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The Application of the PEBBED Code Suite to the PBMR-400 Coupled Code Benchmark – FY 2006 Annual Report

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September 2006

Idaho National Laboratory

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The Application of the PEBBED Code Suite to the PBMR-400 Coupled Code Benchmark - FY2006 Annual Report

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ABSTRACT

This document describes the recent developments of the PEBBED code suite and its application to the Pebble-Bed Modular Reactor (PBMR)-400 Coupled Code Benchmark. This report addresses a FY2006 Level 2 milestone under the Next Generation Nuclear Plant (NGNP) Design and Evaluation Methods Work Package. The milestone states "Complete a report describing the results of the application of the integrated PEBBED code package to the PBMR-400 coupled code benchmark." The report describes the current state of the PEBBED code suite, provides an overview of the benchmark problems to which it was applied, discusses the code developments achieved in the past year, and states some of the results attained. Results of the steady state problems generated by the PEBBED fuel management code compare favorably to the preliminary results generated by codes from other participating institutions and to similar non-benchmark analyses. Partial transient analysis capability has been achieved through the acquisition of the NEM-THERMIX code from Pennsylvania State University (PSU). Phase I of the task has been achieved through the development of a self-consistent set of tools for generating cross sections for design and transient analysis and in the successful execution of the steady state benchmark exercises.

1. INTRODUCTION

1.1 STATEMENT OF THE MILESTONE

The PEBBED (Ref 1) Code Suite is under development at the Idaho National Laboratory (INL) for the design and analysis of pebble-bed high temperature reactor (PBR) cores. To validate the accuracy of the code, the INL has participated in the Organization for Economic Cooperation and Development (OECD) / Nuclear Science Committee (NSC)-sponsored Working Group on the PBMR-400 Coupled Code Benchmark. The Benchmark is also under construction and the results of the steady-state exercises are being compiled for publication in 2006 and 2007. The transient exercises have been defined but have been analyzed by only a couple of the Working Group participants as of the end of FY2006. Nonetheless, Phase I of the effort (code suite identification and steady-state exercise completion) is described in this report as specified in the NGNP Methods milestone," Complete a report describing the results of the application of the integrated PEBBED code package to the PBMR-400 coupled code benchmark."

This milestone documents the progress made under the NGNP Design and Evaluation Methods Work Package (# GI0204L01). Part of this Work Package addresses the development of a pebble-bed core simulation analysis capability centered about the INL code PEBBED. Toward this end, specific FY06 activities performed included:

- completing the pebble dynamics model development and computation of pebble flow parameters,
- completing the addition of transient capability through the coupling of NEM-THERMIX to PEBBED,
- completing the integration of cross-section generation through the coupling of PEBBED with COMBINE, and
- the evaluation of the PBMR-400 benchmark with the enhanced PEBBED suite.

This report specifically addresses the last bullet but describes activities associated with the others as well. A description of the other activities is provided in separate reports as specified in the Work Package.

1.2 REVIEW OF THE PEBBED CODE SUITE

PEBBED (Ref 1) is the preferred code for pebble-bed physics analysis in the U.S. Originally, designed for rapid scoping studies, it has been enhanced with higher fidelity thermal fluid and spectral modules to the extent that favorable comparisons to computational and experimental PBR integral benchmarks. It is, however, a code under development. For example, the original PEBBED used a user-supplied, static set of microscopic cross sections for each isotope and simple one-dimensional thermal fluid computations to estimate fuel temperature. This was adequate to demonstrate the PEBBED principle – that of an internally consistent equilibrium cycle analysis of recirculating pebble bed reactors. The considerable spectral variations about the core were not captured with this simple set and accuracy was limited. Because of the considerable variations in temperature and material composition (burnup) over the dimensions of the core, accurate design and analysis calculations require that core physics and thermal-hydraulic calculations occur in concert and be linked by cross sections generated on-line using interpolation tables or an embedded spectrum code. Efforts began in 2005 to couple PEBBED to spectrum codes (COMBINE and MICROX) for cross section generation and to a thermal fluid code (THERMIX) for heat transfer and gas dynamics. This work has been completed to some extent but the coupling is not yet optimized.

PEBBED is still mainly a core design and fuel management code; it converges upon a steady-state (asymptotic) burnup, flux, and temperature profile by iteratively solving the neutron diffusion and depletion codes and a known fuel recirculation pattern. The novel approach used in PEBBED to couple pebble flow and burnup makes it amenable to the application of sophisticated optimization techniques. This was demonstrated in 2003 with the conceptual design of a passively safe 600 thermal megawatt (MWt) Very High Temperature Reactor (Ref. 2).

Power transients, however, require the solution of the time-dependent diffusion equation and the explicit computation of the nuclide densities of only a few short-lived isotopes such as xenon-135. In its current state, PEBBED does not possess a transient solver although it can perform a basic post-SCRAM conduction cooldown analysis using a user-supplied decay heat trajectory. Development of a time-dependent version of the nodal diffusion solver is underway at the INL as part of a separate advanced methods research program. A beta version of this solver will be tested in FY07. As a temporary measure supported by NGNP Methods funding, the NEM-THERMIX code has been acquired from Penn State University with the support of Professor Kostadin Ivanov. Testing of the code on pebble bed reactor models occurred at both Penn State and the INL in FY2006.

Other capabilities and limitations of the PEBBED suite are described in the following sections. In the aggregate, these tools provide the INL and DOE with a basic capability to model a pebble-bed reactor fuel cycle and many severe transients (Figure 1). This report will also show, however, that much work remains to be done.

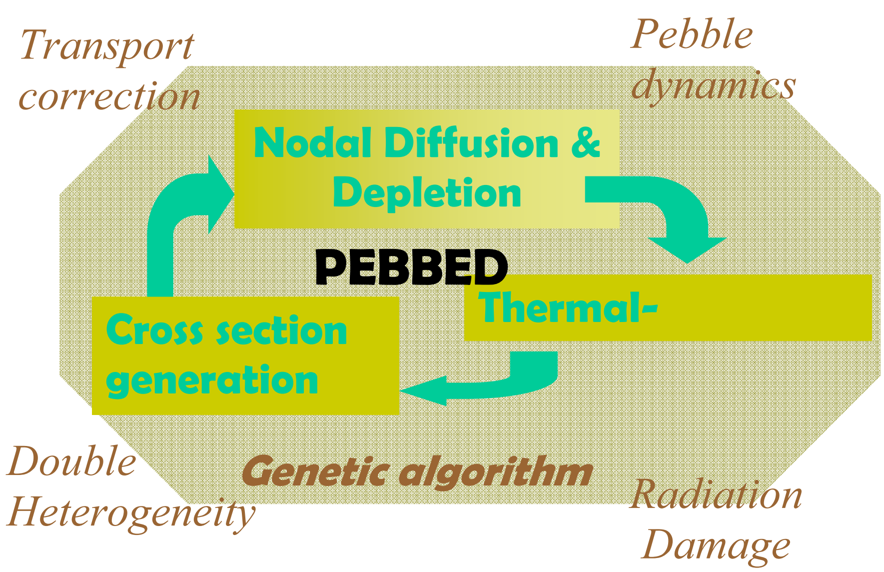


Figure 1: PEBBED Computational Scheme with Enhancements (Current and in Progress).

PEBBED-COMBINE-THERMIX

Although PEBBED does possess an embedded thermal fluid analysis capability for computing fuel temperature, a more sophisticated thermal-hydraulic capability has been achieved with the coupling of PEBBED to THERMIX. THERMIX-KONVEK is a two-dimensional (R-Z) thermal-hydraulic code developed specifically for the German HTR program and thus contains correlations and material properties for the PBR. THERMIX-KONVEK is a two-dimensional (R-Z) thermal-hydraulic code developed at Kernforschungsanslage Jülich GmbH in Germany. It possesses correlations and material properties designed to support the German HTR program and thus is well-suited to PBR analysis. It is a key component of the VSOP reactor analysis code suite used in Germany and South Africa for their PBR work. THERMIX solves the equations of heat transfer in gases, liquids, and solids using power density and fluence data supplied by a reactor physics code. It has been successfully employed for PBR thermal-hydraulics benchmark calculations.

With the help of a student from Purdue University, THERMIX-KONVEK was coupled to PEBBED through an interface program (Ref. 3). The combined code runs successfully on steady-state and simple post-shutdown transient problems. THERMIX is now an option in PEBBED for thermal analysis; the original thermal module in PEBBED still remains operational as an alternative option. Benchmark problems were run comparing the results of the two thermal analysis options.

The magnitude and variation in temperatures and burnup across a PBR have a profound effect on reaction rates such that thermal-hydraulic calculations must be performed along with cross section feedback in order to achieve reasonable levels of accuracy. With help from Penn State University, a scheme involving direct interpolation between cross sections tabulated for different core conditions was implemented in PEBBED during the summer of 2004. Local parameters (temperature and buckling) are used to generate microscopic cross sections for user-delineated regions of the neutronic model. These interpolation tables were generated with the spectrum code MICROX (Ref. 4). PEBBED retains the option of reading MICROX data either directly from its output files or tabulated as a function of various state parameters.

Cross sections can also be generated using the INL code COMBINE (Ref. 5). The code can be called from PEBBED using scripts and thus cross sections for each local region (or *spectral zone*) in the model can be generated on the fly. This allows for more significant changes to the core model during the design phase without the risk of moving beyond the range of validity of the pre-computed interpolation tables. In FY06, however, the capability to generate interpolation tables using COMBINE was also developed with the help of a student from Idaho State University. This development of this capability is described in detail in a companion NGNP report. A number of options now exist for generating local cross section data for use in PEBBED design and analysis.

In parallel developments, methods for computing Dancoff factors for pebble-bed fuel and for simulating pebble flow were undertaken in 2005 and 2006. In 2005, the code PEBDAN was written to compute Dancoff factors that take into account the double heterogeneity of the fuel and the ransom distribution of both pebbles and particles. This code was partially integrated into the PEBBED suite in 2006 but the full implementation is not yet complete. Work also progressed on PEBBLES, a pebble motion code that uses a molecular dynamics to compute the movement of pebbles during normal and accident conditions. Eventually, data from PEBBLES will be used to enhance the PEBBED code so that it can model time-dependent burnup profiles in three dimensions. This capability is needed to simulate the behavior of cores from initial (fresh core) criticality all the way to its asymptotic burnup state and to account for the physical effects of azimuthally distributed flow loading and discharge patterns. Currently, PEBBED can analyze only the initial startup and asymptotic cores and assumes azimuthal pebble flow symmetry (even though the neutronics can be solved in three dimensions). A full description of the PEBBLES effort is contained in a companion report.

Also in FY06 a scheme and code was developed by guest scientist Richard Sanchez to improve the accuracy of the cross sections generated using COMBINE. This enhancement is described in a companion NGNP report.

NEM-THERMIX

As mentioned above, PEBBED is currently a steady state fuel management and core design tool; it does not yet possess a time-dependent neutronics solver. Such a solver is being developed at the INL but a third-party code (NEM-THERMIX) was acquired as a short-term option for performing transient PBR analysis. Burnup information is embedded in these cross sections; NEM does not possess a depletion capability so it cannot perform fuel management and core design like PEBBED.

NEM is a 3-D multi-group nodal code developed at The Pennsylvania State University for modeling both steady state and transient core conditions. It utilizes a transverse integration procedure and is based on the partial current formulation of the nodal balance equations. The code has options for modeling of 3-D Cartesian, cylindrical and hexagonal geometry. The cylindrical option utilizes fourth-order polynomial expansions of the 1-D transverse-integrated flux distribution in the R-, Z- and θ-directions. It is important to note that the detailed treatment of the effects of azimuthally dependent reactor control rods requires a full three-dimensional representation of the PBMR. The NEM code has been coupled with THERMIX-DIREKT (a more recent version of THERMIX) using serial integration approach. The spatial mesh overlays are exact in R-Z geometry and provide a capability for different spatial meshing in neutronics and thermal-hydraulics models. The temporal coupling is based on the same time step size used by NEM and THERMIX-DIREKT with the time step determined by the later code. During both steady state and at each time step a coupling iteration loop is performed between neutronics and thermal-hydraulic calculations upon reaching a defined convergence in temperature distribution. The cross-section dependencies on feedback parameters are modeled through linear surface interpolation in multi-dimensional tables.

NEM-THERMIX uses macroscopic cross sections generated using MICROX, COMBINE, or other spectrum software. With COMBINE, an internally consistent path exists for burnup and transient analysis (Figure 2).

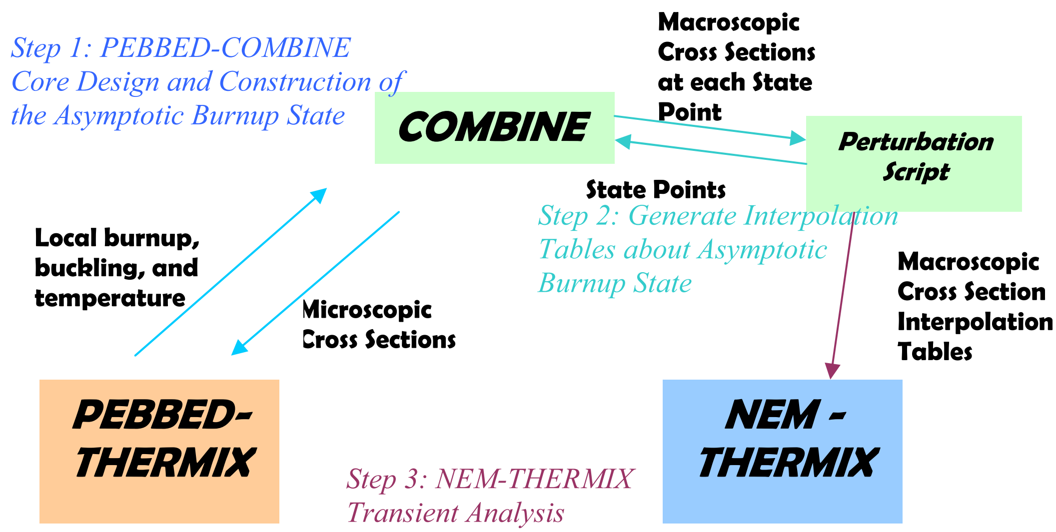


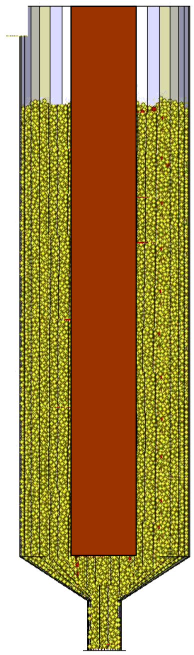
Figure 2: Self-consistent Core Design and Transient Analysis for the PBR.

An accurate asymptotic burnup state is achieved with a COMBINE-PEBBED-THERMIX integrated analysis. Microscopic cross sections are generated for the PEBBED burnup calculations and updated in an iterative process until eigenvalue and source convergence is obtained. Nuclide concentration data for the each local spectral zone are then used to generate macroscopic cross sections at user-specified temperature and buckling states. This data is written to files as interpolation tables that are used in subsequent NEM-THERMIX transient analyses. Only short-lived nuclides such as xenon-135 are tracked explicitly in NEM; the long-lived isotopes do not vary significantly from the values computed by PEBBED.

This package is not considered optimal. The NEM nodal solver uses a polynomial expansion technique while the PEBBED solver uses either finite different or an analytical nodal formulation. This may lead to subtle differences in the flux solutions. Also, the THERMIX modules used with PEBBED and NEM use different gas dynamics algorithms (KONVEK vs. DIREKT) that may yield different temperature profiles. As a result, a critical state computed by PEBBED may not yield a critical initial condition in the NEM analysis. Furthermore, although THERMIX is a widely used standard for PBR thermal fluid analysis, it is still a two-dimensional code; it does not yet posses the capability to analyze three-dimensional phenomena such a single rod ejections. For that matter, the INL is exploring the replacement of THERMIX with RELAP-3D. Although this will take some improvements to RELAP such as the addition of appropriate heat transfer correlations, the end result will be a 3-D PBR transient analysis capability that can also easily be expanded to model full PBR power plant systems.

In FY06, scripts were written to build and execute COMBINE input files using the spectral zone data supplied by PEBBED and to write the computed macroscopic cross sections into tables for subsequent interpolation by NEM.
While debugging and optimization of the code coupling is still in progress, the basis elements of a complete PBR core design and transient analysis capability now exist and are being applied to the PBMR-400 Coupled Code Benchmark.

2. DESCRIPTION OF THE PBMR 400 COUPLED CODE BENCHMARK



The Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development has accepted, through the Nuclear Science Committee, the inclusion of the Pebble-Bed Modular Reactor coupled neutronics/thermal hydraulics transient benchmark problem as part of their official activities.

The deterministic neutronics, thermal-hydraulics and transient analysis tools and methods available to design and analyze PBMRs have, in many cases, lagged behind the state of the art compared to other reactor technologies. This has motivated the testing of existing methods for HTGRs but also the development of more accurate and efficient tools to analyze the neutronics and thermal-hydraulic behavior for the design and safety evaluations of the PBMR. In addition to the development of new methods, this includes defining appropriate benchmarks to verify and validate the new methods in computer codes.

The benchmark is complementary to other on-going or planned efforts in the reactor physics community. The PBMR 400MW core design is also a test case in the International Atomic Energy Agency's (IAEA) Coordinated Research Programme #5 (IAEA CRP-5) but important differences exist between the test case definitions and approaches.

Figure 3: Conceptual Drawing of the PBMR-400 Core with Inner Reflector

The OECD benchmark includes additional steady-state and transient cases including reactivity insertion transients not included in the CRP-5 effort. Furthermore it makes use of a common set of cross sections (to eliminate uncertainties between the usage of different cross section libraries by different codes) and includes specific simplifications to the design to limit the need for participants to introduce approximations in their models. Some of the details of the benchmark are still being worked out and thus it remains an unpublished draft. The important specifications and exercises have been defined and are described in Ref. 6. This document is included as an Appendix.

2.1 DESCRIPTION OF THE REACTOR MODEL

The reference design for the PBMR-400 benchmark problem is derived from the PBMR 400MW design of the demo unit. A detailed description of the plant neutronic design has been published (Ref. 7). Several simplifications were made to the design in this specification in order to limit the need for any further approximations to a minimum. During this process care has been taken to ensure that all the important characteristics of the reactor design were preserved. This ensures that the results from the benchmark will be representative of the actual design's characteristics.

Core Geometry

Simplifications made for the benchmark problem make the core design essentially two-dimensional (r,z). These include flattening of the pebble bed's upper surface and the removal of the bottom cone and de-fuel channel that results in a flat bottom reflector. Flow channels within the pebble bed have been simplified to be parallel and at equal speed. Control rods in the side reflector are modeled as a cylindrical skirt (also referred to as a grey curtain) with a given boron concentration. Only one of the transient cases, the single control rod ejection event, requires a three-dimensional model. In this case an equivalent boron concentration is defined for a specific mesh or region where the control rods are situated.

Thermal-hydraulic simplifications include the specification of stagnant helium (no mass flow) between the side reflector and barrel and the barrel and RPV. Stagnant air (no mass flow) is defined between the RPV and heat sink (outer boundary). The coolant flow is simplified to the main engineered flow paths, i.e. upwards flow from the inlet below the core within a porous ring in the side reflector and downwards flow through the pebble bed to the outlet plenum. No reflector cooling or leakage paths were defined. In the fixed central reflector the 10 cm hole in the middle, the cooling dowels and cooling slits were also removed. Other engineered coolant flows excluded are the control rod cooling flow, the core barrel leakage flow and the cooling effect of the core barrel conditioning system (CBCS) that would keep the barrel temperature within a temperature range during operation. The geometry of the simplified PBMR-400 is shown in **Figure 4.**

	0	10	41	73.6	80.55	92.05	100	117	134	151	168	185	192.95	204.45	211.4	225	243.6	260.6	275	287.5	292.5	310	328	462	463
-235		10	31	32.6	6.95	11.5	7.95	17	17	17	17	17	7.95	11.5	6.95	13.6	18.6	17	14.4	12.5	5	17.5	18	134	1
-200	35	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	He	RPV	Air	RCCS
-150	50	CC	CC	CC	CC	RSS	CC	TR	TR	TR	TR	TR	SR	RCS	SR	SR	SR	SR	SR	He	CB	He	RPV	Air	RCCS
-100	50	CC	CC	CC	CC	RSS	CC	TR	TR	TR	TR	TR	SR	RCS	SR	SR	SR	SR	SR	He	CB	He	RPV	Air	RCCS
-50	50	CC	CC	CC	CC	RSS	CC	TR	TR	TR	TR	TR	SR	RCS	SR	SR	SR	SR	SR	He	CB	He	RPV	Air	RCCS
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100	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
150	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
200	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
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1535	35	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	He	RPV	Air	RCCS

CORE LAYOUT DEFINITIONS

F	REACTOR CORE CONTAINING THE FUEL
V	HELIUM GAP BETWEEN FUEL AND TOP REFLECTOR: VOID
CC	CENTRAL REFLECTOR: GRAPHITE
TR	TOP REFLECTOR: GRAPHITE
BR	BOTTOM REFLECTOR: GRAPHITE
SR	SIDE REFLECTOR: GRAPHITE
RCS	REACTOR CONTROL SYSTEM CHANNEL : GRAPHITE / GREY CURTAIN AREA
RSS	RESERVE SHUTDOWN SYSTEM CHANNEL : GRAPHITE / GREY CURTAIN AREA
IP	INLET PLENUM TOP / BOTTOM : GRAPHITE
RC	RISER CHANNEL IN SIDE REFLECTOR : GRAPHITE
OP	OUTLET PLENUM BOTTOM : GRAPHITE
He	STAGNANT HELIUM
TP	TOP PLATE : IRON : ADIABATIC BOUNDARY
BP	BOTTOM PLATE : IRON : ADIABATIC BOUNDARY
CB	CORE BARREL : IRON
RPV	REACTOR PRESSURE VESSEL : IRON
Air	STAGNANT AIR
RCCS	REACTOR CAVITY COOLING SYSTEM : 20C TH BOUNDARY
	NEUTRONIC BOUNDARY CONDITIONS

Figure 4: Geometry of the PBMR-400 Benchmark.

Cross Sections

Input data for the neutronic modules is provided in the form of macroscopic cross sections in two energy groups (fast and thermal). Other data needed for the transient calculation are supplied as well (microscopic absorption cross sections for xenon, six-group delayed neutron precursor parameters). For the stand-alone steady-state neutronic benchmark (S-1), a single set of macroscopic cross sections for 110 compositions is supplied in an electronic file. The user is urged also to attempt various treatments of the helium-filled regions (the gas plenum above the core and the helium inlet riser) as simple diffusion theory fails in these void regions. The benchmark provides so-called *directional* diffusion coefficients derived from transport theory that can be used in place of the single-valued diffusion coefficients given in the cross section table.

The stand-alone steady-state thermal-hydraulic benchmark (S-2) does not require cross sections. The steady-state coupled benchmark problem (S-3) requires tables of cross sections for each of 114 spectral zones. Each spectral zone has a specified composition that is constant except for the xenon concentration. The cross sections are tabulated as a function of fuel temperature, moderator temperature, thermal and fast buckling, and xenon concentration. These states are computed for each spectral zone during the computation and new cross sections are then interpolated from the tables. Two sets of cross section tables are provided; one with buckling dependence and one without. The same data sets are then used for the transient problems (T-1 through T-6).

The cross sections supplied for the benchmark were generated using the MICROX code.

2.2 STEADY STATE PROBLEMS

The steady state exercises are designed to test separately the individual neutronic and thermal fluid modules and also to test the coupling algorithm. The first exercise is the neutronic steady state problem S-1. Temperature variations across the core are captured in the static macroscopic cross section data. Users report the core eigenvalue, the flux profiles for each energy group, and the total core leakage. The participants are free to determine the calculational mesh but are strongly urged to demonstrate spatial convergence of the solutions.

The stand-alone steady state thermal-hydraulic exercise (S-2) requires no neutronic solution. The local power densities are provided as input along with other material specifications, heat transfer correlations for the pebble-bed, and gas flow boundary conditions. Participants must compute the temperature distribution, outlet temperature, core pressure drop, and heat loss rate at the constant temperature boundary of the model. Once again participants are free to specify the computational mesh.

The steady-state coupled problem uses an interpolation algorithm developed at Penn State University for producing macroscopic cross sections as a function of up to five local parameters. The algorithm requires that the local equilibrium xenon concentration be computed but no other nuclide concentration calculations are necessary. Participants must compute the solid and gas temperature distributions, outlet temperatures, core pressure drop, and heat loss rate to the reactor cavity cooling system.

Exercise S-3 is also used as the starting point (initial condition) of the transient cases.
These exercises have been defined to an extent such that comparisons between various codes and solution techniques have been carried out. Preliminary results have been provided to the OECD-NEA sponsor and discussed during meetings of the Working Group. They have been neither

confirmed nor published so any results included in the next chapter are to be considered speculative and not for further distribution.

2.3 TRANSIENT PROBLEMS

The focus of the benchmark is on the modeling of the transient behavior of the PBMR core. Six exercises, covering the range from slow to fast neutronic transients, as well as feedback effects from thermal-hydraulic parameters and fission products, are included. The maturity of the transient cases is less than that of the steady state cases at this point in the progress of the Working Group and only one or two of the participants has provided preliminary results. Indeed, as THERMIX is most widely used thermal fluids code for the PBR and yields only a two-dimensional (R-Z) solution, most participants (including the INL) must engage in some code development even to complete the entire set.

A summary of the test exercises, some with various sub-cases, with a short description of each is given below:

1. Depressurized Loss of Forced Cooling (DLOFC) without SCRAM (T-1)
   The event is a Depressurized Loss of Forced Cooling in a very short time. A linear reduction in reactor inlet coolant mass flow from nominal (192.7 kg/s) to 0.0 kg/s is assumed over 13 seconds. No external flow after this step. During the same time a linear reduction in the reactor helium outlet pressure from nominal (90 bar) to 1 bar is postulated. The effects of natural convection are to be excluded in this case for simplicity. Since no SCRAM signal is assumed re-criticality should occur after some time.

2. Depressurized Loss of Forced Cooling (DLOFC) with SCRAM (T-2)
   The event is the same as Exercise 1 but with a reactor SCRAM after the depressurization phase of 13 second. At that time all control rods are fully inserted over 3 seconds to SCRAM the reactor. No re-criticality is expected but all other conditions and assumptions remain unchanged.

3. Pressurized Loss of Forced Cooling (PLOFC) with SCRAM (T-3)
   The event is a Pressurized Loss of Forced Cooling (PLOFC) with SCRAM. The effects of natural convection are included in this case. The time sequence of the event is similar to Exercise T-2 with a linear reduction of the mass flow to zero over 13 seconds. In this case a linear reduction in reactor helium outlet pressure from nominal (90 bar) to 60 bar takes place over 13 seconds. After the pressure equalization phase is completed, natural convection may start that will lead to some internal mass flow. No external mass flow is allowed. Also after 13 seconds all control rods are fully inserted over 3 seconds to SCRAM the reactor.

4. 100%-40%-100% Power Load Follow (T-4)
   The event simulates load follow in the plant with a fast change in the power from 100% to 40%, and after some time, back to 100%. The main effect is of course the xenon transient due to the power changes but other feedback effects such as the Doppler temperature also play a role. Two scenarios should be considered. In the first no control rod movement is allowed while in the second scenario the control-rods are moved to maintain a critical core within a given reactivity band width. No decay heat effects will be taken into account during the transient so that the heat is only from fission.

To assess the xenon behavior the xenon concentrations during these two cases are included in the output.

5. Reactivity Insertions by Control Rod Withdrawal and a beyond design event Control Rod Ejection (T-5). The exercise defines fast reactivity insertion by simulating different control rod withdrawal (CRW) and control rod ejection (CRE) scenarios at hot full power conditions. Note that no decay heat effects will be taken into account during the transient. Since only the core is included in this specification the changes in the inlet and outlet conditions due to the power conversion unit is not included and therefore the inlet mass flow rate, inlet temperature and outlet pressure should be kept constant at nominal conditions. Four different cases are to be analyzed. They are (i) Withdrawal of all 24 control rods at the maximum speed of 1 $cm \cdot s^{-1}$; (ii) Ejection of all 24 control rods over a 0.1 second duration; (iii) Ejection of a single control rods over a 0.1 second duration; and (iv) Ejection of 6 control rods in one quarter of the core over a 0.1 second duration. Sub-cases ii to iv were selected to include the sub-prompt and super-prompt cases even though these events are not possible on the plant and thus only of academic value.

6. Cold Helium Inlet Event (T-6). This exercise simulates a bypass valve opening, with "cold" Helium being injected into the core inlet plenum. A temperature ramp of 50 ^{o}C (i.e. 10% of nominal inlet temperature) is applied over 10 seconds, without changing any other reactor parameters like mass flow, pressure or control rod positions. Thus the reactor inlet temperature is reduced linearly from nominal (500 ^{o}C) to 450 ^{o}C over 10 seconds. It is postulated that a reactor protection system would cause the valve to close again after 300 seconds, and the temperature would return to the nominal value, again over 10 seconds. Note that no decay heat effects will be taken into account during the transient.

For all the transient cases the focus of the results are on maximum and average fuel, moderator and gas temperatures and coolant flow behavior. For the reactivity excursions the core fission power, maximum and power density profiles, and axial offset are of interest. These results are to be presented as a function of time or at specific time points or events.

This ends the summary of the full PBMR-400 Coupled Code Benchmark. In the following chapter, 1) descriptions are provided of specific modifications to the PEBBED code suite that have been implemented to run the exercises, limitations on the ability to run an exercise (if it can be run at all), and results of any successful runs.

3. CODE DEVELOPMENT AND RESULTS

3.1 STEADY STATE NEUTRONICS (S-1)

Figure 5 shows the composition map for the S-1 exercise, the stand-alone, steady state neutronics model. The red region is the active core, the yellow is the reflector, and the blue regions are gas-filled spaces (or voids). The orange region is the control rod curtain and the grey region is the core barrel. Two group macroscopic cross sections were provided in a spreadsheet file named OECD-PBMR-VSOP-Sample.XLS but converted to an ASCII text file (S2samplemac.txt) for reading by PEBBED.

	0	10	41	73.6	80.55	92.05	100	117	134	151	168	185	192.95	204.45	211.4	225	243.6	260.6	275	287.5	292.5
-200		10	31	32.6	6.95	11.5	7.95	17	17	17	17	17	7.95	11.5	6.95	13.6	18.6	17	14.4	12.5	5
-150	50	1	1	1	1	1	1	1	1	1	1	1	1	2	1	1	1	1	1	0	3
-100	50	1	1	1	1	1	1	1	1	1	1	1	1	2	1	1	1	1	1	0	3
-50	50	1	1	1	1	1	1	1	1	1	1	1	1	2	1	1	1	1	1	0	3
0	50	1	1	1	1	1	1	0	0	0	0	0	1	2	1	1	1	1	1	0	3
50	50	1	1	1	1	1	1	101	201	301	401	501	1	2	1	1	1	1	1	0	3
100	50	1	1	1	1	1	1	102	202	302	402	502	1	2	1	1	1	1	1	0	3
150	50	1	1	1	1	1	1	103	203	303	403	503	1	2	1	1	1	1	1	0	3
200	50	1	1	1	1	1	1	104	204	304	404	504	1	1	1	1	1	1	1	0	3
250	50	1	1	1	1	1	1	105	205	305	405	505	1	1	1	1	1	1	1	0	3
300	50	1	1	1	1	1	1	106	206	306	406	506	1	1	1	1	1	1	1	0	3
350	50	1	1	1	1	1	1	107	207	307	407	507	1	1	1	1	1	1	1	0	3
400	50	1	1	1	1	1	1	108	208	308	408	508	1	1	1	1	1	1	1	0	3
450	50	1	1	1	1	1	1	109	209	309	409	509	1	1	1	1	1	1	1	0	3
500	50	1	1	1	1	1	1	110	210	310	410	510	1	1	1	1	1	1	1	0	3
550	50	1	1	1	1	1	1	111	211	311	411	511	1	1	1	1	1	1	1	0	3
600	50	1	1	1	1	1	1	112	212	312	412	512	1	1	1	1	1	1	1	0	3
650	50	1	1	1	1	1	1	113	213	313	413	513	1	1	1	1	1	1	1	0	3
700	50	1	1	1	1	1	1	114	214	314	414	514	1	1	1	1	1	1	1	0	3
750	50	1	1	1	1	1	1	115	215	315	415	515	1	1	1	1	1	1	1	0	3
800	50	1	1	1	1	1	1	116	216	316	416	516	1	1	1	1	1	1	1	0	3
850	50	1	1	1	1	1	1	117	217	317	417	517	1	1	1	1	1	1	1	0	3
900	50	1	1	1	1	1	1	118	218	318	418	518	1	1	1	1	1	1	1	0	3
950	50	1	1	1	1	1	1	119	219	319	419	519	1	1	1	1	1	1	1	0	3
1000	50	1	1	1	1	1	1	120	220	320	420	520	1	1	1	1	1	1	1	0	3
1050	50	1	1	1	1	1	1	121	221	321	421	521	1	1	1	1	1	1	1	0	3
1100	50	1	1	1	1	1	1	122	222	322	422	522	1	1	1	1	1	1	1	0	3
1150	50	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	3
1200	50	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	3
1250	50	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	3

Figure 5: Composition Map of the PBMR-400 Core.

PEBBED allows for a number of options for reading cross sections. Microscopic cross for individual isotopes can be written directly into the input file, they can be read from the auxiliary files, one file for each spectral zone, generated by MICROX or COMBINE, or they can be interpolated from state point tables generated from a suitable spectrum code. For this exercise, however, the format of the spreadsheet file provided in the benchmark was not compatible with any of these. A new subroutine was thus added to read the text file mentioned above.

PEBBED has an editing option that will write average cell fluxes, by group, to an auxiliary output file. The template for reporting fluxes and powers to the Working Group, however, specifies a discretization of the R-Z space that does not necessarily match the discretization used in the model. An optional cell merge feature was added to the PEBBED output editing routines that allows the user to cluster cells into large regions for editing. Fluxes and power densities are volume-averaged to obtain the region-wise values.

The PBMR possess a large void region above the pebble-bed and also a large helium riser channel just inside the core barrel. These nominally contain helium gas and are neutronically transparent. Such regions are not well-treated by diffusion theory. One correction that is suggested by the Benchmark authors is the use of directional *diffusion coefficients*, one for the radial direction and one for the axial, instead of a single scalar diffusion coefficient. A method based upon transport theory was developed in Germany for the void region above the core and provides a value that is a function of the geometry of the void. It assumes however that the void is cylindrical and thus its validity for annuli is questionable. Nonetheless, directional diffusion coefficients are offered in the Benchmark as an alternative to the single diffusion coefficients given for these void regions.

PEBBED was modified to accept directional diffusion coefficients in the input deck. Both cases (scalar and directional) were tested in this exercise. Also, a cylindrical nodal solver developed at the INL is being implemented and was also tested against the same solution generated by the finite difference solver in PEBBED. The nodal solver is not fully implemented in that it still assumes a flat source across the nodes. This restriction will be eliminated in FY07.

Table 1 lists some of the preliminary data generated by Workshop participants. There are four PEBBED results:

PBD-1D-FD – finite difference with scalar diffusion coefficients,
PBD-DD-FD – finite difference with direction diffusion coefficients,
PBD-1D-ND – analytical nodal with scalar diffusion coefficients,
PBD-DD-FD – analytical nodal with scalar diffusion coefficients,

Also, preliminary results from other codes are presented:

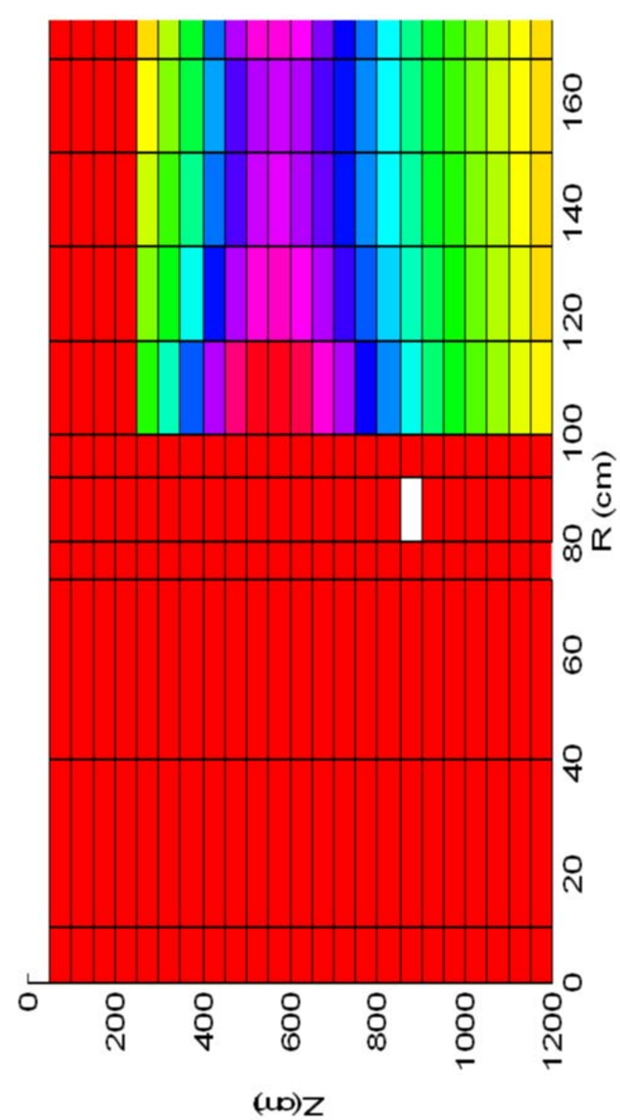
KAERI FDM – a finite difference cylindrical code from the Korean Atomic Energy Reseach Institute
TINTE – a 2-D finite difference synthesis solver developed in Germany and used by PBMR for transient analysis. TINTE uses its own cross section library rather than the library supplied with the Benchmark
Dalton – a 3-D diffusion code from Delft Institute of Technology
PARCS – Finite difference and nodal solver from Purdue

These data are not yet suitable for publication. Figure 6 shows the relative distribution of power in the core (coarse mesh RZ map).

Table 1: Comparison of Eigenvalue, Peak Flux, and Peak Power for S-1 Exercise

Code	PBD-1D-FD	PBD-DD-FD	PBD-1D-ND	PBD-DD-ND	KAERI FDM	TINTE	Dalton	PARCS	**Mean**	**% STD**
k-eff	1.0026	1.0028	1.0034	0.9988	0.9994	0.9982	1.0042	1.0001	**1.0012**	**216**
Maximum Power density (W/cm3)	10.7	10.7	10.6	10.7	10.8	10.4	10.5	10.5	**10.6**	**0.01**
Maximum fast flux (n/cm2/s)	2.12E+14	2.11E+14	2.11E+15	2.14E+15	2.11E+14	2.00E+14	2.07E+14	2.14E+14	**6.88E+14**	**1.21**
Maximum thermal flux (n/cm2/s)	3.27E+14	3.25E+14	3.27E+15	3.33E+14	3.30E+14	2.00E+14	3.22E+14	3.27E+14	**6.79E+14**	**1.44**

Figure 6: Coarse Mesh Power Distribution in the PBMR 400 at Steady State



The PEBBED results indicate the gross effect of the void spaces and the use of directional diffusion coefficients. Figure 7 illustrates the effect in showing the radially averaged fast flux as a function of axial position. The top of the pebble bed is located at z = 200 cm and the void space above it is 50 cm thick (shaded blue).

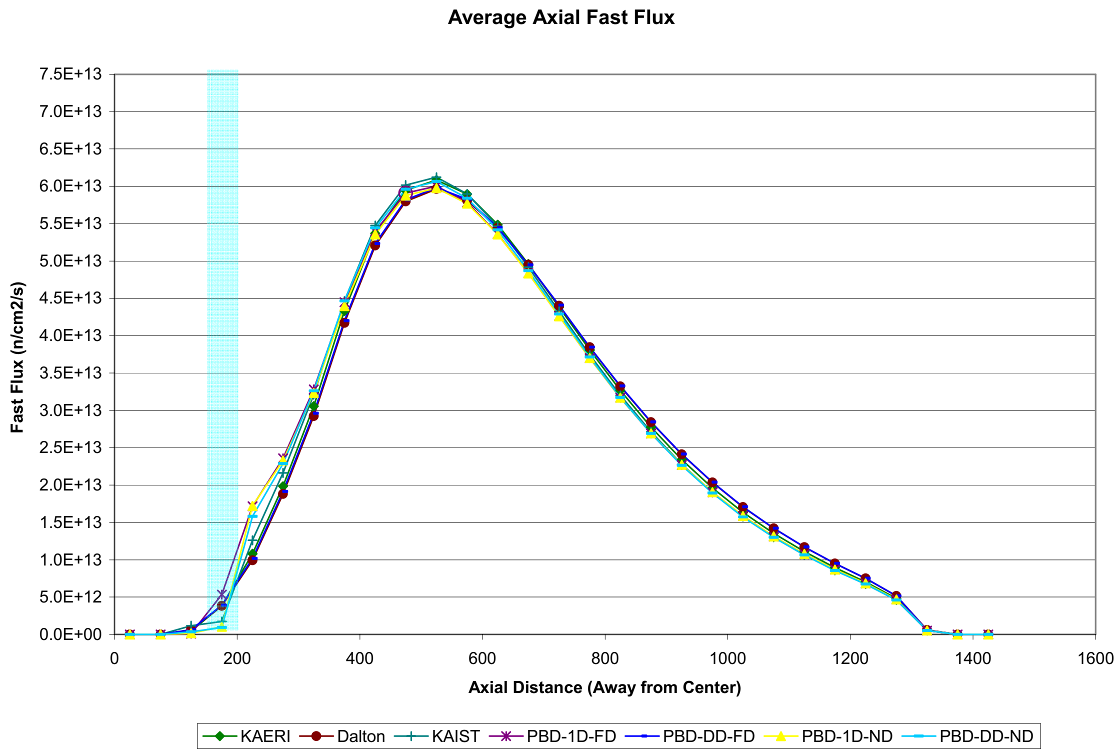


Figure 7: Radially averaged fast flux as a function of core axial height.

The effect of the helium riser next to the core barrel appears to have little effect on the fast flux but a noticeable effect on the thermal flux. The axially averaged fast flux as a function of radial distance from core center is shown in Figure 8 and the corresponding thermal flux is shown in Figure 9.

Diffusion theory is known to be inaccurate in regions far from the core so these results, which were generated from using diffusion codes, will have to be compared to a full core transport solution to have any physical validity.

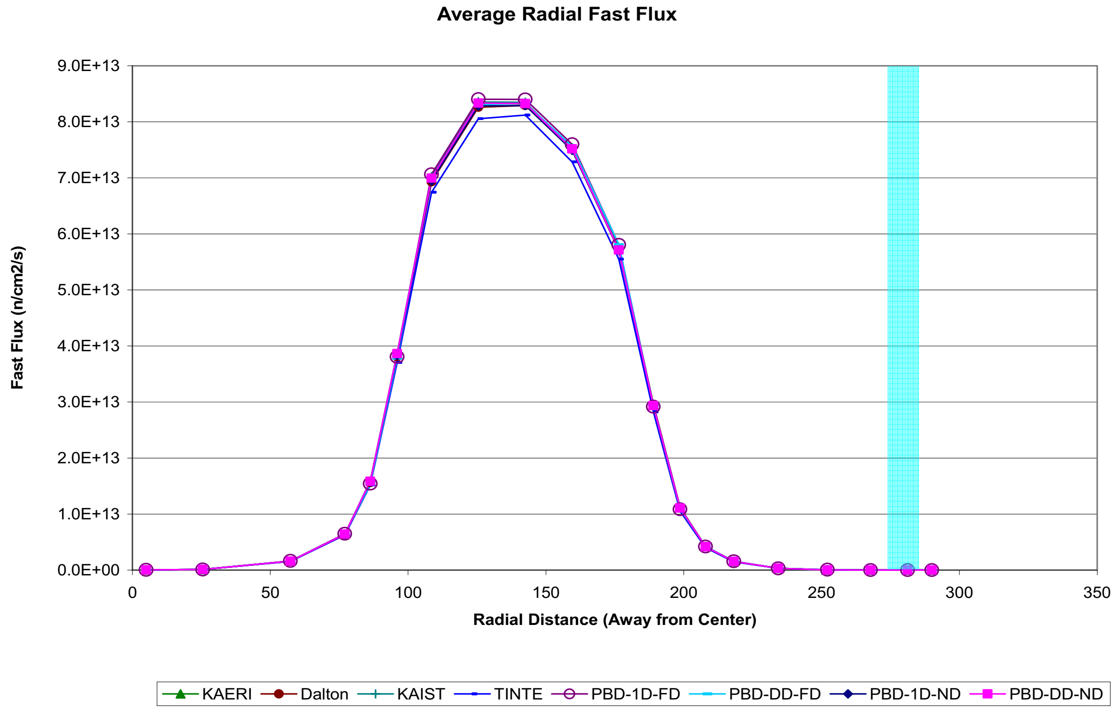


Figure 8: Axially averaged fast flux as a function of distance from core center.

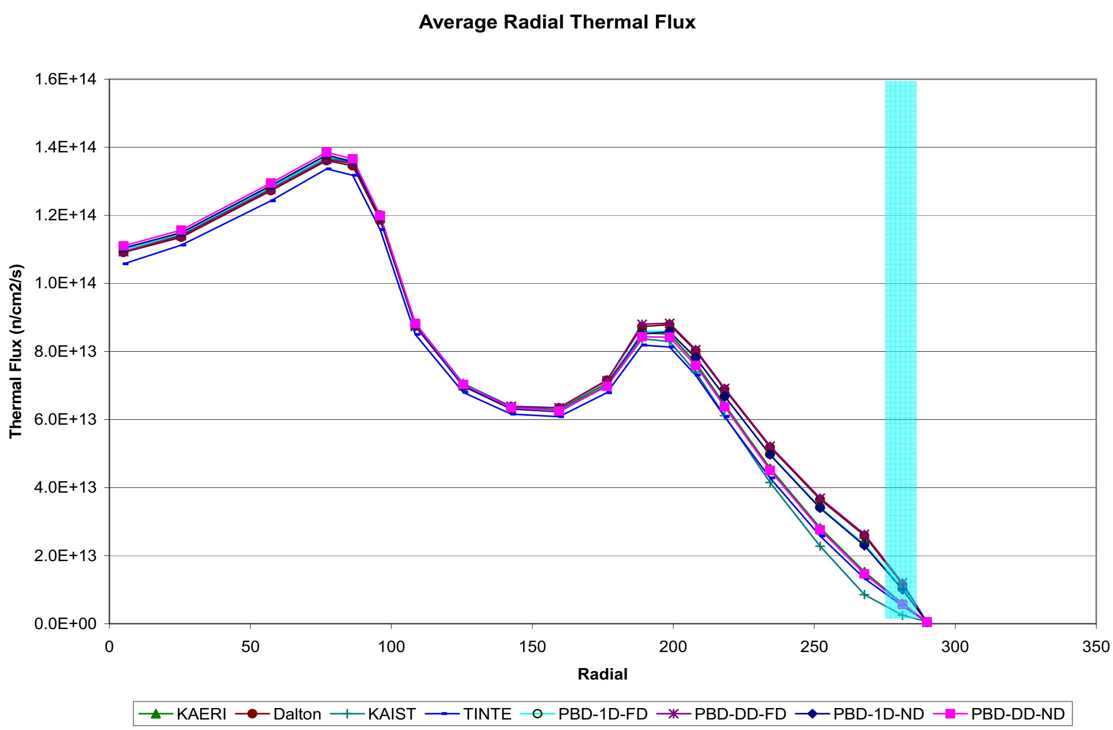


Figure 9: Axially averaged thermal flux as a function of distance from core center.

Figure 10 shows the radially averaged thermal flux as a function of axial position. The effect of the void space above the core is not so significant here (although the KAIST solver appears to have difficulty with it).

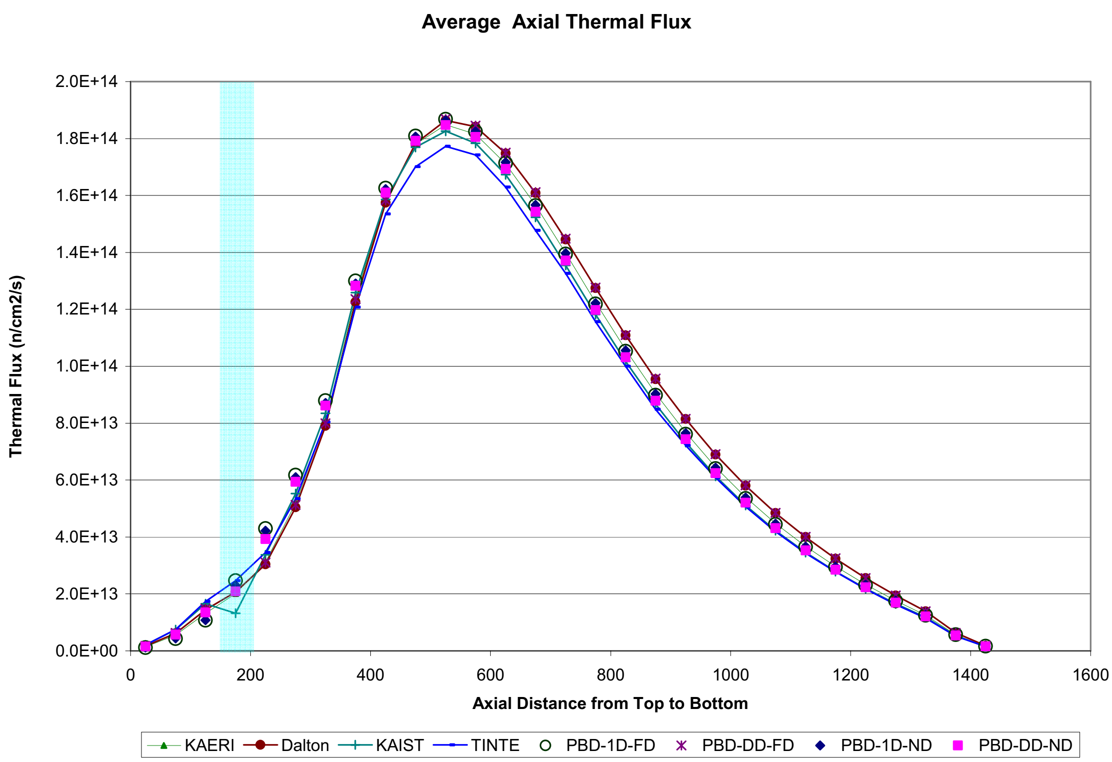


Figure 10: Radially averaged thermal flux as a function of axial location.

All in all, the PEBBED neutronic solutions (nodal and finite difference) compare well with those generated by the other codes applied to the benchmark.

3.2 STEADY STATE THERMAL FLUIDS (S-2)

This test is designed to confirm and compare the thermal-hydraulic component of the benchmark. The core model (see Figure 1 in the Appendix) is more extensive than that of the neutronics exercise as it includes core structures that influence heat removal during operations and during rapid transients (pressure vessel, stagnant air gaps, etc.). A power density map is provided in the benchmark along with basic material properties and coolant flow boundary conditions (See Appendix). Results to be reported include peak temperatures, pressure drops, temperature fields, and flow maps.

The THERMIX solver used in the PEBBED suite is called as a subroutine during a PEBBED run. This particular version of THERMIX was extracted from the VSOP-94 code suite and therefore does not have the input processing and overall computational flow control to run as a stand-alone solver. Therefore, PEBBED was modified to accommodate THERMIX testing by adding in a routine to read a power map (in the format used by PEBBED to write such maps) and set up the geometry and other computational parameters for the THERMIX run without actually performing a neutronics calculation.

Table 2 shows the power density map provided in the benchmark.

Table 2: Power Density (W/cm^3) profile in the PBMR-400

#	Region 1-22	Region 23-44	Region 45-66	Region 67-88	Region 89-110
1	2.57	2.04	1.753	1.529	1.371
2	4.32	3.449	2.968	2.59	2.328
3	6.266	5.113	4.512	4.08	3.841
4	8.221	6.911	6.337	6.123	6.517
5	9.721	8.353	7.806	7.716	8.39
6	10.491	9.155	8.612	8.541	9.234
7	10.547	9.33	8.808	8.732	9.35
8	10.075	9.022	8.542	8.458	8.967
9	9.275	8.398	7.97	7.881	8.28
10	8.318	7.6	7.227	7.138	7.441
11	7.304	6.729	6.411	6.325	6.546
12	6.315	5.86	5.592	5.512	5.669
13	5.4	5.041	4.817	4.744	4.854
14	4.581	4.298	4.112	4.046	4.122
15	3.859	3.636	3.482	3.425	3.475
16	3.232	3.056	2.929	2.879	2.912
17	2.69	2.552	2.448	2.404	2.425
18	2.222	2.113	2.029	1.992	2.004
19	1.815	1.73	1.662	1.631	1.638
20	1.457	1.391	1.336	1.311	1.314
21	1.136	1.087	1.045	1.024	1.023
22	0.872	0.855	0.827	0.799	0.775

Table 3 lists some of the parameters computed by the THERMIX module in PEBBED.

Table 3: Selected Results from the THERMIX-KONVEK Analysis of the S-2 Benchmark

Pressure drop across core (bar)	2.9419
He mass flow rate (kg/s)	193
Average fuel temperature (C)	819
Average moderator temperature (C)	797
Average helium temperature (C)	669
Peak operating fuel temperature (C)	993

Table 4: THERMIX Solid Material Temperature Profile for S-2 Exercise

	0	26.370	52.740	79.110	105.480	131.850	158.220	175.851	193.482	211.113	228.744	246.375	253.538	263.904	270.075	278.466	286.125	293.784	307.184	319.684	324.684	342.184
0	(cm)																					
1.000			20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20
36.000			298.6	294.9	288.9	287.4	284.6	282.5	277.3	271.4	264.8	257.5	249.3	245.3	239	235.1	226.9	214.7	202.4	191	180.2	176
86.000		302.3	302.2	298.5	292.4	290.8	288	285.8	280.6	274.8	268.2	260.9	252.8	248.8	242.6	238.7	230.7	218.8	207	196.4	180.1	176.1
136.000		318.7	318.6	314.5	307.7	306	302.9	300.6	295.1	289	282.5	275.5	267.9	264	258.1	254.4	246.6	235.1	223.9	214	187	183.1
186.000		351.4	351.3	346.6	338.3	336	331.9	328.7	321.2	314.2	307.8	302	296.2	293	287.8	284.2	276.3	263.8	250.9	239.1	208.4	203.5
236.000		402.8	402.8	399	390.6	387.5	380.8	374.7	352.9	340.4	334.5	334.3	340.7	341.7	339.1	336.1	327.6	312.2	295.4	279.7	242.9	236.4
285.836		468.9	469	473.8	484.8	488.9	497.5	505.4	506.1	505.9	504.7	503	502	479.4	453.4	440.1	418	391.7	366.5	342.4	294.6	284.8
335.672		516.3	516.4	519.3	524.5	525.8	528.1	529.7	525.4	519.3	514.5	510	507	502.7	497.2	494.7	492.1	495.7	483.8	434.9	363.1	346.6
385.508		551.9	551.9	552.4	552.6	552.5	552.1	551.7	545	535.4	528.6	523.3	520.3	517.7	513.7	511.4	507.3	502.9	494.9	449	381.3	364.3
435.344		585.8	585.8	585.3	584.2	583.8	583.1	582.4	573.6	560.9	552.4	547.1	544.8	538.7	530.1	525	515.2	502.5	493.7	449.9	384.8	368.3
485.180		621.6	621.6	621.2	620.4	620.2	619.7	619.4	608.6	593	583.4	579.8	579	567.6	551.7	542.6	525.4	503.3	494.1	450.6	386.1	369.7
535.016		659.1	659.1	659.1	659.1	659.1	659.1	659.1	646.7	628.5	617.9	615.5	615.8	598.7	575.2	561.6	536.3	504.1	494.2	450.9	386.6	370.3
584.852		696.5	696.5	696.9	697.7	697.9	698.3	698.6	685	664.6	652.9	651.2	652.1	629.5	598.4	580.5	547.2	504.8	494.4	451	386.8	370.5
634.688		732.2	732.2	732.9	734.2	734.5	735.1	735.6	721.3	699.3	686.8	685.3	686.4	658.6	620.4	598.4	557.5	505.5	494.5	451.2	387	370.6
684.524		764.9	764.9	765.8	767.3	767.7	768.5	769.1	754.4	731.6	718.3	716.7	717.6	685.1	640.5	614.8	566.9	506	494.6	451.3	387.1	370.8
734.360		794.1	794.2	795.1	796.7	797.1	797.9	798.5	783.9	760.7	746.8	744.9	745.4	708.7	658.4	629.3	575.3	506.6	494.7	451.4	387.2	370.8
784.196		819.6	819.6	820.6	822.1	822.5	823.2	823.8	809.7	786.5	772.2	769.7	769.8	729.4	674	642.1	582.6	507	494.8	451.5	387.3	370.9
834.032		841.4	841.4	842.3	843.7	844.1	844.8	845.3	831.7	808.9	794.4	791.2	790.7	747.2	687.5	653.1	588.9	507.3	494.9	451.6	387.3	371
883.868		859.8	859.8	860.6	861.8	862.2	862.8	863.2	850.3	828.2	813.6	809.7	808.6	762.4	699	662.5	594.3	507.6	495	451.6	387.4	371.1
933.704		875.1	875.1	875.8	876.9	877.2	877.7	878.1	866	844.7	830	825.5	823.8	775.4	708.8	670.4	598.9	507.8	495.1	451.7	387.5	371.1
983.540		887.7	887.7	888.3	889.3	889.5	890	890.3	878.9	858.5	844	838.9	836.7	786.3	717.1	677.1	602.7	508	495.2	451.8	387.5	371.2
1033.376		898	898	898.5	899.3	899.6	899.9	900.3	889.6	870.2	855.8	850.2	847.5	795.5	724	682.8	605.9	508.1	495.3	451.9	387.6	371.2
1083.212		906.3	906.3	906.8	907.5	907.6	908	908.2	898.3	879.9	865.8	859.7	856.5	803.2	729.8	687.5	608.6	508.2	495.4	451.9	387.7	371.3
1133.048		912.9	912.9	913.3	913.9	914.1	914.3	914.6	905.4	887.9	874.1	867.6	864	809.6	734.7	691.4	610.8	508.2	495.4	452	387.7	371.3
1182.884		918	918	918.4	918.9	919	919.3	919.5	910.9	894.4	881	874.2	870.3	814.9	738.6	694.7	612.7	508.2	495.5	452	387.8	371.4
1232.720		921.9	921.9	922.2	922.6	922.8	923	923.1	915.2	899.7	886.6	879.5	875.4	819.2	741.9	697.3	614.1	508.2	495.6	452.1	387.8	371.4
1282.556		924.5	924.5	924.8	925.2	925.4	925.6	925.7	918.4	903.7	891	883.8	879.3	822.5	744.4	699.3	615.2	508.2	495.6	452.2	387.9	371.5
1332.392		926	926	926.3	926.8	926.9	927.1	927.2	920.4	906.8	894.5	887.1	882.7	825.3	746.4	700.9	616.1	508.1	495.7	452.2	387.9	371.5
1382.392		926.3	926.3	926.7	927.5	927.8	928.3	928.8	922.4	909.2	897.1	889.6	883.8	825.9	746.6	700.9	616	508	495.8	452.3	388	371.6
1432.392		925.1	925.1	925.2	925.1	925	924.7	924.5	918.4	905.9	894.2	886.4	873.3	817.9	741.3	696.9	613.8	507.8	495.8	452.4	388.1	371.7
1482.392		923.5	923.5	924	924.6	924.7	924.9	925.1	919	906.5	894.7	887	874.2	818.4	741.5	697	613.7	506.5	496	452.6	388.4	372.1
1532.392		920.1	920.1	921.5	923.3	923.7	924.3	924.7	918.7	906.2	894.5	886.7	873.5	820.1	746.4	703.5	622.6	516.4	494.2	452.1	389.2	372.9
1582.392		911.4	911.5	914.7	920.1	921.6	924.2	926.2	920.2	907.3	895.4	887.8	875	827.6	762.9	726.1	658.8	577.3	515	467.1	399.2	381.4
1632.392		889.9	890	894.8	903.6	906.1	910.9	914.7	910.8	901	890.5	881	869.6	822.2	758.7	722.9	658.1	579.5	516	467.4	398.6	380.8
1682.392		849.3	849.4	853	860.9	863.7	869.6	874.7	873.5	867.1	857.1	844	827.6	779.7	718.2	684.4	624.5	552.7	494.7	450	384.1	367.6
1732.392			794.6	790.4	782.2	779.6	774.5	770.1	757.7	740.9	719.1	691.6	657.2	638	608	589.3	551.8	500.7	455.4	418.7	359.8	345.8
1767.392			756.8	748.4	733.4	729.1	721.1	714.6	698.4	678.5	654.7	627	595.3	579.2	554.8	539.5	508.5	464.4	423.4	388.4	345.5	332.8
1768.392			747.6	738.3	721.9	717.4	708.8	702.1	685.1	664.7	640.7	613.2	582.2	566.6	543	528.2	498.1	454.9	413.7	377.5	344.6	331.8

Data from the other benchmark participants was not available for comparison when this report as written. Data for the actual PBMR-400 model provided to the DOE by PBMR (Ref. 9) is shown n Table 5 for comparison. Note that the benchmark model is significantly simpler than the actual power plant and thus differences are expected. For example, the actual PBMR-400 will have an independent pressure vessel cooling system separate from the main core coolant flow. This is not modeled in the benchmark. PBMR design calculations also assume at least 10% bypass flow around the core. No bypass flow was assumed for the benchmark. Values are also included for a third PEBBED-THERMIX run that assumed 10% bypass flow. This data was generated for a study of the temperature of the pressure vessel for the NGNP and will be presented in a paper (Ref. 10) at the HTR-2006 conference.

Table 5: Benchmark Results vs. Design Data for the PBMR-400

	THERMIX Benchmark Result	PBMR Design Value	INL RPV Study of the PBMR
Maximum Fuel Temperature (C)	993	1079	1043
Maximum Core Barrel Temperature (C)	399	428	488
Maximum Pressure Vessel Temperature (C)	305	280	342

These results indicate the importance of accurately determining and modeling the bypass flow around the core. Comparisons with other benchmark results are needed to confirm the accuracy of the THERMIX calculations.

3.3 COUPLED STEADY STATE NEUTRONICS AND THERMAL FLUIDS (S-3)

The third steady-state problem tests the coupling between the neutronic and thermal fluid models. The coolant flow boundary conditions of the previous exercise are used along with a cross section interpolation tables with which the neutronic model can compute the power density maps. The initial temperature profile is not known so an initial guess at the profile is used to start the iterative process that leads to the final flux-power-temperature solution.

Five-dimensional tables are used to represent the instantaneous variation in cross-section due to changes in the reactor. The cross section models are designed to cover the initial steady state conditions and the expected ranges of change of the 5 selected instantaneous feedback parameters in the transients to be simulated in the benchmark. Cross sections were generated for all the combinations of the given state parameters. The five state parameters are:

- Fuel temperature
- Moderator temperature
- Fast buckling
- Thermal buckling
- Xenon concentration

In all of the fuel material cross section tables, there were four fuel temperatures, seven moderator temperatures, three fast bucklings, three thermal bucklings and three Xenon number densities while for all the non-fuel materials no fuel temperature or xenon variations were included. The ranges chosen for each parameter were selected based on the reactor conditions for normal operation as well as for accident conditions. For instance, the fuel temperature ranges from 300K to 2400K.

The set was generated using MICROX using equilibrium core number densities specified in the benchmark with two energy groups separated at 2.38 eV. Two sets of cross sections were generated: the full 5-independent variable set described above and a reduced set in which the buckling dependence was omitted and all of the cross sections were generated assuming no fast or thermal leakage from the spectral zone.

Exercise 3 is the steady-state starting condition of all the Transient cases. The detailed results thus only need to be given once and not repeated for each transient case. Results to be edited are 1) spatial maps of the maximum and average fuel temperature, 2) maximum and average moderator temperature, 3) power density, 4) relative pressure, 5) mass flow, and 6) thermal conductivity. Single parameter values to be edited are the axial power offset and k-eff. Not all of these results are provided in this report but they will be included in the OECD publication for the Benchmark.

As with the S-1 benchmark, four PEBBED-THERMIX models were executed. They are:

1) NB-1D: No buckling dependence and a single diffusion coefficient for the void regions,
2) NB-DD: No buckling dependence and a single diffusion coefficient for the void regions,
3) B-1D: No buckling dependence and a single diffusion coefficient for the void regions,
4) B-DD: No buckling dependence and a single diffusion coefficient for the void regions.

Table 6 lists some of the integral parameters estimated by PEBBED-THERMIX.

Table 6: Selected PEBBED-THERMIX results for the S-3 exercise

	NB-1D	NB-DD	B-1D	B-DD
Core Eigenvalue (k_{eff})	1.06149	1.07221	1.08371	1.09403
Maximum Fuel Temperature (C)	995	988	994	987
Average Fuel Temperature (C)	820	819	819	816
Peak Power Density (W/cm^3)	11.9	11.5	12.1	11.7
Peak Thermal Flux (n/cm^2-s)	2.15E14	2.22E14	2.22E14	2.09E14
Peak Fast Flux (n/cm^2-s)	3.31E14	3.26E14	3.26E14	3.20E14
Ratio of Core Leakage to Total Loss (% of neutrons lost)	15.2	14.9	15.3	14.7

The table indicates the effect of the leakage spectrum on local cross sections. Capturing the leakage spectrum, even with a rudimentary buckling treatment, changes the cross sections enough to have a significant effect on core reactivity. The core eigenvalue is about 2000 pcm higher with the buckling correction. The temperature appears to be less affected.

Preliminary results for the S-3 exercise were also generated using NEM-THERMIX. Full flux and power maps will be included in the benchmark publication but a core eigenvalue of 1.07971 was computed for a model that used the zero-buckling cross sections and scalar diffusion coefficients (Ref. 11). This result will be confirmed in FY07 but is within the range of variation observed in the PEBBED cases. This result also reveals an issue with the cross section set. The nuclide densities used to generate the interpolation tables were obtained from a VSOP calculation that was adjusted to yield a critical core. The cross sections computed using MICROX clearly yield a supercritical core. This inconsistency will need to be addressed by the Working Group as the S-3 case is to be used as the initial condition for the transient cases.

Figures 11 and 12 illustrate the flux variations in the PBMR core. The significant gradients, especially in the radial direction, confirm the considerable cross-zone leakage that is not captured in infinite-cell spectrum calculations.

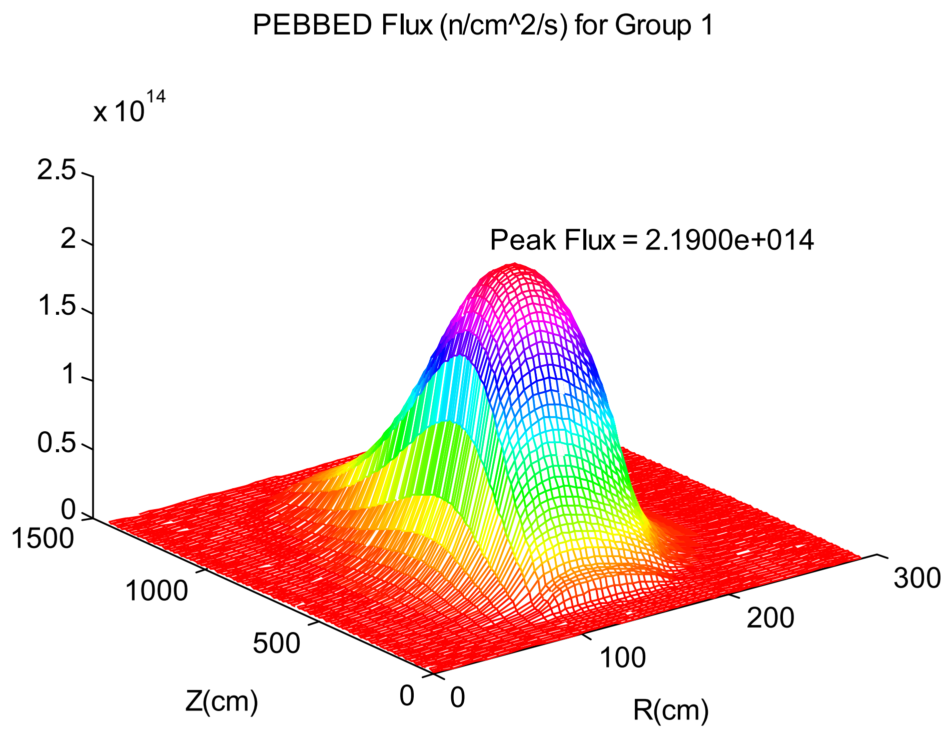


Figure 11: Fast flux profile in the PBMR-400 Benchmark (NB-1D)

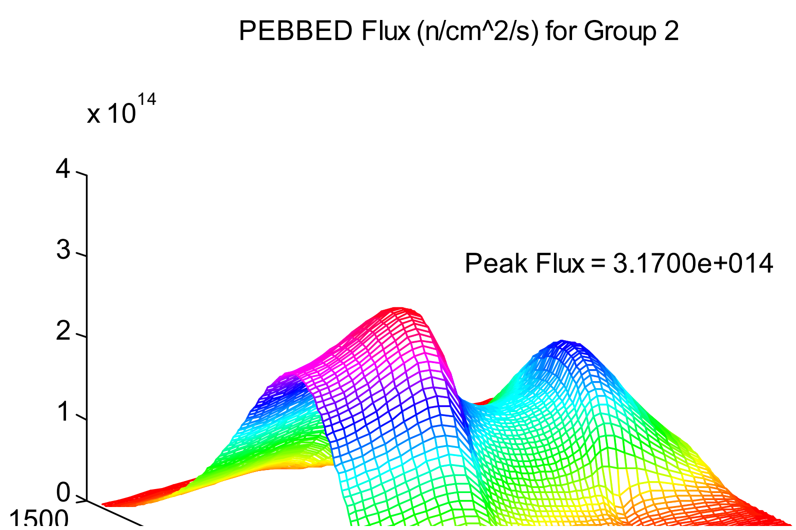


Figure 12: Thermal flux profile in the PBMR-400 Benchmark (NB-1D)

The minor differences between the peak flux values shown in the plots and those in the table are a result of the averaging process. The table values are peaks over the common coarse mesh specified for benchmark reporting while the plot values are the peaks from the fine neutronic mesh used in the PEBBED model.

Figure 13 shows the radial flux profile (averaged over the core). Note the flux gradients at the core-reflector interfaces. The fuel zones adjacent to the reflector receive a significant thermalized neutron stream from the reflectors. In-leakage of this sort implies a negative buckling that many spectrum codes (including MICROX and COMBINE version 6) do not accommodate. A companion NGNP report contains a summary of the improvements made to COMBINE (for version 7) to treat negative bucklings as a leakage source in the B-1 approximation to the transport equation.

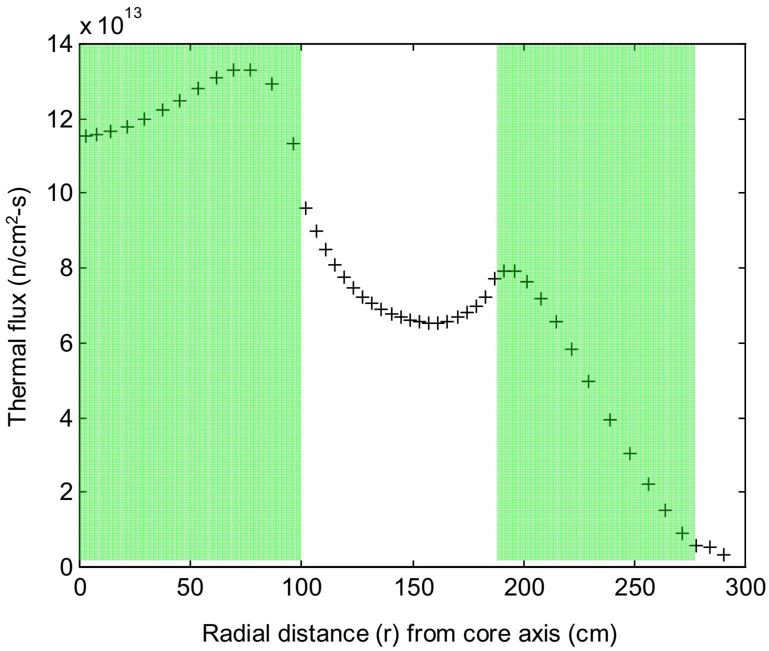


Figure 13: Axially averaged radial thermal flux profile in the PBMR-400 benchmark

THERMIX plots were also generated. Figure 14 shows the temperature profile in the core and inner reflector. The inner reflector (0 cm < r < 100cm) profile tracks that of the core (100 cm < r < 185 cm) as there is no significant cooling mechanism present. The coolant inlet temperature of the PBMR-400 is 500 ^{o}C and the target outlet temperature (assuming no bypass) is 900 ^{o}C.

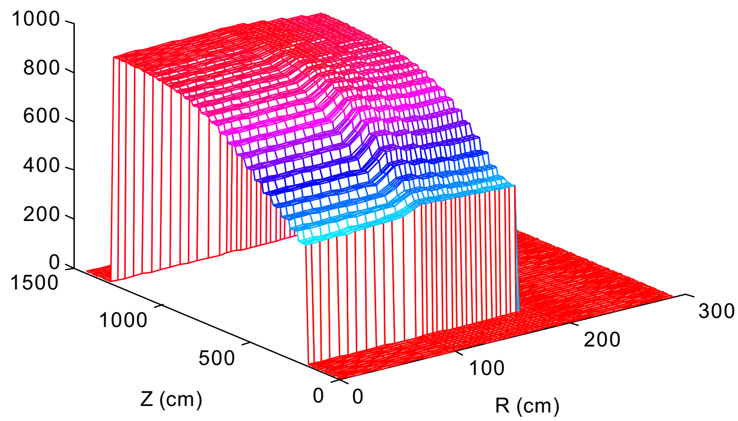


Figure 14: Graphite temperature field in the inner reflector and core

Tables 7a and 7b show the coolant flows by position in the core. Table 7a lists the radial (cross flow) with the inlet helium flow entering from the top and right.

Table 7a: Radial coolant flow in the core (kg/s)

z (cm)	**0**	-7.06	-20.80	-31.24	-31.83	-14.33
	50	-6.10	-21.21	-45.07	-85.31	-151.65
	100	-1.32	-3.88	-5.75	-5.90	-2.71
	150	-0.03	-0.11	-0.12	-0.03	0.01
	200	0.04	0.08	0.08	0.04	0.00
	250	0.03	0.06	0.05	0.02	-0.01
	300	0.02	0.04	0.03	0.01	-0.01
	350	0.02	0.03	0.02	0.01	-0.01
	400	0.01	0.02	0.02	0.01	-0.01
	450	0.01	0.01	0.01	0.01	-0.01
	500	0.01	0.01	0.01	0.01	0.00
	550	0.00	0.00	0.00	0.00	0.00
	600	0.00	0.00	0.00	0.00	0.00
	650	0.00	-0.01	0.00	0.00	0.00
	700	0.00	-0.01	-0.01	0.00	0.00
	750	-0.01	-0.01	-0.01	0.00	0.00
	800	-0.01	-0.02	-0.01	0.00	0.01
	850	-0.01	-0.02	-0.01	0.00	0.01
	900	-0.02	-0.02	-0.01	0.00	0.02
	950	-0.02	-0.02	-0.01	0.00	0.02
	1000	-0.03	-0.02	-0.01	0.01	0.03
	1050	-0.03	-0.02	-0.01	0.01	0.04
	1100	-0.03	-0.03	-0.02	0.00	0.03
	1150	0.00	0.00	0.00	0.00	0.00
	1200	0.00	0.00	0.00	0.00	0.00
	1250	0.00	0.00	0.00	0.00	0.00
	1300	0.00	0.00	0.00	0.00	0.00
	1350	0.00	0.00	0.00	0.00	0.00
	1400	-0.14	-0.37	-0.47	-0.40	-0.16

100 117 134 151 168 185

r (cm)

Table 7b shows the corresponding helium flow rates in the axial direction. In the core itself the axial flow is roughly four orders of magnitude greater than the radial. This small amount of cross flow is a result of the high pressure drop through a packed bed of pebbles. The axial flow density (kg/s/cm^2) is actually quite uniform (<2% variation) in the radial direction so that each pebble is subject to the same flow stream regardless of location or power produced.

Table 7b: Axial coolant flow in the core (kg/s)

	0	7.06	6.67	3.76	-3.17	-14.33
	50	20.22	22.29	22.37	18.98	12.29
	100	27.64	32.45	37.85	43.80	50.52
	150	28.99	33.67	38.43	43.19	47.81
	200	28.98	33.65	38.38	43.11	47.81
	250	28.91	33.60	38.37	43.11	47.79
	300	28.85	33.56	38.36	43.10	47.77
	350	28.80	33.53	38.34	43.09	47.74
	400	28.77	33.50	38.33	43.07	47.72
	450	28.74	33.48	38.31	43.06	47.70
	500	28.72	33.46	38.29	43.04	47.68
z (cm)	**550**	28.71	33.44	38.27	43.02	47.67
	600	28.70	33.42	38.25	43.01	47.67
	650	28.70	33.42	38.23	42.99	47.66
	700	28.71	33.41	38.22	42.98	47.66
	750	28.72	33.41	38.21	42.98	47.66
	800	28.74	33.42	38.21	42.98	47.67
	850	28.76	33.44	38.23	42.99	47.69
	900	28.80	33.47	38.25	43.02	47.73
	950	28.84	33.52	38.29	43.06	47.78
	1000	28.89	33.57	38.34	43.12	47.84
	1050	28.96	33.63	38.40	43.18	47.92
	1100	29.03	33.71	38.48	43.26	48.00
	1150	29.06	33.74	38.51	43.29	48.03
	1200	29.06	33.74	38.51	43.29	48.03
	1250	29.06	33.74	38.51	43.29	48.03
	1300	29.06	33.74	38.51	43.29	48.03
	1350	29.06	33.74	38.51	43.29	48.03
	1400	14.53	16.88	19.26	21.65	24.03
	100	**117**	**134**	**151**	**168**	**185**
			r (cm)			

Without the results from other codes for comparison, little can be claimed about the validity of the PEBBED-THERMIX values. Better conclusions can be drawn after the results from the participants are submitted and compiled in FY07. The S-1 neutronic results do indicate fair agreement with other codes, however, and the S-2 results are consistent with those generated for more complex PBMR models.

3.4 TRANSIENT CASES

Although the steady state cases are informative and necessary, the transient exercises are the focus of the Benchmark. The six cases have been defined in sufficient detail for the participants to build and execute models but some minor issues remain to be resolved. These will be addressed in the second phase of the benchmark exercise that is scheduled to commence in FY07. Preliminary results for some of the cases have been generated using TINTE (PBMR). NEM-THERMIX has been used to generate transient results for the PBMR-268 benchmark that preceded the current activity but a number of issues arose when it was applied to the PBMR-400. These coding issues are being resolved collaboratively by Penn State and the NIL and are discussed in a companion milestone report. Testing of NEM-THERMIX on these transient problems is expected in the coming months.

As mentioned in the first section, PEBBED is currently unable to model transient cases in general because it does not yet possess a time-dependent neutronics solver. There is one transient for which PEBBED has been designed to simulate, that of the Depressurized Loss of Fluid Condition (DLOFC) with Scram. This is also known as a Depressurized Conduction Cooldown because decay heat is transferred from the core by (mainly) radial conduction and thermal radiation across gaps. Because the peak DLOFC fuel temperature is a fundamental design parameter, PEBBED-THERMIX contains a module for simulating this transient through the use of a programmed decay heat curve. The algorithm assumes that the decay heat source shape is the same as that of the steady state power profile but its magnitude decays away according to a specified trajectory. Figure 15 shows two trajectories that are available for use in PEBBED. The PBMR trajectory is based upon the German DIN standard and is the default correlation in THERMIX.

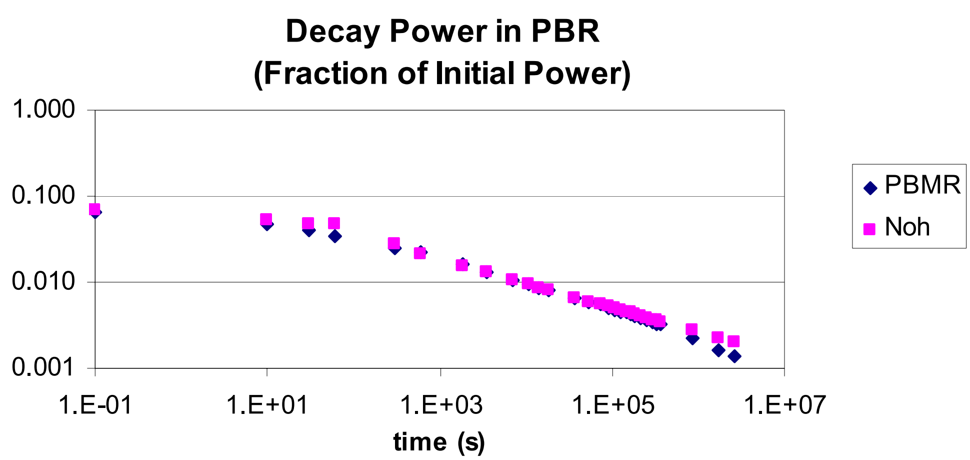


Figure 15: Decay heat trajectories (fraction of steady state power) used in PEBBED.

Coolant flow is assumed to cease immediately at the start of the transient; a conservative assumption. The pressure of the gas during the transient is specified by the user.

A scram is assumed to occur because this simple DLOFC model cannot simulate the re-criticality that is likely to occur after xenon decays away and the core temperature decreases. Such a simulation requires a proper transient analysis that will be achieved with the maturity of NEM-THERMIX. Also, the actual DLOFC with Scram exercise assumes that the pressure and flow drop linearly over a 13 second interval at the start of the transient. The instantaneous drop assumed in the PEBBED-THERMIX model is unrealistically abrupt and should yield a higher peak temperature than the ramp model.

With the S-3 computed power profile, PEBBED-THERMIX computed a peak DLOFC fuel temperature of 1690 ^{o}C that occurs 60 hours after shutdown. This is higher than the 1600 ^{o}C design value for the actual PBMR (Ref. 7) but it is not an unexpected result given the assumption of instantaneous pressure and flow drop. The 60 hour interval is consistent with the PBMR design value.

Figure 16a shows the temperature field in the core at steady state (0 h) while Figure 16b shows the temperature field at 60.5 hours after shutdown.

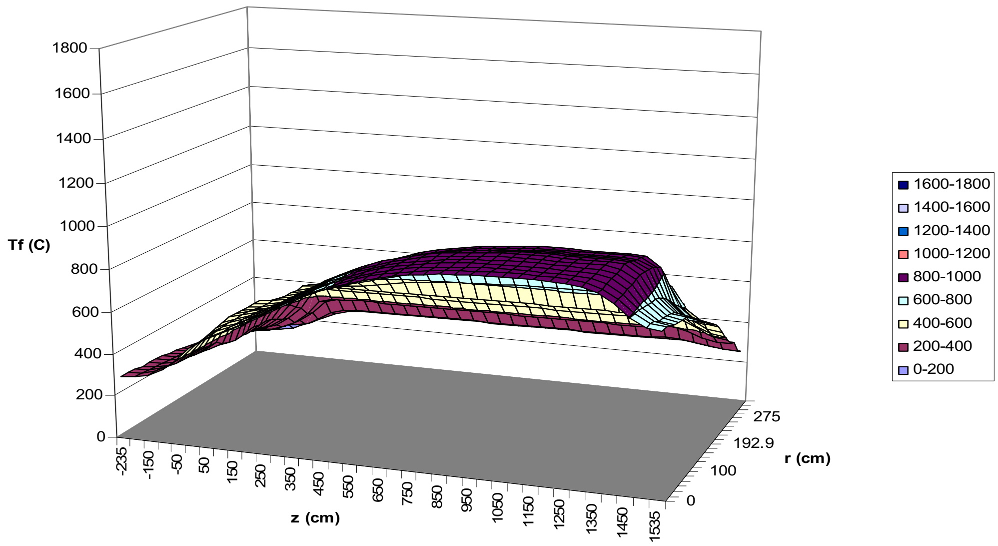


Figure 16a: Core temperature map at steady state (0h into DLOFC).

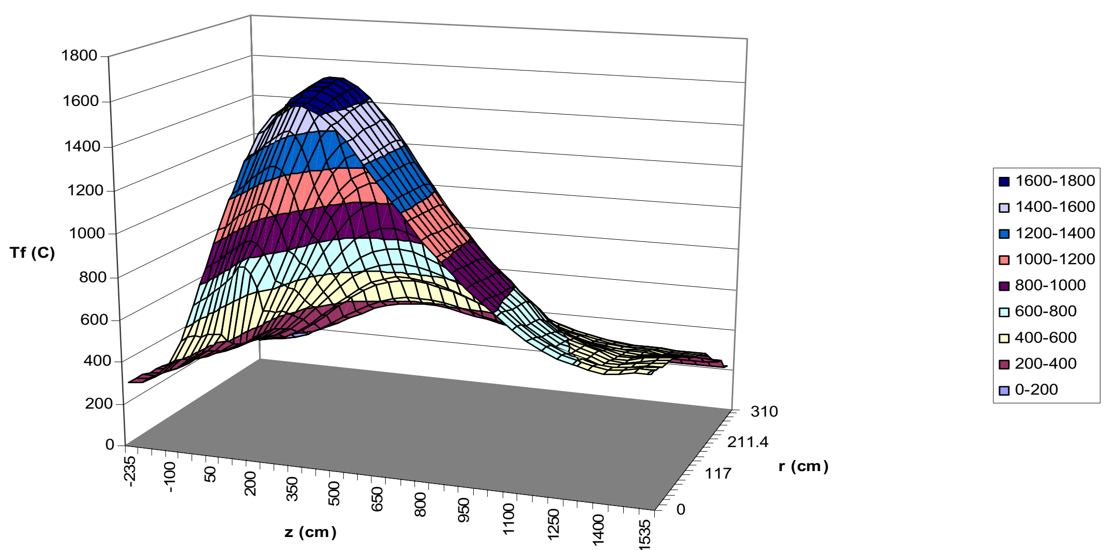


Figure 16b: Core temperature map at 60h into DLOFC.

The second plot indicates how the DLOFC peak temperature profile tracks that of the initial power distribution rather than the initial temperature profile.

Again, this data needs to be compared with the results of other codes but they are qualitatively sound.

No results are yet available for the other transient exercises. Debugging and testing of the NEM-THERMIX code will continue in FY07 with sufficient funding after which a full analysis of the benchmark exercises will be performed and published. Alternatively, if the kinetic version of the PEBBED solver is also available, it will be coupled to a thermal fluid solver and tested against these problems.

4. CONCLUSIONS AND FURTHER DEVELOPMENTS

The diffusion solver in PEBBED has undergone some testing and appears to be suitable for pebble bed reactor design and analysis. It produces core eigenvalues and flux profiles comparable to other established diffusion codes on well defined problems (the S-1 exercise). In FY06 it was modified to accept directional diffusion coefficients that may yield improved accuracy in core models that include large gas plenums.

Cross sections for the benchmark problems were provided by PBMR using the MICROX code. PEBBED is capable of reading MICROX data but in FY06 the COMBINE code was enhanced to make it more suitable for in-line generation of cross sections codes for high temperature reactor applications. A script was written that automatically generates state point cross sections for interpolation by PEBBED or NEM-THERMIX.

PEBBED is coupled to THERMIX-KONVEK, a legacy PBR thermal-hydraulics solver developed at Research Center Jülich in Germany and part of the VSOP94 code package. THERMIX-KONVEK solves the equations of heat transfer (THERMIX) and gas dynamics (KONVEK) in two dimensions (R-Z). It contains correlations and material properties appropriate for PBR simulation.

VSOP99 uses a newer version of THERMIX coupled with the gas dynamics solver DIREKT. THERMIX-DIREKT is used by a number of institutions for PBR analysis. Penn State University sponsored an effort to couple it to the transient neutronics solver NEM and the coupled code has been provided to the INL to enable PBR transient simulation. The NEM-THERMIX solver has been used successfully to model the earlier PBMR-268 core model but the coupling algorithms contained model-specific elements that prevented its application to the PBMR-400. In FY06, students at Penn State and Idaho State Universities cooperated to remove these elements and make the solver more flexible. Work is just about complete on this task and testing will conducted in the early part of FY07 using the problems in the PBMR-400 Benchmark.

The INL spectrum code COMBINE has been used to generate microscopic cross sections for PEBBED analysis and in FY06 a method was developed to use COMBINE to generate state-variable-dependent macroscopic cross sections for NEM analysis as well. An internally consistent mechanism now exists for generating cross sections for both core design and safety analysis computations.

The PEBBED-THERMIX code has been applied to the steady state exercises in the PBMR-400 Coupled Code Benchmark. While results from other participants are not yet available for comparison, PEBBED results appear physically plausible and consistent with the results of other PBR analyses.

In the near term (the next 2 years), the NEM-THERMIX code can provide transient capability that coordinates well with the capabilities of the fuel design code PEBBED. In the long term, a kinetic version of the PEBBED solver will yield a more accurate and compatible tool.

The THERMIX solvers used with PEBBED and NEM have a long history of PBR analysis having been developed for the German HTR program. THERMIX, however, remains a two-dimensional solver and thus is of limited use in certain types of PBR transients. There are some efforts underway (not at the INL) to write a three-dimensional version of THERMIX. THERMIX is not a DOE code, however, and thus would be difficult to maintain and modify for regular use. A more suitable long-term approach would be to adapt the INL code RELAP5-3D for PBR use by adding appropriate correlations and material libraries. RELAP already possesses a mature architecture or linking with other codes. The PEBBED solvers could be incorporated into this scheme with little difficulty. Ultimately this would provide the DOE with an independent and wholly owned PBR analysis capability. Planning and initial assessments were performed in FY06 to couple PEBBED to RELAP. This work will continue in FY07 should adequate funding be provided.

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Appendix A
The OECD/NEA/NSC PBMR Coupled Neutronics/Thermal Hydraulics Transient Benchmark: The PBMR-400 Core Design

APPENDIX A

Description of the PBMR-400 Core Design

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Abstract

The Pebble Bed Modular Reactor (PBMR) is a High-Temperature Gas-cooled Reactor (HTGR) concept to be built in South Africa. As part of the verification and validation program the definition and execution of code-to-code benchmark exercises are important.

The Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development (OECD) has accepted, through the Nuclear Science Committee (NSC), the inclusion of the PBMR coupled neutronics/thermal hydraulics transient benchmark problem in its program.

The OECD benchmark defines steady-state and transients cases, including reactivity insertion transients. It makes use of a common set of cross sections (to eliminate uncertainties between different codes) and includes specific simplifications to the design to limit the need for participants to introduce approximations in their models.

In this paper the detailed specification is explained including the test cases to be calculated and the results required from participants.

KEYWORDS: Pebble bed modular reactor, PBMR, Coupled Neutronics, Thermal Hydraulics, Transient, OECD Benchmark

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Appendix A
The OECD/NEA/NSC PBMR Coupled Neutronics/Thermal Hydraulics Transient Benchmark: The PBMR-400 Core Design

1. INTRODUCTION

The Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development (OECD) has accepted the Pebble-Bed Modular Reactor (PBMR) coupled neutronics/thermal hydraulics transient benchmark problem as part of their program.

The PBMR is a High-Temperature Gas-cooled Reactor (HTGR) concept, which has attracted the attention of the nuclear research and development community. The deterministic neutronics, thermal-hydraulics and transient analysis tools and methods available to design and analyze PBMRs have, in many cases, lagged behind the state of the art compared to other reactor technologies. This has motivated the testing of existing methods for HTGRs but also the development of more accurate and efficient tools to analyze the neutronics and thermal-hydraulic behavior for the design and safety evaluations of the PBMR. In addition to the development of new methods, this includes defining appropriate benchmarks to verify and validate the new methods in computer codes.

The scope of the benchmark described in this paper is to establish a well-defined problem, based on a common given set of cross sections, to compare methods and tools in core simulation and thermal hydraulics analysis with a specific focus on transient events through a set of multi-dimensional computational test problems.

In addition, the benchmark exercise has the following objectives:

1. Establish a standard benchmark for coupled codes (neutronics/thermal-hydraulics) for PBMR design.
2. Code-to-code and methods comparison using a common cross section library – this is very important for Verification and Validation and part of the PBMR licensing process.
3. Obtain a detailed understanding of the phenomena that is important to model during the different transient events.
4. Benefit from the use of different methods and also different approaches to the test exercises.
5. Obtain an understanding of the limitations of the tools and the effects of approximations introduced.
6. Organize special sessions at conference or a special issue of a publication to give exposure to HTGR methods and designs.
7. Serve as the vehicle for future benchmarks based on experimental facilities or eventually the PBMR demonstration unit.

The OECD benchmark is of course not the first effort to verify the methods and codes used for the PBMR design or more generally for HTGRs. The tools and methods available today have continuously been validated against experiments and operating reactors throughout its development although the formalized procedures required today was not in general use. Some benchmark problem definitions and experimental facilities do of course exist for HTRs, including a few existing for pebble bed reactors. This includes, amongst others, the Proteus pebble bed critical experiments [1] and ASTRA facility [2,3] as examples of critical assemblies, the HTR 10 reactor in operation at Institute of Nuclear Energy Technology, Tsinghua University, Beijing, China [4], reactors that operated in Germany in the past such as the AVR (Arbeitsgemeinschaft Versuchsreaktor GmbH – a 15MWe pebble bed experimental reactor built at the FZJ site, Jülich and operated from December 1967 till 1988), and several code-to-code comparisons performed as part of the IAEA CRP-5 (Co-ordinated Research Project (CRP) on "Evaluation of HTGR Performance") [5,6] and similar programs. Some transient experiments were also performed at the AVR [7] and others include simulations with codes still in use today [8]. All of these contributed to the benchmarking and V&V of coupled neutronics/core thermal-hydraulics tools used in pebble bed reactor designs. The current transient benchmark specification with all the different transient cases is the first based on the 400 MWth PBMR design with its annular core design with the fixed graphite central column. In previous work, based on the older PBMR 268 MWth dynamic central column design [9], similar transient cases were analyzed. This benchmark was restricted to only a few participants and the specific behavior of the PBMR 400 MWth design required a new definition and the OECD acceptance has given it wider exposure. The lessons learned from these initial efforts are now applied to the OECD benchmark.

2. THE BENCH MARK DEFINITION

The reference design for the PBMR-400 benchmark problem is derived from the PBMR 400MW design of the demo unit. A detailed description of the plant design and specifically the reactor core neutronics design has been published [6, 10, 11]. Several simplifications were made to the design in this specification in order to limit the need for any further approximations to a minimum. During this process care has been taken to ensure that all the important characteristics of the reactor design were preserved. This ensures that the results from the benchmark will be representative of the actual design's characteristics.

2.1 Simplifications Introduced

The simplifications made for the benchmark problem make the core design essentially two-dimensional (r,z). It includes flattening of the pebble bed's upper surface and the removal of the bottom cone and de-fuel channel that results in a flat bottom reflector. Flow channels within the pebble bed have been simplified to be parallel and at equal speed. Control rods in the side reflector are modeled as a cylindrical skirt (also referred to as a grey curtain) with a given B_{10} concentration. Only one of the transient cases, the single control rod ejection event, requires a three-dimensional model. In this case an equivalent boron concentration is defined for a specific mesh or region where the control rods are situated.

Thermal-hydraulic simplifications include the specification of stagnant helium (no mass flow) between the side reflector and barrel and the barrel and RPV. Stagnant air (no mass flow) is defined between the RPV and heat sink (outer boundary). The coolant flow is simplified to the main engineered flow paths, i.e. upwards flow from the inlet below the core within a porous ring in the side reflector and downwards flow through the pebble bed to the outlet plenum. No reflector cooling or leakage paths were defined. In the fixed central reflector the 10 cm hole in the middle, the cooling dowels and cooling slits were also removed. Other engineered coolant flows excluded are the control rod cooling flow, the core barrel leakage flow and the cooling effect of the core barrel conditioning system (CBCS) that would keep the barrel temperature within a temperature range during operation.

The effect of excluding specific coolant flows is to some extend balanced by the assumption that all heat sources (from fission) will be deposited locally, i.e. in the fuel and that no other heat sources exist outside the core (for example neutron absorption in the control rods). Simplifications are also made in the material thermal properties in as far as constant values are employed or specific correlations are employed.

2.2 Geometrical Description

The benchmark reactor unit geometry description is given in Figure 1 with the general material layout shown. The mesh dimensions (r, z) as well as the general material regions of the core are shown

Appendix A
The OECD/NEA/NSC PBMR Coupled Neutronics/Thermal Hydraulics Transient Benchmark: The PBMR-400 Core Design

The figure represents half of the reactor with a symmetry axis on the zero radius line in the centre of the reactor. The pebble bed core is the 85 cm thick annulus represented by “F”. Just above the fuel is a “void” area (that is of course filled with helium). The graphite reflector has been divided into four regions called the Central Column (CC), the Top Reflector (TR), the Bottom Reflector (BR) and the Side Reflector (SR). The central column has a radius of 100 cm and the side reflector a thickness of 90 cm. Beyond the side reflector is a helium gap (He) between the graphite blocks of the SR and core barrel (CB). This is followed by another Helium gap (He) and the Reactor Pressure Vessel (RPV). Outside the RPV and air gap of 134 cm is found before the Reactor Cavity Cooling System (RCCS) is defined as the outer boundary of the benchmark model. Above the top reflector of 150 cm the 35 cm thick Top Plate (TP) is the upper boundary. Similarly the Bottom Plate (BT) forms the lower boundary of the problem below 400 cm of bottom reflector. The effective core height is 1100 cm with a helium filled cavity at the top of 50 cm. The core effective volume that can be filled with fuel is thus 83.7155 m^3.

The helium coolant path is bordered by the solid lines shown within the figure. The side reflector contains the lower inlet plenum (IP) where the coolant gas enters and flow upward through the Riser Channels (RC) into the upper inlet plenum (IP). The gas then flow down through the core, through slits in the bottom reflector into the outlet plenum from where it enters into the power conversion unit (PCU). The side reflector also contains the Reactivity Control System channels (RCS) while the Central Column contains the Reserve Shutdown System channels (RSS). In the current benchmark definition the RSS is never filled with any neutron absorber material and is therefore treated the same as the rest of the Central Column. Only the upper few meshes of the RCS are typically filled by the control rods (see shaded area) while the rest of the axial meshes are then assumed to be the same as the side reflector.

Figure 1: Core layout and identification

	0	10	41	73.6	80.55	92.05	100	117	134	151	168	185	192.95	204.45	211.4	225	243.6	260.6	275	287.5	292.5	310	328	462	463
-235		10	31	32.6	6.95	11.5	7.95	17	17	17	17	17	7.95	11.5	6.95	13.6	18.6	17	14.4	12.5	5	17.5	18	134	1
-200	35	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	TP	He	RPV	Air	RCCS
-150	50	CC	CC	CC	CC	RSS	CC	TR	TR	TR	TR	TR	SR	RCS	SR	SR	SR	SR	SR	He	CB	He	RPV	Air	RCCS
-100	50	CC	CC	CC	CC	RSS	CC	TR	TR	TR	TR	TR	SR	RCS	SR	SR	SR	SR	SR	He	CB	He	RPV	Air	RCCS
-50	50	CC	CC	CC	CC	RSS	CC	TR	TR	TR	TR	TR	SR	RCS	SR	SR	SR	SR	SR	He	CB	He	RPV	Air	RCCS
0	50	CC	CC	CC	CC	RSS	CC	V	V	V	V	V	SR	RCS	SR	SR	SR	SR	SR	He	CB	He	RPV	Air	RCCS
50	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	IP	RCS	IP	IP	IP	RC	SR	He	CB	He	RPV	Air	RCCS
100	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
150	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
200	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
250	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
300	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
350	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
400	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
450	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
500	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
550	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
600	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
650	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
700	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
750	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
800	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
850	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
900	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
950	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
1000	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
1050	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
1100	50	CC	CC	CC	CC	RSS	CC	F	F	F	F	F	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
1150	50	CC	CC	CC	CC	RSS	CC	BR	BR	BR	BR	BR	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
1200	50	CC	CC	CC	CC	RSS	CC	BR	BR	BR	BR	BR	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
1250	50	CC	CC	CC	CC	RSS	CC	BR	BR	BR	BR	BR	SR	RCS	SR	SR	SR	RC	SR	He	CB	He	RPV	Air	RCCS
1300	50	CC	CC	CC	CC	CC	CC	BR	BR	BR	BR	BR	SR	SR	SR	SR	SR	IP	SR	He	CB	He	RPV	Air	RCCS
1350	50	CC	CC	CC	CC	CC	CC	BR	BR	BR	BR	BR	SR	SR	SR	SR	SR	SR	SR	He	CB	He	RPV	Air	RCCS
1400	50	CC	CC	CC	CC	CC	CC	OP	OP	OP	OP	OP	SR	SR	SR	SR	SR	SR	SR	He	CB	He	RPV	Air	RCCS
1450	50	CC	CC	CC	CC	CC	CC	BR	BR	BR	BR	BR	SR	SR	SR	SR	SR	SR	SR	He	CB	He	RPV	Air	RCCS
1500	50	CC	CC	CC	CC	CC	CC	BR	BR	BR	BR	BR	SR	SR	SR	SR	SR	SR	SR	He	CB	He	RPV	Air	RCCS
1535	35	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	BP	He	RPV	Air	RCCS

CORE LAYOUT DEFINITIONS

F	REACTOR CORE CONTAINING THE FUEL
V	HELIUM GAP BETWEEN FUEL AND TOP REFLECTOR: VOID
CC	CENTRAL REFLECTOR: GRAPHITE
TR	TOP REFLECTOR: GRAPHITE
BR	BOTTOM REFLECTOR: GRAPHITE
SR	SIDE REFLECTOR: GRAPHITE
RCS	REACTOR CONTROL SYSTEM CHANNEL : GRAPHITE / GREY CURTAIN AREA
RSS	RESERVE SHUTDOWN SYSTEM CHANNEL : GRAPHITE / GREY CURTAIN AREA
IP	INLET PLENUM TOP / BOTTOM : GRAPHITE
RC	RISER CHANNEL IN SIDE REFLECTOR : GRAPHITE
OP	OUTLET PLENUM BOTTOM : GRAPHITE
He	STAGNANT HELIUM
TP	TOP PLATE : IRON : ADIABATIC BOUNDARY
BP	BOTTOM PLATE : IRON : ADIABATIC BOUNDARY
CB	CORE BARREL : IRON
RPV	REACTOR PRESSURE VESSEL : IRON
Air	STAGNANT AIR
RCCS	REACTOR CAVITY COOLING SYSTEM : 20C TH BOUNDARY
	NEUTRONIC BOUNDARY CONDITIONS

2.3 CROSS SECTION LIBRARY

An important characteristic of the benchmark is the use of a common set of cross sections. The data is represented as various sets of two-group macroscopic cross section data representing different fuel regions (with different mixtures of burned pebbles), reflector and control rod regions. The cross sections are stored in multi-dimensional tables that include cross terms. The cross sections are tabulated as a function of (and all combinations of) five state-parameters namely fuel temperature, moderator temperature, fast and thermal buckling (representing the leakage spectral effects) and xenon concentration. All cross terms are included implying linear interpolation on a 5-dimensional space.

All of the fuel material cross section tables have data for the five state parameters with cross section data at four fuel temperatures, seven moderator temperatures, three fast bucklings, three thermal bucklings and three Xenon number densities. The non-fuel materials have no fuel temperature or xenon variations. The ranges chosen for each parameter were selected based on the reactor conditions for normal operation as well as for accident conditions. The current data ranges are given in Table 1.

Table 1: State parameters and ranges used in benchmark cross section library

Parameter	Range of values
Fuel temperature	300K, 800K, 1400K, 2400K
Moderator temperature	400K, 600K, 800K, 1100K, 1400K, 1800K, 2400K
Fuel regions:	
Fast buckling	-1.0×10^{-6}, 1.0×10^{-4}, 4.0×10^{-3}
Thermal buckling	-1.4×10^{-3}, -2.0×10^{-5}, 5.0×10^{-5}
Reflector regions:	
Fast buckling	-6.5×10^{-3}, -1.0×10^{-4}, 0.0
Thermal buckling	-1.1×10^{-3}, 5.0×10^{-5}, 1.0×10^{-4}
Xenon concentration	0.0, 3.78×10^{-13}, 9.44×10^{-8} [# / barn cm]

Tests to confirm the appropriateness of the state-parameter set, its range and to ensure that the number of data points is adequate for linear interpolation must still be finalized for all transient cases. One such an example is that the fuel temperature should be interpolated as the square root of the temperatures.

The use of the fuel and moderator temperatures as state parameters to tabulate cross sections are well known for most reactor types while the use of xenon, or other parameters to quantify the spectrum effects are also often used. In graphite moderated reactors and specifically pebble-bed reactors with its mixture of fuel pebbles, the environmental effects are very important. This is largely due to the large mean free path lengths and the transparency of the fuel pebbles. It is thus important to introduce the environment effects in the fine group spectrum analysis by representing the cell leakage in some way. The method used in VSOP99 and TINTE [12] is by representing the broad group leakage from the core diffusion calculation as few group buckling terms in the fine group cell calculation (GAM module of VSOP99) or polynomial representation (TINTE). For implementation in the benchmark specification the following definition is used.

Buckling is defined as follow: $\beta^2 = \dfrac{L}{D.\phi.V}$ [cm^{-2}];

where β^2 is the Buckling; L is the total out leakage from a given mesh or region; D the diffusion coefficient; ϕ the average flux and V the region volume. Note that a net inflow of neutrons will lead to a negative leakage value and thus a negative buckling. In the case of a negative buckling a necessary condition for a positive flux in each fine group is that $\left|D\beta^2\right| < \Sigma_r$.

This condition can easily be violated if for example an assumption of a constant fine-group buckling is used. In the two-group representation used for the benchmark, this should not be a problem but such cases had to be circumvented in the library creation process.

The library contains all the cross sections and kinetic parameters needed to perform the steady-state and transient cases. The current data set includes the following data for fast and thermal energies:

1. Diffusion coefficient, [cm]
2. Macroscopic absorption, [cm-1]
3. Macroscopic nu-fission, [cm-1]
4. Macroscopic fission, [cm-1]
5. Macroscopic Scattering (to the other group) [cm-1]
6. Inverse velocity, [s.cm-1]
7. Fraction Beta(1) of delayed neutrons, [dimensionless]
8. Fraction Beta(2) of delayed neutrons, [dimensionless]
9. Fraction Beta(3) of delayed neutrons, [dimensionless]
10. Fraction Beta(4) of delayed neutrons, [dimensionless]
11. Fraction Beta(5) of delayed neutrons, [dimensionless]
12. Fraction Beta(6) of delayed neutrons, [dimensionless]
13. Kappa, Energy release per fission, [MeV]
14. Microscopic absorption of Xenon , [cm2]
15. Iodine yield [dimensionless]
16. Xenon yield [dimensionless]

The last two quantities are not energy dependent and are given after the fast and thermal set of cross sections and data on the library. The five-dimensional interpolation routines required to read and interpolate the data are provided to the benchmark participants.

3. THE CALCULATIONAL CASES

3.1 Steady State Cases

The steady-state calculational cases were designed to test the correct implementation of the benchmark code to code verification cases in a systematic way. For example, in Exercise 1 a simplified cross section set is provided to verify the correct implementation of the cross section lookup tables into the different code packages. It also enables participants to use card input cross section data that is available in many codes. Participants must perform mesh refinement calculations to ensure a converge solution and report the k_{eff}, two-group fluxes and region powers in the provided spreadsheet template.

Exercise 2 is defined to test the implementation of the thermal hydraulic data in the different codes. A two-dimensional heat source distribution is provided as input and used to verify the thermal-hydraulic performance of the models. This includes a wide variety of correlations and constants that includes the pebble-bed effective conductivity, material heat capacities, helium coolant mass flow distribution and the heat transfer from the fuel spheres to the coolant to name a few. Results that need to be compared include the outlet gas temperature, pressure drop over the core, average and detailed two-dimensional maps of the fuel, graphite and gas temperatures.

A final steady-state case, Exercise 3, is an integrated test of the combined neutronics thermal-hydraulics models. It utilizes the multi-dimensional cross section library which includes full feedback on fuel and moderator temperatures, the leakage conditions of the material or cross section spectrum region and the xenon concentration. This also requires a model that determines the iodine and xenon concentrations explicitly. Exercise 3 represents the starting condition of all the transient cases and good agreement in these results is essential to assure a good platform for the transient cases.

3.2 TRANSIENT CASES

The focus of the benchmark is on the modeling of the transient behavior of the PBMR core. Six exercises, covering the range from slow to fast neutronic transients, as well as feedback effects from thermal-hydraulic parameters and fission products, are included. A summary of the test exercises, some with various sub-cases, with a short description of each is given below:

7. Depressurized Loss of Forced Cooling (DLOFC) without SCRAM
   The event is a Depressurized Loss of Forced Cooling in a very short time. A linear reduction in reactor inlet coolant mass flow from nominal (192.7 kg/s) to 0.0 kg/s is assumed over 13 seconds. No external flow after this step. During the same time a linear reduction in the reactor helium outlet pressure from nominal (90 bar) to 1 bar is postulated. The effects of natural convection are to be excluded in this case for simplicity. Since no SCRAM signal is assumed re-criticality should occur after some time.

8. Depressurized Loss of Forced Cooling (DLOFC) with SCRAM
   The event is the same as Exercise 1 but with a reactor SCRAM after the depressurization phase of 13 second. At that time all control rods are fully inserted over 3 seconds to SCRAM the reactor. No re-criticality is expected but all other conditions and assumptions remain unchanged.

9. Pressurized Loss of Forced Cooling (PLOFC) with SCRAM
   The event is a Pressurized Loss of Forced Cooling (PLOFC) with SCRAM. The effects of natural convection are included in this case. The time sequence of the event is similar to Exercise 2 with a linear reduction of the mass flow to zero over 13 seconds. In this case a linear reduction in reactor helium outlet pressure from nominal (90 bar) to 60 bar takes place over 13 seconds. After the pressure equalization phase is completed, natural convection may start that will lead to some internal mass flow. No external mass flow is allowed. Also after 13 seconds all control rods are fully inserted over 3 seconds to SCRAM the reactor.

10. 100%-40%-100% Power Load Follow
    The event simulates load follow in the plant with a fast change in the power from 100% to 40%, and after some time, back to 100%. The main effect is of course the xenon transient due to the power changes but other feedback effects such as the Doppler temperature also play a role. Two scenarios should be considered. In the first no control rod movement is allowed while in the second scenario the control-rods are moved to maintain a critical core within a given reactivity band width. No decay heat effects will be taken into account during the transient so that the heat

is only from fission. To assess the Xenon behavior the Xenon concentrations during these two cases are included in the output.

11. Reactivity Insertions by Control Rod Withdrawal (CRW) and a beyond design event Control Rod Ejection (CRE). The exercise defines fast reactivity insertion by simulating different CRW and CRE scenarios at hot full power conditions. Note that no decay heat effects will be taken into account during the transient. Since only the core is included in this specification the changes in the inlet and outlet conditions due to the power conversion unit is not included and therefore the inlet mass flow rate, inlet temperature and outlet pressure should be kept constant at nominal conditions. Four different cases are to be analyzed. They are (i) Withdrawal of all 24 control rods at the maximum speed of 1 $cm.s^{-1}$; (ii) Ejection of all 24 control rods over a 0.1 second duration; (iii) Ejection of a single control rods over a 0.1 second duration; and (iv) Ejection of 6 control rods in one quarter of the core over a 0.1 second duration. Sub-cases ii to iv were selected to include the sub-prompt and super-prompt cases even though these events are not possible on the plant and thus only of academic value.

12. Cold Helium Inlet Event. This exercise simulates a bypass valve opening, with "cold" Helium being injected into the core inlet plenum. A temperature ramp of 50 ^{o}C (i.e. 10% of nominal inlet temperature) is applied over 10 seconds, without changing any other reactor parameters like mass flow, pressure or control rod positions. Thus the reactor inlet temperature is reduced linearly from nominal (500 ^{o}C) to 450 ^{o}C over 10 seconds. It is postulated that a reactor protection system would cause the valve to close again after 300 seconds, and the temperature would return to the nominal value, again over 10 seconds. Note that no decay heat effects will be taken into account during the transient.

For all the transient cases the focus of the results are on maximum and average fuel, moderator and gas temperatures and coolant flow behavior. For the reactivity excursions the core fission power, maximum and power density profiles, and axial offset are of interest. These results are to be presented as a function of time or at specific time points or events.

4. CONCLUDING REMARKS, STATUS, AND FUTURE WORK

The OECD PBMR Coupled Neutronics/Thermal Hydraulics Transient Benchmark based on the PBMR-400 Core Design has reached a mature level of definition and has been well supported. Two official meetings have already taken place at the OECD/NEA headquarters in Paris. The first workshop was held on 16th and 17th June 2005 at the OECD headquarters in Paris, followed by a second workshop on the 26th and 27th of January 2006 at the NEA headquarters. At the first meeting, attended by 24 participants from 12 countries, the benchmark was introduced and discussed in detail. For the next meeting clarifications and missing detail was added to the specification and results templates were provided. Results of the first two steady-state exercises were presented and discussed during the second meeting. These results, from thirteen different participating groups, are the subject of an accompanying paper [13]. The third formal workshop is planned for 1st and 2nd February 2007. The current plan is to finalize the benchmark in 2009.

The benchmark exercise is an important initiative to verify the different implementations of HTR physics phenomena especially during postulated transients. It already plays an important role in the verification of the codes and methods used to evaluate pebble bed reactors transient events. Many of the phenomena and issues discussed as part of the benchmark exercises provide insight into the shortcomings of some of the methods used today and will also be used to create the basis for future more advanced methods and codes.

5. ACKNOWLEDGEMENTS

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