was an improvement nonetheless, and an improved 600-MW(thermal) VHTR design was produced.⁶³ Shortly thereafter, an option to vary and optimize the uranium enrichment was implemented.

The problem was addressed again using the integrated PEBBED-THERMIX-COMBINE code. The eigenvalue and maximum DLOFC temperature targets are similar to those of the previous case, but the restriction on the total diameter was relaxed. A block graphite inner reflector with variable radius was added. The base case geometry for the optimization was the core that resulted from the earlier study report,⁶² and the genes were allowed to fluctuate about those values (see Table VI).

The neutronics model contains 5640 computational nodes and 44 spectral zones. The feed fuel pebbles each contain 9 g of 8% LEU to be burned to 80 MWd/kg HM. Neither the enrichment nor the discharge burnup were allowed to vary. An estimated pebble flow rate of 5990 pebbles/day was specified so that each pebble would pass through the core about eight times. The thermal-fluid model was designed for an outlet pressure of 90 bars and inlet and outlet coolant temperatures of 600 and 1000°C, respectively.

The desired traits were a “critical” eigenvalue of about 1.03 (to compensate for the poisoning by fission

TABLE VI
Gene Domain for the 600-MW(thermal)
Pebble Bed VHTR

Gene	Range
Inner reflector radius (cm)	120 to 160
Pebble bed width (cm)	80 to 120
Outer reflector width (cm)	50 to 100
Height of active core (cm)	950 to 1200

products not modeled explicitly) and a maximum DLOFC fuel temperature of <1590°C. An outer reflector radius fitness profile was constructed not to drive the design toward a specific value but rather to give marginal rewards to smaller diameters. The GT-MHR pressure vessel has an outer radius of ~383 cm, so the fitness function was designed to penalize any dimension larger than this. The contribution of this trait to the overall fitness is shown in Fig. 13.

After five generations, the best individual possessed the traits shown in Table VII. The corresponding values for the General Atomics prismatic GT-MHR are shown in parentheses.

A core with most of the desired traits was obtained after a few generations. Allowing the algorithm to proceed for a few more generations yields a slightly “fitter” model, but the differences would probably be within the computational uncertainties of the models and methods. The radial core dimensions are comparable to the General Atomics design, but note the considerably taller core. The ability of the pebble bed to conduct heat safely away in the event of a loss of coolant is hindered somewhat by the voids between pebbles, as compared to a prismatic reactor of comparable dimensions and power. The core must be made larger in order to decrease the overall power density and prevent an excessive temperature increase. The taller core also will have a larger pressure drop that will require greater coolant pumping power.

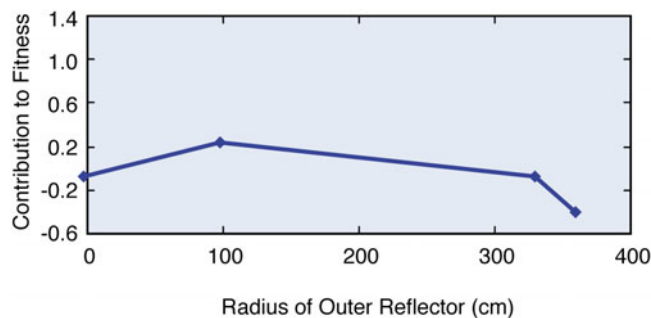


Fig. 13. Outer reflector radius contribution to the 600-MW(thermal) pebble bed VHTR fitness function.

TABLE VII
Properties of Optimized 600-MW(thermal)
Pebble Bed VHTR

Property	Result of Genetic Algorithm Search
Core height (cm)	1105 (793)
Inner reflector radius (cm)	153 (148)
Core annulus width (cm)	90.6 (93.5)
Outer reflector width (cm)	53.8
Pressure vessel outer diameter (cm)	752 (766)
Core eigenvalue	0.9694
Feed enrichment (%)	8.0
Maximum steady-state fuel temperature (°C)	1113
Maximum DLOFC-state fuel temperature (°C)	1589
Discharge burnup (MWd/kg HM)	80.0

The core multiplication factor (k_{eff}) target was not achieved. The feed enrichment is not sufficient to overcome the leakage from a core of this size. Two solutions to this deficiency were attempted: decreasing the discharge burnup and increasing the feed enrichment. Allowing the discharge burnup to drop to 43.6 MWd/kg HM yielded the target eigenvalue of 1.029. The peak DLOFC temperature rose slightly to 1590°C at the limit but is still acceptable. Likewise, the maximum operating fuel temperature rose a few degrees to 1118°C. Fixing the discharge burnup again at 80 MWd/kg HM but increasing the enrichment had a similar outcome. A feed enrichment of 10.4% yielded the target equilibrium eigenvalue of 1.029. The peak DLOFC temperature in this case increased a few degrees over the original result to 1595°C, and the peak operating fuel temperature increased to 1118°C. The temperature differences between these cases are well within the uncertainty from other parameters and modeling assumptions.

A viable design is therefore achieved and can be examined in detail with methods of higher resolution.

V. CONCLUSIONS

Automated design optimization of recirculating PBRs is demonstrated with the PEBBED code. PEBBED uses a description of pebble flow and mixing that enables even complex pebble loading and recirculation schemes to be described in terms of a few well-defined core parameters. Examples of schemes that have been proposed were documented in this study, but even more sophisticated PBR fuel cycles have been explored and will be the subject of future publications.

Gross core parameters can be manipulated in a numerical optimization with the PEBBED algorithm being used to couple the diffusion and burnup equations. Stochastic design optimization of various types of PBR cores is demonstrated using a genetic algorithm. Viable core designs have been obtained for PBRs subjected to rather challenging constraints. Other plant constraints (materials, fuels, and power conversion systems) as well as external factors also determine the economics of the PBR, but the PEBBED approach can ensure that the core itself can be tuned to satisfy the design constraints.

Although the genetic algorithm was chosen as the optimization technique, primarily for its ease of implementation, other techniques, stochastic or otherwise, may prove to be more effective at obtaining a satisfactory design with less computational effort. The PEBBED algorithm is amenable to use with these tools as well. Likewise, the individual solvers (neutronics, thermal fluids, and spectrum generators) can be updated or replaced with more sophisticated tools as they become available.

The technique described within assumes a fixed-fuel design and thus omits a potentially significant degree of freedom in core optimization. Preliminary work at INL indicates the considerable benefits of optimizing the moderating ratio in PBR fuel by adjusting the number of particles per pebble as part of the core geometry optimization technique described in this paper. That work will be described in a follow-on paper. Still another degree of freedom is the design of the TRISO particle itself. Studies have indicated that the optimization of the fuel kernel size and composition can improve fuel performance and increase the consumption of plutonium and other actinides.^{64,65} As has already been demonstrated for the corresponding LWR process,⁵¹ a proper nonlinear optimization integrating TRISO, pebble, and core design can greatly improve the economics and safety of future PBRs and facilitate extensive deployment.

ACKNOWLEDGMENTS

This work was supported by the DOE, Office of Nuclear Energy, Science, and Technology, under DOE Idaho Operations Office contract DE-AC07-99ID13727. Parts of this work (the novel recirculation algorithm, the optimization capability, and the development of the nodal diffusion solver) were supported by a DOE Nuclear Engineering Research Initiative grant (NERI-02-195). The coupling of PEBBED with THERMIX and COMBINE was conducted at INL with the support of the NGNP project (project 23843). All sources of support are gratefully acknowledged.

REFERENCES

1. "Critical Experiments and Reactor Physics Calculations for Low-Enriched High Temperature Gas Cooled Reactors,"

- IAEA TECDOC 1249, International Atomic Energy Agency (2001).
2. A. J. GOODJOHN, "Summary of Gas-Cooled Reactor Programs," *Energy*, **16**, 1/2, 79 (1991).
 3. K. R. SCHULTZ, L. C. BROWN, G. E. BESENBRUCH, and C. J. HAMILTON, "Large-Scale Production of Hydrogen by Nuclear Energy for the Hydrogen Economy," presented at National Hydrogen Association Annual Mtg., Washington, D.C., March 4–6, 2003.
 4. W. KUHR, C. BOLTHRUNIS, and M. CORBETT, "Economics of Process Heat Applications," *Proc. Int. Congress Advances in Nuclear Power Plant (ICAPP '06)*, Reno, Nevada, June 4–8, 2006, American Nuclear Society (2006) (CD-ROM).
 5. R. SCHULTEN, "Pebble-Bed HTRs," *Ann. Nucl. Energy*, **5**, 8–10, 357 (1978).
 6. G. H. LOHNERT and H. REUTLER, "The Modular HTR—A New Design of High-Temperature Pebble-Bed Reactor," *Nucl. Energy*, **22**, 3 (June 1983).
 7. H. FREWER, W. KELLER, and R. PRUSCHEK, "The Modular High-Temperature Reactor," *Nucl. Sci. Eng.*, **90**, 411 (1985).
 8. M. T. SIMNAD, "The Modular HTGR: Its Possible Role in the Use of Safe and Benign Nuclear Power," *Climate Change and Energy Policy: Proc. Int. Conf. Global Climate Change: Its Mitigation Through Improved Production*, Los Alamos, New Mexico, October 21–24, 1991, American Institute of Physics/Springer (1992).
 9. P. E. MacDONALD, J. W. STERBENTZ, R. L. SANT, P. D. BAYLESS, R. R. SCHULTZ, H. D. GOUGAR, R. L. MOORE, A. M. OUGOUAG, and W. K. TERRY, "NGNP Preliminary Point Design—Results of the Initial Neutronics and Thermal-Hydraulic Assessments," INEEL/EXT-03-00870, Rev. 1, Idaho National Engineering and Environmental Laboratory (Sep. 2003).
 10. A. KADAK and R. BALLINGER, "MIT Modular Pebble Bed Reactor (MPBR)," *Proc. 2nd Int. Topl. Mtg. High Temperature Reactor Technology (HTR-2004)*, Beijing, China, September 22–24, 2004.
 11. X. YAN, K. KUNITOMI, T. NAKATA, and S. SHIOZAWA, "GTHTR300 System Design Features and Performance," *Proc. 1st Int. Topl. Mtg. High Temperature Reactor Technology (HTR-2002)*, Petten, the Netherlands, April 22–24, 2002.
 12. Z. ZHANG, Z. WU, Y. XU, Y. SUN, and F. LI, "Design of a Chinese Modular High-Temperature Gas-Cooled Reactor (HTR-PM)," *Proc. 2nd Int. Topl. Mtg. High Temperature Reactor Technology (HTR-2004)*, Beijing, China, September 22–24, 2004.
 13. D. HITTNER, E. BOGUSCH, D. BESSON, D. BUCKTHORPE, V. CHAUVET, M. A. FÜTTERER, A. VAN HEEK, W. VON LENZA, M. PHÉLIP, J. PIRSON, W. SCHEUER-MANN, and D. VERRIER, "RAPHAEL, A European Project for the Development of VHTR Technology for Industrial Process Heat Supply and Cogeneration," *Proc. 3rd Int. Topl. Mtg. High Temperature Reactor Technology (HTR-2006)*, Johannesburg, South Africa, October 1–4, 2006.
 14. M. J. GOUGE, "Closed Cycle Gas Turbine Nuclear Power Plant for Submarine Propulsion," *Naval Engineers J.*, November 1995.
 15. G. CROMMELIN, "The NEREUS Installation," *Proc. Int. Gas Turbine and Aeroengine Congress and Exhibition*, Indianapolis, Indiana, June 1999, ASME.
 16. P. LOBET, R. SEIGEL, A. C. THOMPSON, R. J. BEADNELL, and P. A. BEELEY, "A High Temperature Reactor for Ship Propulsion," *Proc. 1st Int. Topl. Mtg. High Temperature Reactor Technology (HTR-2002)*, Petten, the Netherlands, April 22–24, 2002.
 17. H. NABIELEK, W. SCHENK, W. HEIT, A. W. MEHNER, and D. T. GOODIN, "The Performance of High-Temperature Reactor Fuel Particles at Extreme Temperatures," *Nucl. Technol.*, **84**, 62 (1989).
 18. R. SCHULTEN, "Twenty Years of AVR High-Temperature Reactor Operation," *Atomwirtschaft-Atomtechnik*, **34**, 4, 166 (Apr. 1989).
 19. U. COLAK, L. BREY, and M. METHNANI, "Status of the IAEA Coordinated Research Project on HTGR Core Physics and Thermal Hydraulics Benchmarks (Crp-5)," *Proc. 3rd Int. Topl. Mtg. High Temperature Reactor Technology (HTR-2006)*, Johannesburg, South Africa, October 1–4, 2006.
 20. E. TEUCHERT, U. HANSEN, and K. HAAS, "VSOP—Computer Code System for Reactor Physics and Fuel Cycle Simulation," JÜL-1649, Kernforschungsanlage Jülich (Mar. 1980).
 21. F. REITSMA, H. J. RÜTTEN, and W. SCHERER, "An Overview of the FZJ Tools for HTR Core Design and Reactor Dynamics, The Past, Present, and Future," *Proc. Topl. Mtg. Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications*, Palais des Papes, Avignon, France, September 12–15, 2005.
 22. J. OPPE, J. KUIJPER, J. DE HAAS, E. VERKERK, and H. KLIPPEL, "Modeling of Continuous Reload HTR Systems by the PANTHERMIX Code System," *Proc. Int. Mtg. Mathematics Methods for Nuclear Applications, Mathematics and Computation*, Salt Lake City, Utah, September 2001, American Nuclear Society (2001) (CD-ROM).
 23. T. D. NEWTON, "The Development of Modern Design and Reference Core Neutronics Methods for PBMR," presented at European Nuclear Conf. (ENC 2002), Lille, France, October 2002.
 24. B. BOER, J. L. KLOOSTERMAN, D. LATHOUWERS, and T. H. J. VAN DER HAGEN, "In-Core Fuel Management

- Optimization of Pebble-Bed Reactors,” *Ann. Nucl. Energy*, **3**, 1049 (2009).
25. F. REITSMA, “The Pebble Bed Modular Reactor Layout and Neutronics Design of the Equilibrium Cycle,” *Proc. Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments (PHYSOR 2004)*, Chicago, Illinois, April 25–29, 2004, American Nuclear Society (2004) (CD-ROM).
26. W. K. TERRY, H. D. GOUGAR, and A. M. OUGOUAG, “Novel Method for the Deterministic Design, Analysis, and Optimization of the In-Core Fuel Cycle of a Recirculating Pebble-Bed Reactor,” *Ann. Nucl. Energy*, **29**, 1345 (2001).
27. H. D. GOUGAR, W. K. TERRY, A. M. OUGOUAG, and K. N. IVANOV, “Design of Pebble-Bed Reactor Using Genetic Algorithms,” *Proc. Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments (PHYSOR 2004)*, Chicago, Illinois, April 25–29, 2004, American Nuclear Society (2004) (CD-ROM).
28. J. ZGLICZYNSKI, A. NEYLAN, and D. KAPICH, “The Gas-Turbine Modular Helium Reactor (GT-MHR) Offers Potential for Stretch Capability to 300Mwe per Reactor Module,” presented at 1993 Int. Joint Power Generation Conf., Kansas City, Missouri, October 1993.
29. P. H. LIEM, “Design Procedures for Small Pebble-Bed High Temperature Reactors,” *Ann. Nucl. Energy*, **23**, 3, 207 (1994).
30. A. M. OUGOUAG and W. K. TERRY, “Development of a Nodal Method for the Solution of the Neutron Diffusion Equation in General Cylindrical Geometry,” INEEL/EXT-2002-489, Idaho National Engineering and Environmental Laboratory (Apr. 2001).
31. A. M. OUGOUAG and W. K. TERRY, “Analytical Solution of the Neutron Diffusion Equation in Three-Dimensional Cylindrical Geometry for Application in a Nodal Method,” *Proc. Int. Topl. Mtg. Nuclear and Mathematical Computational Sciences (M&C 2003)*, Gatlinburg, Tennessee, April 6–10, 2003, American Nuclear Society (2003) (CD-ROM).
32. RELAP5-3D CODE DEVELOPMENT TEAM, “RELAP5-3D Code Manual Code Structure, System Models, and Solution Methods,” INEEL-EXT-98-00834, Vol. 1, Rev. 2.3, Idaho National Engineering and Environmental Laboratory (Apr. 2005).
33. W. Y. YOON, R. A. GRIMSEY, D. W. NIGG, and R. L. CURTIS, “COMBINE7.0—A Portable ENDF/B-VII.0 Based Neutron Spectrum and Cross-Section Generation Program,” INL/EXT-08-14729, Idaho National Laboratory (Sep. 2008).
34. “NJOY99.0: Code System for Processing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B Data,” Los Alamos National Laboratory; PSR-480 Radiation Safety Information Computational Center (1999).
35. J. L. KLOOSTERMAN and A. M. OUGOUAG, “Spatial Effects in Dancoff Factor Calculations for Pebble-Bed HTRs,” *Proc. Topl. Mtg. Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications*, Palais des Papes, Avignon, France, September 12–15, 2005.
36. J. LIEBEROTH and A. STOJADINOVIC, “Neutron Streaming in Pebble Beds,” *Nucl. Sci. Eng.*, **76**, 336 (1980).
37. H. GERWIN and W. SCHERER, “Treatment of the Upper Cavity in a Pebble-Bed High-Temperature Gas-Cooled Reactor by Diffusion Theory,” *Nucl. Sci. Eng.*, **97**, 9 (1987).
38. R. MPHAHLELE, A. M. OUGOUAG, K. IVANOV, and H. GOUGAR, “Spectral Zone Determination for Pebble Bed Reactor Cores Using Diffusion Theory Spectral Indices,” *Proc. 4th Int. Topl. Mtg. High Temperature Reactor Technology (HTR-2008)*, Washington, D.C., September 28–October 1, 2008.
39. A. M. OUGOUAG, F. RAHNEMA, H. HIRUTA, D. ZHANG, C. WEMPLE, and D. NIGG, “Development of a Method for Neutronics Treatment of Non-Multiplying Zone in Pebble Bed Reactors,” *Proc. 3rd Int. Topl. Mtg. High Temperature Reactor Technology (HTR-2006)*, Johannesburg, South Africa, October 1–4, 2006.
40. W. K. TERRY, A. OUGOUAG, F. RAHNEMA, and M. MCKINLEY, “Effects of Spatial Variations in Packing Fractions on Reactor Physics Parameters in Pebble-Bed Reactors,” *Proc. Int. Topl. Mtg. Nuclear and Mathematical Computational Sciences (M&C 2003)*, Gatlinburg, Tennessee, April 6–10, 2003, American Nuclear Society (2003) (CD-ROM).
41. H. D. GOUGAR, W. K. TERRY, and A. M. OUGOUAG, “Matrix Formulation of Pebble Circulation in the PEBBED Code,” *Proc. 1st Int. Topl. Mtg. High Temperature Reactor Technology (HTR-2002)*, Petten, the Netherlands, April 22–24, 2002.
42. F. REITSMA, W. JOUBERT, A. OUGOUAG, and H. GOUGAR, “Investigation of Power Peaking in the PBMR Pebble Bed Reactor,” *Proc. Topl. Mtg. Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications*, Palais des Papes, Avignon, France, September 12–15, 2005.
43. A. M. OUGOUAG, F. REITSMA, H. D. GOUGAR, W. JOUBERT, and W. K. TERRY, “PEBBED Analysis of Hot Spots in Pebble-Bed Reactors,” *Proc. Topl. Mtg. Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications*, Palais des Papes, Avignon, France, September 12–15, 2005.
44. “Formation Loading Cones—Analysis,” FZJ-ISR-RC-5010/2001, Forschungszentrum Jülich (2001).
45. A. M. OUGOUAG, J. J. COGLIATI, and J.-L. KLOOSTERMAN, “Methods of Modeling the Packing of Fuel Elements in Pebble Bed Reactors,” *Proc. Topl. Mtg. Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications*, Palais des Papes, Avignon, France, September 12–15, 2005.

46. A. HAWARI and J. CHEN, "On-Line Interrogation of Pebble Bed Reactor Fuel," *Nuclear Science Symposium Conference Record*, 2004 IEEE, Vol. 1, p. 206 (Oct. 2004).
47. N. A. BARRICELLI, "Esempi numerici di processi di evoluzione," *Methodos*, 45 (1954).
48. H. J. BREMERMANN, "Optimization Through Evolution and Recombination," *Self-Organizing Systems-1962*, pp. 93–106, M. YOVITS, G. T. JACOBI, and G. D. GOLDSTEIN, Eds., Spartan Books, Washington D.C. (1954).
49. I. RECHENBERG, "Evolutionsstrategie—Optimierung technischer Systeme nach Prinzipien der biologischen Evolution," PhD Thesis (1971) [reprinted by Fromman-Holzboog (1973)].
50. H.-P. SCHWEFEL, *Numerische Optimierung von Computer-Modellen mittels der Evolutionsstrategie: mit einer vergleichenden Einführung in die Hill-Climbing- und Zufallsstrategie*, Birkhäuser (1977).
51. J. HOLLAND, "Genetic Algorithms," *Sci. Am.*, **66** (July 1992).
52. P. POON and G. PARKS, "Application of Genetic Algorithms to In-Core Nuclear Fuel Management Optimization," *Proc. Joint Int. Conf. Mathematical Models and Supercomputing in Nuclear Applications*, Karlsruhe, Germany, April 1993.
53. M. DeCHAINED and M. FELTUS, "Nuclear Fuel Management Optimization Using Genetic Algorithms," *Nucl. Technol.*, **111**, 109 (1995).
54. F. ALIM, K. IVANOV, and S. LEVINE, "GA Loading Pattern and Burnable Poison Placement Optimization Technique for PWR," *Ann. Nucl. Energy*, **35**, 1, 93 (2008).
55. F. ALIM, K. IVANOV, and S. LEVINE, "Simultaneous Optimization of Loading Pattern and Burnable Poison Placements for the TMI-1 Reactor," *Ann. Nucl. Energy*, **35**, 1, 113 (2008).
56. S. YILMAZ, K. IVANOV, S. LEVINE, and M. MAHGEREFTEH, "Genetic Algorithm Application for Burnable Poison Placement in PWRs with Optimized $\text{UO}_2/\text{Gd}_2\text{O}_3$ Fuel Pin Configurations," *Nucl. Technol.*, **156**, 180 (2006).
57. W. E. HART, "Evolutionary Pattern Search Algorithms," SAND-95-2293C, CONF-960820-1, Sandia National Laboratories (Sep. 1995).
58. D. E. GOLDBERG, *Genetic Algorithms in Search, Optimization, and Machine Learning*, Addison-Wesley, Reading, Massachusetts (1989).
59. L. MASSIMO, *The Physics of High-Temperature Reactors*, Pergamon Press, Oxford (1976).
60. R. C. POTTER, "Gas Turbine-Modular Helium Reactor (GT-MHR) Conceptual Design Description Report," Project No. 7658, General Atomics (July 1996).
61. S. M. M. REZA, E. A. HARVEGO, M. RICHARDS, A. SHENOY, and K. L. PEDDICORD, "Design of Alternative Configuration of Coolant Inlet Flow for Modular High Temperature Helium Cooled Reactor," *Proc. Int. Congress Advances in Nuclear Power Plant (ICAPP '06)*, Reno, Nevada, June 4–8, 2006, American Nuclear Society (2006) (CD-ROM).
62. H. GOUGAR, A. M. OUGOUAG, W. K. TERRY, and R. M. MOORE, "Conceptual Design of a Very High Temperature Pebble-Bed Reactor," *Proc. Topl. Mtg. Global 2003*, New Orleans, Louisiana, November 16–20, 2003, American Nuclear Society (2003) (CD-ROM).
63. H. D. GOUGAR, C. B. DAVIS, G. HAYNER, and K. D. WEAVER, "Reactor Pressure Vessel Analysis of Candidate Very High Temperature Reactor Designs," *Proc. 3rd Int. Topl. Mtg. High Temperature Reactor Technology (HTR-2006)*, Johannesburg, South Africa, October 1–4, 2006.
64. H. J. RÜTTEN and K. A. HAAS, "Research on the Incineration of Plutonium in a Modular HTR Using Thorium-Based Fuel," *Nucl. Eng. Des.*, **195**, 353 (2000).
65. T. K. KIM, T. A. TAIWO, R. N. HILL, and W. S. YANG, "A Feasibility Study of Reactor-Based Deep-Burn Concepts," ANL-AFCI-155, Argonne National Laboratory (Aug. 2005).