Coupled Neutronics/Thermal-hydraulics Calculations for the Safety Analysis of the PBMR

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This paper presents an overview of the safety analysis of the pebble-bed reactor using the advanced coupled-code NEM-THERMIX. This coupled code is a combination of the Nodal Expansion Method code (NEM), a 3-D neutronics code developed at Penn State, and THERMIX-DIREKT, a 2-D HTR thermal-hydraulics code. The coupled code is used in this work to illustrate the importance of coupled neutronics/thermal-hydraulics calculations when analyzing the safety of high temperature gas-cooled reactors. Using this code, it is demonstrated that the neutronics behavior is sensitive to cross section changes due to temperature and spectrum feedback effects. The spatial dependence of these effects is very important to be modeled and hence, coupled calculations are inevitable in establishing and building a safety case for the high temperature gas-cooled reactors of a pebble-bed type like the PBMR.

KEYWORDS: pebble-bed, NEM, NEM-THERMIX, transients

1. Introduction

Pebble-Bed Modular Reactors (PBMR) with re-circulating fuel are gaining wide acceptance as a viable alternative to traditional reactor concepts. Passive safety features, simplicity of operation, a stable waste form, and more efficient use of the fuel are making PBMR a very attractive candidate for next generation nuclear power plants. This reactor concept has yet to mature, particularly with regard to the coupled deterministic neutronics thermal-hydraulics methods available to design and analyze PBMRs. These methods have lagged behind the state of the art compared to other reactor technologies. This fact motivates the efforts to develop more accurate and highly efficient computational tools to conduct the coupled neutronics thermal-hydraulics analysis of the reactor's behavior for the design and safety evaluation of PBMRs. Such developments must invariably incorporate coupled multidimensional deterministic neutronics and thermal-hydraulics calculations that will provide adequate analysis capabilities to be used to advance the level of maturity of this innovative reactor concept. This paper presents an on-going work in the development of such advanced methods and schemes. The definition of appropriate benchmarks to verify and validate the coupled computer codes is also addressed.

2. Motivation for this work

The Pennsylvania State University (PSU) has been developing and coordinating several international coupled neutronics/thermal-hydraulics benchmarks problems such as the OECD/NRC PWR MSLB [1] Benchmark, the OECD/NRC BWR TT

Benchmark [2], and the OECD/DOE/CEA VVER-1000 Coolant Transient Benchmark [3]. The accomplishment of the afore-mentioned projects involved extensive development and usage of advanced coupled neutronics and thermal-hydraulics codes. These codes, models and available plant data were used in other research projects to test the viability of new schemes and techniques in the framework of efficient parallel computing algorithms. In regard to PBMRs PSU has been involved in a collaborative research effort with the South African PBMR Company and Purdue University addressing the benchmarking of core simulation methods through a set of multi-dimensional computational test problems. [4] The intention was to develop these test problems into High Temperature Gas Reactor (HTGR) benchmarks similar to the well-known IAEA PWR steady-state benchmarks. The developed test problems were analyzed with three different codes: VSOP [5], NEM, [6] and PARCS. [7]. For different test-problems analyzed with these three codes the comparison of the results has shown good agreement. This agreement has confirmed the suitability of NEM in analyzing PBMR cores. The steady-state analysis for these test problems has been concluded and some results have been published [8].

Following the good agreement obtained between the three codes, the logical extension of this work would be to move to the next step, which is to perform transient analysis of the PBMR taking into account the appropriate thermal-hydraulics feedback. The modeling of PBMR feedback effects is based on the following considerations:

1. The nuclear power production is coupled with spectrum- averaged cross section changes due to temperature and spectrum feedback effects. The temperature is governed by nuclear heat production, heat transport in the coolant gas, heat conductivity in the fuel and graphite, and radiation
2. The large heat capacity of the graphite causes overall temperature changes to be slow. But even small temperature changes in the particles and in the inner part of the fuel elements results in sensitive feedback to the nuclear behavior or neutronics.
3. The core temperature has to be treated in a heterogeneous way. The heat produced in the coated particles is transferred very rapidly into the graphite matrix, the inner part of the spherical fuel elements. From there it is transported to the fuel elements surface, where it must be removed by the coolant gas, global heat conduction, or radiation
4. In order to accurately model the reflector feedback to the neutronics, one needs at least two dimensions (r-z geometry)

From the PSU perspective, this necessitates coupling the NEM code with a suitable core thermal-hydraulics code and analyzing a series of test problems with the coupled code. Recently, a collaborative agreement between PSU, the PBMR Company and NRG in the Netherlands has been established. The essence of this collaboration is basically to extend the efforts of the first benchmark exercise to transient analysis. The core thermal-hydraulics code Thermix-Direkt [9] presently used in the Netherlands by NRG is coupled with NEM and the coupled code is being used to analyze the transient test problems. It is then envisioned that the results obtained will be compared to the results obtained by the PBMR with their TIme-dependent Neutronics and TEmperatures (TINTE) [10] code, which performs the dynamic nuclear and thermal calculation in two dimensions, and the NRG Panthermix code [11] for code-to-code verification purposes.

3. The computer code system

In the analysis several calculational tools have been used to model the PBMR. Three computer programs (codes) and the associated interfaces have been assembled at PSU to establish a complete code system for use in HTGR safety analysis:

i. NJOY/MICROR/MICROX-2 package: for cross section processing and generation;
ii. NEM: for three-dimensional (3-D) steady-state and transient core neutronics calculations;
iii. Thermix-Direkt: for calculation of the pebble-bed core thermal-hydraulics.

In the following sections we discuss each one of these codes, in terms of their capabilities models and qualification.

3.1 The NJOY/ MICROR/MICROX-2 package

NJOY is a data processing code, which processes the Evaluated Nuclear Data Files ENDF/B-VI. The code produces two output files: the Pointwise Evaluated Nuclear Data File (PENDF) and the Groupwise Evaluated Nuclear Data File (GENDF). MICROR is an NJOY reformatting module, which uses the PENDF and GENDF data from NJOY as input. Three output files are generated: FDTAPE, GARTAPE and GGTAPE. These three output files contain the fast, resonance and thermal cross sections, and are used as input in MICROX-2. MICROX-2 is a one-dimensional two-region lattice cell code. It solves the neutron slowing down and thermalization equations, and produces the broad group neutron cross sections. The two regions of the cell are coupled by collision probabilities based on a spatially flat neutron emission. The Dancoff factor and buckling are utilized to correct the one-dimensional cell calculations for multi-dimensional lattice effects. The Dancoff factor for an infinite medium was calculated using the method outlined in [12].

$$C = \frac{1}{1 + \Sigma_t^M \bar{l}_M} \tag{1}$$

$$\bar{l}_M = 4\frac{4/3\,\pi(R_2^3 - R_1^3)}{4\pi R_1^2} \tag{2}$$

C is the Dancoff factor

Σ_t^M is the total macroscopic cross section of the outer shell (graphite)

$\bar{l}_M$ is the mean chord length of the moderator region

R_1 is the radius of the fuel region

R_2 is the radius of the moderator/coolant region

MICROX-2 was developed and tested at the Paul Scherrer Institute in Switzerland. Extensive verification and validation of this code was performed with experiments from the HTR PROTEUS configuration at PSI [13] and [14]. At the PSU a further verification of this code package was performed using the benchmark exercise developed at the Massachusetts Institute of Technology (MIT). The benchmark specifications, outlined in [15], is based on the Swiss PROTEUS LEUPRO-1 fuel cell. The fuel for this benchmark was enriched to 16.75%. The results produced by

MICROX-2 code were compared to the MCNP results from this benchmark and a good agreement between the codes was observed [15].

3.2 The nodal expansion method code (NEM)

NEM [6] is a 3-D multi-group nodal code developed at PSU for modeling both steady state and transient core conditions based on the nodal expansion method. This method for solving the nodal equations in three dimensions was developed by Finnemann [16]. It utilizes a transverse integration procedure and is based on the partial current formulation of the nodal balance equations. The leakage term in the one-dimensional transverse integrated equations is approximated using a standard parabolic expansion using the transverse leakages in three neighboring nodes. The nodal coupling relationships are expressed in partial current formulation and the time dependence of the neutron flux is approximated by a first order, fully explicit, finite difference scheme. This method has shown to be very efficient although it lacked the precision of the advanced nodal codes. Recently an upgrade of the method has been completed, replacing the fourth order polynomial expansion with a semi-analytical expression utilizing a more accurate approximation of the transverse leakage. 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 distributions in the R-, Z- and θ-directions.

3.2.1 Verification of the NEM code for PBMR analysis

The NEM cylindrical option has been verified using the Dodd's benchmark problem [17]. It is important to note that the detailed treatment of the effects of azimuthally dependent PBMR control rods requires a full three-dimensional representation.

As mentioned above the standalone NEM code has also been verified for high temperature gas-cooled reactors of the pebble-bed type through a joint benchmark exercise between the PBMR Company, PSU, and Purdue University. In the benchmark exercise, a realistic model of equilibrium PBMR reactor core with a thermal power of 268 MWt is defined. A bottom cone area, directing pebble flow to a central de-fueling chute, and a 10-pass fuel management system were introduced. The cross-section data sets used were however obtained from VSOP on the CITATION material mesh (r,z), which implies that the flow speed variations and non vertical flow lines (due to the bottom cone) were already taken into account (by volume weighting and averaging) in the cross-section sets prepared. In this problem, there are 286 regions, and thus 286 cross section sets of which 225 of them are within the fuel region. The core is 350 cm wide and 850 cm high, with varying mesh sizes for both the axial and the radial directions. This problem as mentioned above was simulated by all participants using different codes. As it can be seen in Fig. 1 the obtained results are in good agreement.

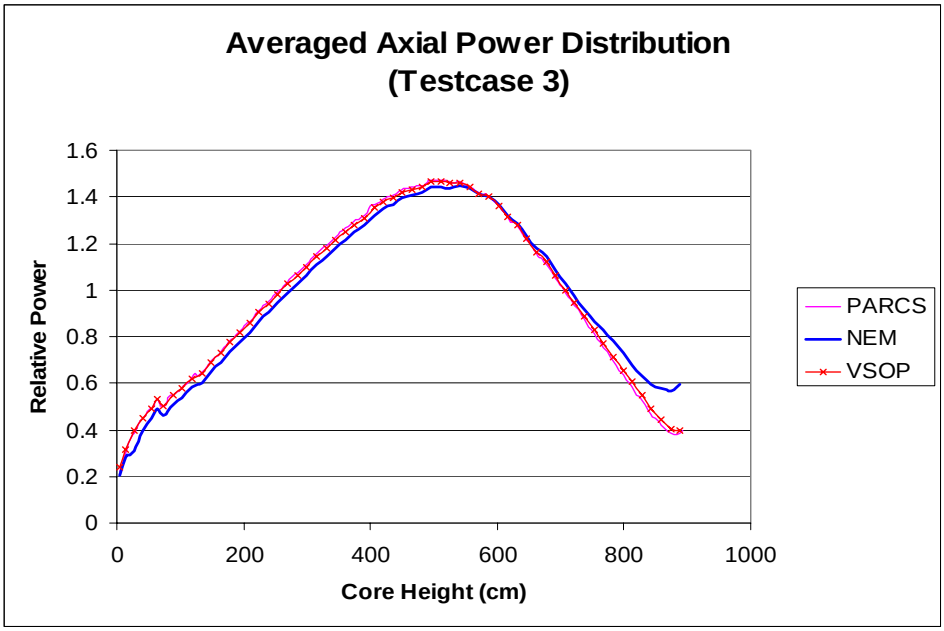

Figure 1. Axial power distribution comparison between Purdue, PSU and PBMR Company

3.2.2 Recent developments

There are ongoing developments and improvements of the NEM code at PSU connected with the HTR applications. Recently, a method of modeling the directional diffusion coefficients to account for the anisotropy of the flux in the void region at the top of the pebble-bed have been implemented in NEM and are being tested. This approach considers the cylindrical void region as a diffusion region with real geometry and artificial constants. In a void region, only the diffusion coefficients are present since both scattering and absorption reaction cross sections are equal to zero. Since transport calculations are too expensive for routine calculations, it is desirable to develop methods to do diffusion treatment of these voids with a certain degree of accuracy. Gerwin and Scherer [18] tried to find the diffusion treatment of such a region and as pointed out above, such regions without any moderation and any reaction can only be treated with scattering and absorption reaction cross-sections equal to zero. Only diffusion coefficients can be used in such a region. The challenge is to choose these constants in a certain way for an optimal description of the cavity. According to this method, the diffusion constant can be represented by two directional diffusion coefficients, which are calculated as functions of radial and axial dimensions of the cavity.

Another recent capability incorporated in NEM is the model to accurately model the xenon-induced power oscillations in the PBMR core. Using this model, it is possible to design an optimum reactor core in terms of the height-to-diameter (H/D) ratio, while ensuring that the core is not susceptible to such transients, and in case such oscillations occur, one can predict whether these will be damped or not.

3.3 The Thermix-Direkt code

The Thermix-Direkt code calculates in *(R, Z)* co-ordinates, the temperature distribution in the pebble-bed due to heat transport by conduction, radiation and convection (natural and forced), given the power distribution and coolant flow

conditions. The code can perform both steady-state and transient calculations. Relations for the conduction or heat transfer coefficients in the pebble-bed are partly empirical, partly exact with fitted parameters [19]. These relations have been validated by numerous experiments with the AVR test reactor, which date back into the seventies.[20] In addition, tests with non-nuclear pebble-beds in the seventies and eighties have also been utilized in order to validate the code. The Thermix-Direkt code as the name suggests is a combination of two codes: Thermix, which solves the heat conduction equation for the solid materials and Direkt, which solves the equations describing heat transfer by convection. Over the years, Thermix-Direkt has been used and validated for core thermal hydraulics, and has been coupled with neutronics codes such as Panther to perform transient analysis of a few HTR designs, e.g the Dutch ACACIA design, the German HTR-Modul among others.

3.3.1 Verification of the Thermix-Direkt Code for PBMR analysis

The standalone version of the Thermix-Direkt code was verified for use in PBMR analysis though simple standalone cases at Penn State. In fact, an extensive verification (and validation) of this code was performed in Germany many years ago for the AVR reactor. At Penn State, the whole idea behind this verification was to test this version of the code as we have never used it before, especially for the PBMR. This was done through the recent PBMR 268 MWt benchmark effort between the PBMR Company, NRG, and PSU. For this work, a standalone Thermix-Direkt calculation was performed to test the capability of the code. As this was a stand-alone simulation, a flat power distribution in the core was assumed. Two calculations were performed with Thermix-Direkt, the first one being a steady state simulation with the core operating at nominal power. The second simulation is a Loss of Forced cooling (DLOFC) without convection. The DLOFC case presupposes a depressurization of the system to 1 bar. Such a scheme could result from the rupture (guillotine break) of the manifold connecting the power conversion unit (PCU) to the reactor. Helium will flow out of the containment into the reactor building until pressures are stabilized at 1 bar (from 60 bar). The main output of these runs is to confirm if whether the maximum fuel temperatures will remain below the recommended limit, i.e. 1600 deg. Celsius. The Fig.2 shows the graphical depiction of the maximum and average fuel temperatures for the transient decay heat accumulation without convection.

3.4 The NEM-THERMIX coupled code

The tasks comprising this coupling involved a careful analysis of the input and output data for the two codes involved in the coupling and a determination of the most efficient temporal and spatial coupling algorithms. The advantage of NEM as compared to Panthermix is the possibility for exact spatial mesh overlays since both NEM and Thermix-Direkt utilize cylindrical geometry modeling. Appropriate coupling interfaces have been developed and tested. Two approaches have been implemented and compared for efficiency: sequential (code integration) and parallel (utilizing the PVM resources). The obtained results indicate that the PVM coupling on a single processor shows about 2 times better efficiency in terms of the CPU time as compared to the sequential coupling. The result of this research activity provides the PBMR community with the advanced capability of a nodal diffusion neutronics solver coupled with a validated core thermal-hydraulics code. This coupled code, NEM-THERMIX, can be deployed for the analysis of PBMR transients with greater accuracy, reliability, and computational efficiency than the existing methodologies.

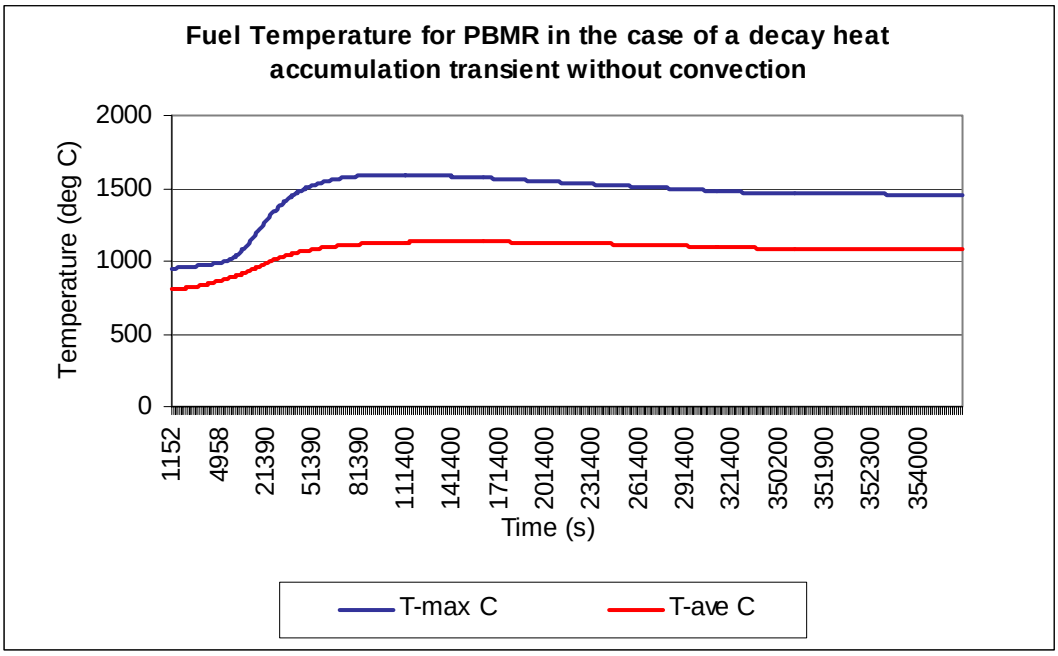

Figure 2: Results from stand-alone Thermix-Direkt testing and verification

3.4.1 Transient cross section modeling

A HTR feedback model has been developed to account for the feedback effects of temperature and spectrum and was implemented into NEM. The four parameters of interest in the model are fuel temperature (T_f), moderator temperature (T_m), coolant temperature (T_c) and spectrum (S). Two software packages have been developed as part of this new feedback model. The first package automatically generates a macroscopic cross section library for a given PBMR core model using MICROX-2. This library contains sets of macroscopic 4-D cross section tables for each composition. Users can specify the ranges of the feedback parameters as well as the number of reference points themselves. Once this information is selected it is stored at the beginning of the cross section library. This information is read by NEM together with the reference cross section values. This library contains tables for transport, absorption, fission, production and scattering cross sections. The second software package reads the tables and interpolates in them to obtain the macroscopic cross section values for each spectral zone (core region) and for each broad energy group. This package interacts with NEM in the following way: first, the cross section library is read once at the beginning of the calculation process and stored in the NEM arrays. During the calculation process for each spatial node of the NEM core model, four parameters representative of this node are passed to the feedback module. While the temperature values are provided from the Thermix-Direkt calculation the spectrum representative parameter (leakage – buckling or albedo) is provided from the NEM calculation. Using these values, four-dimensional tables are then interpolated for the appropriate macroscopic cross section values. The updated macroscopic cross sections are passed back to NEM to perform core calculations, pass the power distribution to Thermix-Direkt and getting the relevant thermal-hydraulics data in turn, and this calculational loop continues.

3.4.2 The spatial coupling scheme used in the coupled code

The coupling scheme between NEM and Thermix-Direkt adopted in this work is a one-to-one scheme. In this scheme, a two dimensional (r, z) neutronics mesh is superimposed on the two-dimensional (r,z) thermalhydraulics mesh, forming mesh overlays. For the theta (azimuthal) direction, NEM divides the core into thirty-six azimuthal sectors, each 10^0. This is necessary for the 3-D modeling of control rods located in the side reflectors for the current PBMR model. This mesh overlay can clearly be seen in the figure 3 below, which is the actual model used for the calculations.

3.4.3 Verification of the coupled code

From a safety and licensing point of view, every new reactor design has to uphold certain safety requirements. This includes proving that the reactor will still maintain the safety limits for any postulated transient, planned or accidental. For the PBMR reactor core, such postulated transients have been analyzed and have included, the Depressurized Loss of Forced Cooling (DLOFC) event, the Total Control Rod Withdrawal (TCRW) event followed by a DLOFC, Water Ingress into the core, Air Ingress, Loss of Flow incident (LOFI) and Load-Follow Transient (100%-40%-100), among others. The main objective is to show that during all of the above transients, the fuel temperature will still remain below 1600^oC. Several codes have been used in different HTR designs to investigate these transients. This step is therefore necessary for the verification of our newly developed code system for analyzing the above transients.

Within the framework of the collaboration we have established with the PBMR Company and NRG, a detailed benchmark specification in the form of physics test problems for some of the above transients has been formulated [7]. These benchmark specifications are currently being used to analyze some of the transients described above. The results our analysis with the NEM-THERMIX coupled code are being compared with the results independently obtained by the PBMR Company using the TINTE code and also with the results from the Panthermix code used at the NRG Company. For the purposes of this paper, some of the results obtained from the NEM-THERMIX calculations are given below. As already mentioned above, one of the events considered as the most severe upset event in a PBMR is the DLOFC.. In modeling this event, a large break in the pressure boundary or pipe work is assumed. This is a highly unlikely event, which assumes that all the coolant is removed from the core to atmospheric pressures. As a result of this break, the removal of heat from the core is impaired and the initial heat-up of the fuel will occur. The negative temperature coefficient of reactivity causes the reactor to become sub-critical and the self-sustaining chain reaction is terminated within a few minutes. Due to the high thermal capacity of the graphite the fuel temperature is increased on average only by 88 °C. Due to the temperature increase and the build-up of ^{135}Xe, the core reactivity is decreased by 1.5 Nile (1 Nile is equal to 100 pcm). The power produced in the core as shown in Fig. 4 is reduced to decay heat, which is mainly due to the decay energy of the short-lived fission products. The calculations also show that during this transient, the maximum temperature of the fuel does not exceed the 1600 deg Celsius limit as shown in Fig. 5.

	0	78.6	110.9	135.7	156.6	175	181	194	215	235	250	275	287	292	300	317	417	418
-231		78.6	32.3	24.8	20.9	18.4	6	13	21	20	15	25	12	5	8	17	100	1
-230	1	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	18
-200	30	13	13	13	13	13	13	13	13	13	13	13	13	12	15	16	17	18
-175	25	7	7	7	7	7	7	7	7	7	7	7	11	12	15	16	17	18
-125	50	9	9	9	9	9	9	9	9	9	3	7	11	12	15	16	17	18
-75	50	2	2	2	2	2	3	3	3	6	3	7	11	12	15	16	17	18
-25	50	2	2	2	2	2	3	3	3	6	3	7	11	12	15	16	17	18
0	25	1	1	1	1	1	3	5	3	6	3	7	11	12	15	16	17	18
50	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
100	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
150	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
200	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
250	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
300	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
350	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
400	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
450	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
500	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
550	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
600	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
650	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
700	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
750	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
800	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
850	50	a	b	c	d	e	3	5	3	6	3	7	11	12	15	16	17	18
900	50	4	4	4	4	4	3	3	3	6	3	7	11	12	15	16	17	18
950	50	4	4	4	4	4	3	3	3	6	3	7	11	12	15	16	17	18
1000	50	4	4	4	4	4	3	3	3	8	3	7	11	12	15	16	17	18
1050	50	4	4	4	4	4	3	3	3	3	3	7	11	12	15	16	17	18
1100	50	10	10	10	10	10	3	3	3	3	3	7	11	12	15	16	17	18
1125	25	7	7	7	7	7	7	7	7	7	7	7	11	12	15	16	17	18
1155	30	14	14	14	14	14	14	14	14	14	14	14	14	12	15	16	17	18
1156	1	19	19	19	19	19	19	19	19	19	19	19	19	19	19	19	19	18

Neutronics

a	Dynamic central column (graphite sheres only)
b	Mixture region with 50:50 ratio of fuel and graphite spheres
c	3rd flow channel with only fuel spheres
d	4th flow channel with only fuel spheres
e	Outer flow channel with only fuel spheres
1	Void area above the pebble bed
2	Top reflector graphite
3	Side reflector graphite
4	Bottom reflector graphite
5	Control rod grey skirt / graphite
6	Side reflector graphite (with helium channels)
7	Carbon side reflector / insulation

Thermal Hydraulics

a	Pebble bed
b	Pebble bed
c	Pebble bed
d	Pebble bed
e	Pebble bed
1	void area above core with vertical helium flow
2	Top reflector porous region with downwards helium flow
3	Side reflector (no helium flow)
4	Bottom reflector porous region with downwards helium flow
5	Control rod region / no flow
6	Porous side reflector graphite (with upward flow in helium channels)
7	Carbon top / side / bottom reflector / insulation
8	Bottom inlet plenum
9	Top Inlet plenum
10	Bottom Outlet plenum
11	Stagnant helium at pressure between side reflector and barrel
12	Barrel
13	Top plate
14	Bottom plate
15	Stagnant helium at pressure between barrel and RPV
16	RPV
17	Air outside RPV
18	Heat sink
19	Adiabatic boundary condition
20	Adiabatic boundary condition

Figure 3: Core model and identification

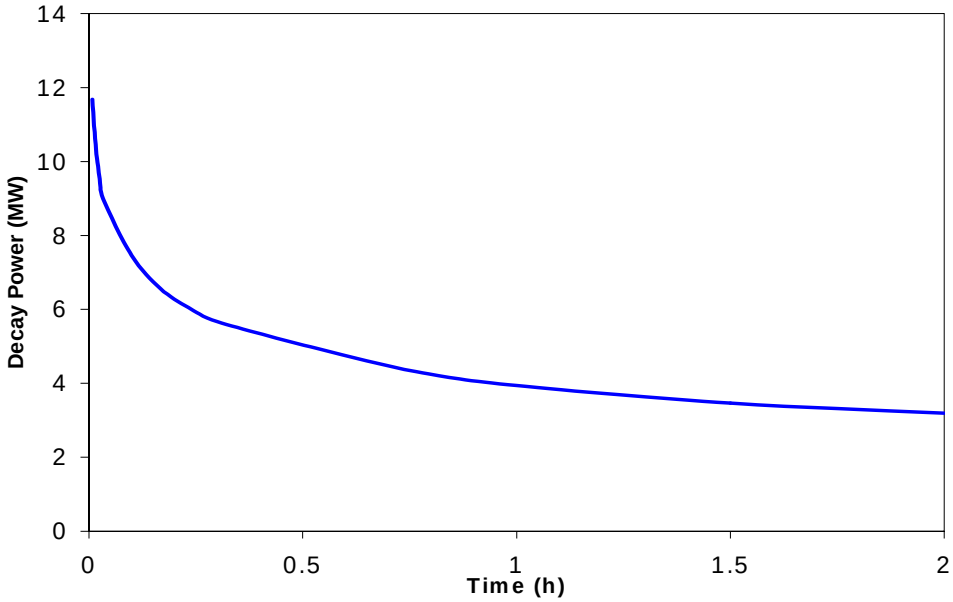

Figure 4. NEM-THERMIX prediction of decay heat removal during the DLOFC transient

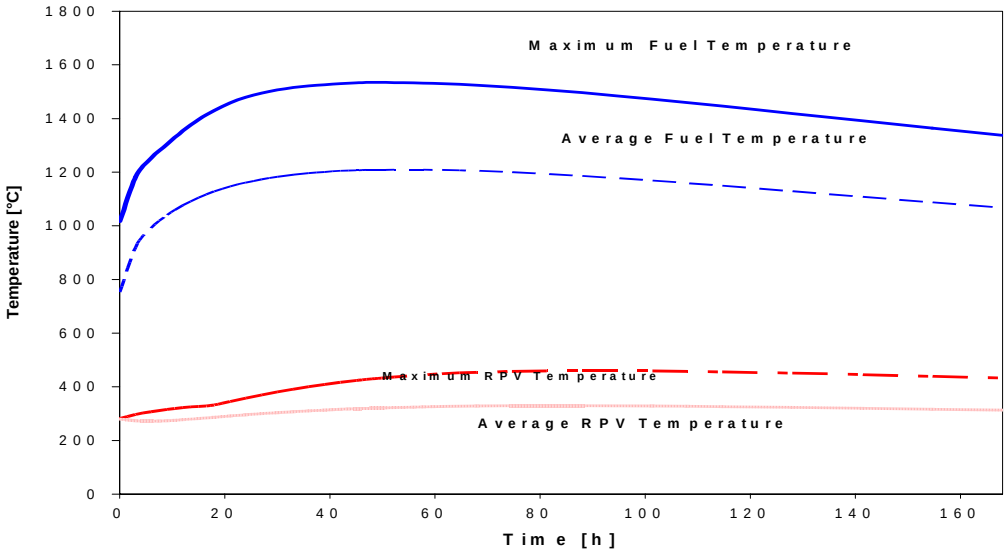

Figure 5. NEM-THERMIX prediction of temperature distribution during the DLOFC transient

4. Conclusions

This work has presented a highlight of ongoing work at PSU on the development of state-of-the-art calculational tools for the analysis of high temperature reactors of the pebble-bed type for the purposes of safety analysis. The work and results shown here have shown that the code system assembled at PSU have the capability and can be deployed for use in the analysis of pebble-bed HTGR safety. As mentioned, this is an

ongoing work and more updates and results will be presented and published in future journal issues and conferences.

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