Development and testing of analytical models for the pebble bed type HTRs

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A B S T R A C T

The pebble bed type gas cooled high temperature reactor (HTR) appears to be a good candidate for the next generation nuclear reactor technology. These reactors have unique characteristics in terms of the randomness in geometry, and require special techniques to analyze their systems. This study includes activities concerning the testing of computational tools and the qualification of models. Indeed, it is essential that the validated analytical tools be available to the research community. From this viewpoint codes like MCNP, ORIGEN and RELAP5, which have been used in nuclear industry for many years, are selected to identify and develop new capabilities needed to support HTR analysis. The geometrical model of the full reactor is obtained by using lattice and universe facilities provided by MCNP. The coupled MCNP-ORIGEN code is used to estimate the burnup and the refuelling scheme. Results obtained from Monte Carlo analysis are interfaced with RELAP5 to analyze the thermal hydraulics and safety characteristics of the reactor. New models and methodologies are developed for several past and present experimental and prototypical facilities that were based on HTR pebble bed concepts. The calculated results are compared with available experimental data and theoretical evaluations showing very good agreement. The ultimate goal of the validation of the computer codes for pebble bed HTR applications is to acquire and reinforce the capability of these general purpose computer codes for performing HTR core design and optimization studies.

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1. Introduction

Gas cooled reactors have been highlighted as a promising option for next generation reactor technology. The advancement and basic concept of the high temperature reactor (HTR) was proposed for the first time in the 40s (Daniels, 1944). In the 1990s, the interest in the HTR concept was substantially revived due to the growing demand for an enhancement of the safety standards of nuclear plants. Currently, the HTRs have been receiving significant attention due to many desired characteristics such as inherent safety, modularity, relatively low cost, short construction period, and easy financing. Above all other possible advantages of the HTR stands its potential to operate as an inherently safe reactor. The concept of 'inherently safe' can be interpreted as the impossibility of the reactor to reach a state where radioactive fission products are set free above the predefined levels. This implicates the usage of passive safety measures, i.e. measures that rely on natural processes to limit core temperatures in situations where all other active control fails, and that do not require human action. Billions of coated particles, called TRISO particle, are formed in which the fuel is dispersed and each forms a containment or the fuel inside, and can be seen as a miniature pressure vessel that can retain fission products (Nabielek et al., 1990). Graphite is the moderator in the core, and can at the same time be utilized as a structure material. Combined with the fact that the coated particles easily transfer heat due to their high surface/volume ratio, the heat transport from fuel to matrix graphite passes off smoothly. High local temperature gradients are avoided in the core. Helium is chosen as coolant in HTRs because it hardly absorbs neutrons, is not activated by neutrons, is chemically inert, does not undergo a phase change, has good heat-exchange properties, and is naturally available in sufficient quantities. Sometimes, the working fluid helium that is heated in the nuclear reactor is offered directly to the energy conversion system (ECS). This implicates the utilization of a gas turbine and a compressor, and therefore the so-called direct Brayton cycle has been chosen as the thermodynamic cycle for the ECS.

This study envisages simple reactor design and operation, and therefore the pebble bed type HTR scheme has been chosen on the following grounds: the excess reactivity in the core is minimal, on-line fuelling is possible by adding fresh fuel pebbles on top of the bed. The qualification, validation and improvement of computational tools and models for the analysis of pebble bed type HTRs are addressed. This effort is based on both reactors and critical facilities applicable to pebble bed type cores. Two facilities, HTR-PROTEUS (Leupro-1 core) of Switzerland and HTR-10 of China,
and one conceptual design from Germany, HTR-PAP20, appear to have the greatest potential for use during this study (Mathews and Chawla, 1990; Xu et al., 2005; Kuijper et al., 1996). The choice of computational tools is also very important. As the HTR is a promising concept for the next generation of nuclear power plants, the nuclear community must have analytical tools that are readily available and are capable to perform conceptual design studies, industrial calculations, safety analyses for licensing, etc. Based on this concept, general purpose computer codes like MCNP, ORIGEN and RELAP5 are selected and used to analyze the core neutronics, thermal hydraulics, fuel depletion study and safety analysis for the HTRs (Briesmeister, 1997; Croff, 1991; Allison and Wagner, 2007). The results are compared with the experiment and the calculations performed by other codes for the particular type of reactor.

### 2. Reactors for benchmarking

Both reactors and critical facilities applicable to pebble bed type cores are considered for this study. HTR fuel is made of spherical pebbles that have an outer graphite shell (0.5 cm thick) surrounding an inner fuel zone (2.5 cm radius). The fuel zone has a graphite matrix in which approximately 8000–20,000 TRISO fuel microspheres are embedded. Each microsphere is coated with a SiC coating, which assures that no fission products are released even at temperatures reaching 1600 °C (anticipated accident temperature) (Nabielek et al., 1990). Depending on the details of the core design, each pebble may contain a total of 5–9 g of UO2. In addition, the 235U enrichment can vary. Brief descriptions of the HTRs considered for this study are given below.

HTR-PAP20 is a conceptual design of FZ Jülich for a small simplified pebble bed reactor of 20 MW where fresh fuel elements (the well-known 6.0 cm diameter pebbles) are added little by little (peu-à-peu) to maintain criticality during operation (Kuijper et al., 1996). No fuel is removed during the life of the core. At the end of life, all fuel elements are unloaded in one step. The initial critical core height, in a cavity of 2.50 m diameter, is about 1 m, using pebbles containing 12 g heavy metal (in UO2, enrichment 10.0%). At the end of core life (about 18 years), the core height is about 4.0 m, when pebbles are added containing fuel at 20% enrichment after initial critical loading.

HTR-PROTEUS experiments involved the investigation of a variety of regular and stochastic pebble bed cores (Mathews and Chawla, 1990). PROTEUS is a zero-power critical facility, which consists of a reactor vessel surrounded by a large graphite reflector with numerous penetrations for control rods and test equipment. It is reconfigurable, and has been used for a variety of reactor simulations. The experiments were carried out using standard 6.0 cm diameter fuel spheres containing TRISO coated fuel particles (CFPs), with 16.76% enriched uranium loading of 5.966 g per sphere. PROTEUS results fill certain gaps in the required experimental data for code validation for advanced gas cooled reactors.

HTR-10 is an experimental 10 MW, pebble bed reactor recently constructed by the Institute of Nuclear Energy Technology in Beijing (Xu et al., 2005). The core is slightly larger than the PROTEUS core (with an inner diameter of 1.80 m and a height of 1.97 m). The 17% enriched fuel is similar to the HTR-PROTEUS fuel, with slightly lower uranium loading of 5 g per fuel sphere. The total number of spheres needed to reach criticality was 16,890, with a fuel-to-moderator sphere ratio (F/M) of 57–43%.

A brief design and core characteristics of these reactors are given in Table 1, and the detailed information can be found elsewhere (Mathews and Chawla, 1990; Xu et al., 2005; Kuijper et al., 1996).

### 3. Computational tools and techniques

#### 3.1. Monte Carlo simulation

##### 3.1.1. Background

Monte Carlo technique is applied for criticality problems for many diverse systems. Monte Carlo simulation is performed for kernels in a fuel sphere and a lattice formed by spheres to generate Dankoff factors and compare them with their analytical estimations (Bende and Hogenbirk, 1999). In this study, criticality analysis based on transport calculations with the Monte Carlo code MCNP4C2 is performed (Briesmeister, 1997). MCNP is a general purpose, continuous energy, generalized-geometry, time-dependent, coupled n particle, neutron, photon and electron, Monte Carlo transport code developed at Los Alamos National Laboratory. Since direct particle paths, energies, and reactions are followed in Monte Carlo simulations, no simplification or assumption is necessary. Other advantages provided by MCNP are to allow flexible geometrical modelling and extensive cross-section libraries. Advances in computer hardware are now making it possible to apply Monte Carlo codes to the modelling of neutron and photon transport in pebble bed reactors.

When spheres are dropped into a large cylinder such as the core of a pebble bed reactor, they pack randomly with a void fraction of approximately 0.39. It requires development of new techniques for representing the randomly packed cores of pebble bed reactors. Because of the large number of spheres in a typical core, the core model must rely on the repeated-geometry feature of the code, in which a unit cell is expanded throughout the volume of the core. However, this raises two questions: (a) how good is a regular

### Table 1

<table>
<thead>
<tr>
<th>Parameters</th>
<th>HTR-PAP20</th>
<th>HTR-PROTEUS</th>
<th>HTR-10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power (MW)</td>
<td>20</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Core radius (m)</td>
<td>4.50</td>
<td>1.00</td>
<td>1.97</td>
</tr>
<tr>
<td>Core height (m)</td>
<td>1.25</td>
<td>0.58</td>
<td>0.90</td>
</tr>
<tr>
<td>Packing fraction (%)</td>
<td>61</td>
<td>74.05</td>
<td>61</td>
</tr>
<tr>
<td>Fuel/moderator ratio</td>
<td>1.0</td>
<td>2.1</td>
<td>0.57:0.43</td>
</tr>
<tr>
<td>Density of UO2 (g/cm³)</td>
<td>10.5</td>
<td>10.88</td>
<td>10.4</td>
</tr>
<tr>
<td>Heavy metal/pebble (g)</td>
<td>12</td>
<td>5.966</td>
<td>5</td>
</tr>
<tr>
<td>Fuel Enrichment (%)</td>
<td>10</td>
<td>16.76</td>
<td>17</td>
</tr>
<tr>
<td>Moderation ratio</td>
<td>315.88</td>
<td>641.43</td>
<td>772.89</td>
</tr>
<tr>
<td>Fuel pebble radius (m)</td>
<td>0.03</td>
<td>0.03</td>
<td>0.03</td>
</tr>
<tr>
<td>No. of kernels/pebble</td>
<td>19810</td>
<td>9393</td>
<td>8335</td>
</tr>
<tr>
<td>UO2 kernel radius (cm)</td>
<td>0.023</td>
<td>0.0251</td>
<td>0.025</td>
</tr>
<tr>
<td>Coating layers (thickness in cm)</td>
<td>PyC/PyC/SiC/PyC</td>
<td>PyC/PyC/SiC/PyC</td>
<td>PyC/PyC/SiC/PyC</td>
</tr>
<tr>
<td></td>
<td>(0.0005/0.004/0.0035/0.0004)</td>
<td>(0.00095/0.003399/0.00353/0.0004)</td>
<td>(0.0009/0.004/0.0035/0.0004)</td>
</tr>
</tbody>
</table>
lattice representation of the random packing and (b) which regular lattice should be used. Several choices of lattice are possible, including simple cubic, body-centered cubic (BCC), face-centered cubic, or hexagonal close packed (HCP). The BCC (or the closely related body-centered tetragonal, BCT) lattice was used before to model different pebble bed cores (Terry, 2001). But it was found that the spheres tend to pack towards an HCP lattice in the core. Therefore, a new technique is applied to develop the HCP lattice that is believed to be the best choice to represent the loose packing typically encountered in pebble bed reactor cores. Every single geometrical detail is included in the model as much as possible.

3.1.2. Fuel pebble

Models for the reactors using MCNP are generated in a way that all reactor components are designed in detail. The initial step is to model the fuel ball having a diameter of 0.06 m. First, a single TRISO particle with UO2 kernel and four outer layers (two inner graphite, a SiC buffer zone, and an outer graphite layers) is created. A lattice in a cubic array in a three-dimensional space is formed with these particles. This lattice is embedded into a spherical volume such that only full TRISO particles are permitted inside the sphere. Volume not occupied by TRISO particles within the sphere is filled with graphite. Then, this spherical volume is covered with a 0.5 cm thick spherical shell made of graphite as in the case of fuel balls. The number of full fuel particles, dimension and composition inside a fuel ball is varied according to the reactor types. The model of a fuel ball is shown in Fig. 1. Graphite moderator balls are also created simply by solid spheres with 6.0 cm of diameter.

3.1.3. Reactor core and periphery

Arrangement of the pebbles in the core is the next step of simulation. This is accomplished by creating hexagonal prism unit cells. These cells are then assembled as layers. The height of a layer is 9.798 cm. Top and bottom planes of hexagonal prisms are flat and contain half spheres. There are seven balls at these faces; one at the centre of the basal plane and six surrounding spheres. These six spheres are not centred at the corners of the hexagons, but rather hexagonal prism side surfaces surround these balls. The intermediate section of each hexagonal prism contains three full balls as well as partial contributions from the neighbouring hexagonal prism cells from all six sides. When neighbouring hexagonal prisms are attached to each other, these partial spheres are completed and make full scale balls. Fuel and moderator balls are selected in each layer according to their presence in the core. For HTR-PROTEUS, the dimension of the hexagonal prism is adjusted to meet the desired packing fraction. Typical structures of cells for different reactor types are shown in Figs. 2–4. These hexagonal prisms are then assembled to form an array to place into the core. The outer boundary of the array is the inner surface of the side reflector. One consequence of the repeated-geometry feature of MCNP is the presence of partial spheres at the core edge, which can overestimate the amount of fuel in the system. This is solved by determining the sphere positions at the core edge explicitly.
However, the top layer is formed only by adding half spheres of each ball present in this layer. Once the model of core region is completed, it is verified that the filling fraction of ball in this region is 61% for HTR-PAP20 and HTR-10 and 74.05% for HTR-PROTEUS. In the case of HTR-10, the cone region and discharge tube are formed by only graphite balls (Jing et al., 2002). These regions are also made by balls arranged in hexagonal geometry. In addition to fuel or moderator balls, there are side, top and bottom reflectors included in the model. The dimension and composition data for different reactor materials including the impurities present in the system can be found elsewhere (Mathews and Chawla, 1990; Xu et al., 2005; Kuijper et al., 1996). Horizontal and vertical cross-sectional views of different HTRs are shown in Figs. 5 and 6.

3.1.4. Extended qualification

Further qualification for the newly developed MCNP models is performed in terms of their capability to represent the randomness encountered in the arrangement of fuel and moderator balls in the core as well as inside a fuel ball in the arrangement of TRISO particles as mentioned earlier. Another Monte Carlo code MVP/GMVP
is used in this process (Nagaya et al., 2005). The MVP/GMVP is a general purpose Monte Carlo code developed in Japan Atomic Energy Agency for neutron and photon transport calculation based on continuous energy. The statistical geometry model available in the code is used to model the random distribution of the coated fuel particles and the pebble bed fuels. The packing fraction is the key parameter to simulate the randomness. Simulations are made for different HTRs using the code, and the results are verified against the newly developed MCNP models.

3.2. Burnup and fuel loading scheme

The burnup and refuelling study for HTR-PAP20 is carried out by the isotope generation and depletion analysis code ORIGEN2.1 (Croff, 1991). ORIGEN uses a matrix exponential method to solve coupled first-order, linear differential equations, where each equation accounts for the generation/depletion of an isotope. The isotopes include activation products, fission products and actinides. The new isotopic concentrations are then passed to MCNP for the next transport step. The combination of MCNP and ORIGEN is useful for predicting isotopic concentrations as functions of burnup and for predicting the reactivity changes associated with burnup. MOCUP (MCNP-ORIGEN Coupled Utility Program) is a coupling program developed by the Idaho National Laboratory (INL) that combines MCNP and ORIGEN, and is used for the plutonium concentration study of pebble bed HTRs (Moore et al., 1995; Terry, 2001). A similar utility program is written in FORTRAN that combines ORIGEN and MCNP so that the updated composition data from ORIGEN after isotope depletion and generation are sent back to MCNP in the form of number densities to generate new MCNP input. The built in $^{235}$U enriched UO$_2$ fuel library having 50,000 MWd/MT$_{HM}$ of burnup is used in ORIGEN calculation. The burnup calculation is performed for the specified number of days of reactor operation at full power.

At the start-up the lower 11 layers of the core (each of them with the height of 9.798 cm) are filled with fuel elements having 10% enrichment. Then, $k_{eff}$ and the core average neutron flux are calculated by MCNP code. The fuel composition data for this height of core along with the calculated flux from MCNP are used to prepare the ORIGEN input to calculate initial burnup for a period of 1 year at constant reactor power. The generated composition data are sent back to MCNP to calculate new $k_{eff}$ value. At this point the refuelling scheme is introduced. This includes adding three more layers of fuels in the core having 20% enrichment (MCNP input is also simulated accordingly), and a new $k_{eff}$ and a set of flux values for both burnt and new batches of fuels are calculated. Two separate inputs are prepared for ORIGEN to calculate composition data for both kinds of fuels after 1 year of full power continuous reactor operation. These data are then used in MCNP to calculate new $k_{eff}$ and flux values. Each time, three layers are filled with 20% enriched fuel. The selection of 10% enriched fuel at the start-up makes the core height around 1 m, and in this way the impact of irregularities in the surface of the bed of spheres on the helium streaming is kept within reasonable bounds (Teuchert et al., 1992). So, just after, the reactor becomes supercritical again. This is the method employed here to calculate the burnup after a single batch refuelling. The technique is also applicable for core life time calculation. At time intervals of 1 year, one layer after the other may be added depending on the requirements of criticality. Filling of the reactor should be finished when 41 layers out of around 46 layers are filled up. At this point, the reactor is kept shut down, and the core is unloaded entirely at a depressurized condition. Clearly, when designing a larger height of the core cavity, the life time of the loading cycle could be extended proportionally.

3.3. Thermal hydraulic analysis

3.3.1. Background

The RELAP5 code is used to analyze the thermal hydraulic characteristics of the pebble bed type high temperature gas cooled reactor. The code is originally designed for transient simulation of the light water cooled power reactors. One of the major differences between gas cooled reactors and LWRs is their moderator. In RELAP5, a generic modelling approach is used that permits simulating a variety of thermal hydraulic components with their control systems. The hydrodynamic model is a two-fluid model for the flow of a two-phase steam–water mixture that allows noncondensible components (e.g. helium) in the steam phase and/or a soluble component in the water phase. It is possible to use RELAP5 with only helium and no steam, and in that case the working fluid only exists in one phase and behaves like an ideal gas. The code provides 110 and 115 cards to list the gasses in the noncondensible mixture and their concentrations (Allison and Wagner, 2007). This has to be used for initial conditions for normal volumes and also for time-dependent volumes.

On the other hand, the code has been validated and tested for a wide range of applications, but for pebble bed type HTGRs virtually no testing and benchmarking has been performed. Therefore, considering that all mass and energy balances are still valid, and that the correct properties of helium is possible to introduce in the
code, it seems that there is no fundamental obligation to using the code with helium as working fluid. For the dynamic reactor behaviour a space-independent point reactor kinetics model is present in RELAP5. The point kinetics formulation requires core-layer averaged temperatures and reactivity feedback coefficients to determine a total reactivity for driving the kinetics calculation of total core power. Once the total core power has been determined, it is then distributed among the core-layers in an invariant manner (fixed power profile).

3.3.2. Model development

The thermal hydraulic analysis of the HTR-PAP20 is performed by the RELAP5/Mod4.0 code for hot full power reactor operating condition at the beginning of life. The components of a nuclear reactor are represented with a user-defined nodalization that contains hydraulic control volumes and junctions that represent flow paths between control volumes and heat structures. The code solves separate continuity, momentum and energy equations for the gas and liquid phases. Each phase can have a different temperature and velocity within a control volume. The code also contains a flexible control system that allows the user to model any physical control system of the real plant. Time-dependent volumes connected with pipe components are used to define the hydrodynamics of this stand-alone reactor (means fixed inlet mass flow rate, pressure and temperature). The time-dependent volumes specify hydraulic conditions, and the time-dependent junction provides mass flow data. During the transient simulation, the pressure is controlled by the exit time-dependent volume. Since the flow is in a closed loop, similar changes are also made in the inlet time-dependent volume. The time-dependent junction is used to model the change in flow rate. The active core has 9 axial regions, each 0.09798 m height and each contains 2594 fuel pebbles. The pertinent parameters necessary for thermal hydraulic analysis of HTR-PAP20 are presented in Table 2.

Heat transfer from working fluid to the enveloping structures, the so-called heat structures, and the conduction towards an outer environment are also modelled. Spherical geometry is used to define the fuel pebbles in the core. The temperature rise in the pebble bed from the centre to the surface is a quadratic function. However, there exist following limitations in the code that require special treatment:

- Heat transfer relations for a pebble bed geometry are not available.
- Relations for the pressure drop over a pebble bed are not available.
- Heat structures cannot have mixed boundary conditions, i.e. transfer heat by conduction and convection at the same boundary.

The following subsections address the necessary steps taken to overcome these drawbacks and also include some other key features relating to the modelling.

### Table 2

Characteristics of HTR-PAP20 used for thermal hydraulic analysis

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactor power (MW)</td>
<td>20.0</td>
</tr>
<tr>
<td>Helium inlet temperature (K)</td>
<td>823</td>
</tr>
<tr>
<td>Helium pressure (MPa)</td>
<td>5.0</td>
</tr>
<tr>
<td>Helium mass flow rate (kg/s)</td>
<td>18.7</td>
</tr>
<tr>
<td>Core diameter (m)</td>
<td>2.5</td>
</tr>
<tr>
<td>Core height (m)</td>
<td>4.5</td>
</tr>
<tr>
<td>Active core height (m)</td>
<td>0.88182</td>
</tr>
</tbody>
</table>

#### 3.3.2.1. Heat transfer relations

In order to describe the heat transfer in the pebble bed correctly, relations must be defined for the heat transfer by forced convection and for the transport by conductance and radiation. These relations do not exist in RELAP5. The Zehner–Schlünder equation has been chosen to tabulate a complex relation that combines the conduction through the pebbles, the conduction through the gas between the pebbles and the conductance by radiation (Zehner and Schlünder, 1972; Barthels and Schürenkramer, 1984). For the heat transfer by forced convection a new Nusselt relation must be defined which will include the ‘porosity’ of the pebble bed. The heat transfer \( Q \) from a pebble to the working fluid is calculated by means of the following equation:

\[
Q = \alpha A \Delta T,
\]

where \( \alpha \) is the mean heat transfer coefficient, \( A \) is the surface area of a pebble in the bed, \( \Delta T \) and \( T_c \) are pebble surface and gas temperatures, respectively. The heat transfer coefficient is defined as

\[
\alpha = \frac{Nu \dot{i}}{d}
\]

where \( Nu \) is the Nusselt number, \( \dot{i} \) is the thermal conductivity of gas and \( d \) is the pebble diameter. The Nusselt number is determined using the following relationship:

\[
Nu = 1.27 \frac{Pr^{1/3}}{e^{1/3}} Re^{0.36} + 0.033 \frac{Pr^{1/2}}{e^{1/7}} Re^{0.86},
\]

where \( Pr \) is the Prandtl number (0.66 for helium gas), \( Re \) is the Reynolds number \((100 < Re < 10^5)\) and \( e \) is the porosity of the pebble bed \((0.36 < e < 0.42)\) (Kugeler and Schulten, 1989). The following expression is used to determine Reynolds number:

\[
Re = \frac{m/A}{\dot{i}},
\]

where \( m \) is the fluid mass flow rate and \( A \) is the cross-sectional area of the core.

All these conditions are fulfilled for the present core. Based on these relations a new set of heat transfer coefficient as a function of temperature are generated and introduced in the RELAP5 model in a tabular form.

#### 3.3.2.2. Pressure drop over pebble bed

In order to model the pressure drop over the pebble bed due to friction, the following relation has been modelled in the control system environment of RELAP5 (KTA Standards, 1986). Every time step the pressure drop is calculated in the form of a control variable which drives the aperture of a valve placed at the exit of the core. The aperture of the valve is such that it causes a pressure drop \( \Delta p \) which is given by

\[
\Delta p = \psi \frac{1 - e}{e^2} H \frac{1}{2 \rho} \left( \frac{m}{A} \right)^2,
\]

where \( \psi \) is the friction coefficient, \( \rho \) is the density of fluid, \( H \) is the reactor height. The following empirical formula is used to derive the friction coefficient \( \psi \) in a pebble bed:

\[
\psi = \frac{320}{(\frac{m}{A})^2} + \frac{6}{(\frac{m}{A})^2 e^2 e^1},
\]

where the Reynolds number is derived from the following equation in terms of dynamic viscosity \( \eta \) of the gas:

\[
Re = \frac{(m/A) d}{\eta}, \quad (10^8 < Re(1 - e) < 10^5).
\]

#### 3.3.2.3. Mixed boundary condition

RELAP5 does not allow an outer surface to have mixed boundary conditions. The surface is either connected to the next mesh of that same heat structure and transports
heat by conduction, or connected to a volume with the working fluid in which case the heat is transported by convection/radiation. This brings a significant inadequacy, and it has implications when modelling the reflector region with the gas ducts. It shields the hot core, and it preheats the helium gas to some extent, thereby recovering most of the heat leaking sideways out of the core. In order to tackle the problem with the coolant channels, two heat structures have been defined, one on each side of the coolant channels (gas duct region shown in Fig. 5). One single annular channel surrounding the core connected with the main flow path has been defined that represents all the ducts. Heat can then be transferred from the hotter to the colder heat structure, but solely by convection of the gas. This way of modelling is very important for transient calculations.

3.3.2.4. Point reactor kinetics. This section describes the parameters required for the point reactor kinetics model in RELAP5. Point reactor kinetic model defines the time behaviour of the neutron population. Combined with the thermal hydraulic core model described above, the dynamics of the reactor can also be performed. The line of approach is as follows: the point reactor kinetics model calculates the integral reactor power having no spatial distribution. The 3D Monte Carlo model is used to calculate the power distribution within the core. The core is divided in nine axial layers, and a portion of the power is allocated to each layer during the steady state conditions. During the transients, the power causes a temperature variation in the layers which introduces a reactivity disturbance. Together with the xenon reactivity contribution, the net reactivity is then fed back into the point reactor kinetics model. Then the kinetic parameters of the model determine the dynamic reactor response at different time steps. It is important to notice that the axial power profile has been chosen to be fixed and has been determined once from the reference core, and the same is applied to the kinetic parameters. The point reactor kinetics model is derived from transport theory in order to obtain a formal and consistent procedure. On the other hand, certain assumptions are required to calculate these parameters using diffusion theory.

3.3.2.5. Thermal conductivity data. Established safety standards are used to calculate thermal properties of HTR-PAP20 reactor materials. Helium and fuel pebble thermal conductivity are very important and require proper representation. For the calculation of the thermal conductivity of helium, the following equation is used:

\[ \lambda = 2.682 \times 10^{-3}(1 + 1.123 \times 10^{-3} \times p)T^{0.71} \times 10^{-4} \times p, \]  

where \( \lambda \) is in W/m K, \( p \) is the pressure in bar, and temperature \( T \) is in K (KTA Standards, 1986).

The thermal conductivity of the fuel pebble, \( \lambda_f \), is derived from the following expressions:

\[ \lambda_f = \frac{2.549 \times 10^{-4}T^{1.545}}{1.163} \text{,} \quad 0 \leq T < 1300 \text{ °C}, \] 
\[ \lambda_f = \frac{2.0 \times 10^{-4}(T - 135.0)^{1.287}}{1.163} \text{,} \quad 1300 \leq T < 2500 \text{ °C}, \]  

where \( \lambda_f \) is in kcal/m h °C and is converted to SI unit accordingly (Yamashita and Zinza, 1990). Other thermal property data for different reactor materials can be found elsewhere (Yamashita and Zinza, 1990).

4. Results and discussion

4.1. Criticality calculations

This section deals with the evaluation of the effective multiplication factor \( k_{\text{eff}} \) for different gas cooled reactors. Continuous energy cross-section data from ENDF/B-VI library are used in the calculation along with the treatment of \( S(\alpha, \beta) \) scattering functions. All materials are specified to be 27 °C. Since the model prepared for MCNP is made of layers, the step size of fuel addition is selected as the height of a layer, i.e. 9.798 cm in order to avoid fractional fuel or moderator balls. One of the items to be determined for the initial steady state cases is the critical core height. The critical core height search is performed in MCNP by calculating the \( k_{\text{eff}} \) at different core height \( H_c \). As \( 1/k_{\text{eff}} \) is, to a very good approximation, a linear function of \( 1/H_c^2 \), the critical value of \( H_c \) can be easily obtained. The evaluation of critical core height for HTR-PAP20 is shown in Fig. 7. The critical core height is found to be 82.15 cm which is in very good agreement with the reference value of 82.0 cm (Kuijper et al., 1996). This represents that the newly developed model for HTR-PAP20 is working extremely well.

The effective multiplication factors calculated by MCNP and MVP/GMVP codes for different HTRs are tabulated in Table 3. The calculations are performed for benchmark critical core heights of those reactors. The results are compared with the available experimental and theoretical values. It is observed that the calculated results are in very good agreement with those of experiment and reference values. This establishes that the developed models in MCNP are representing the heterogeneity of pebble bed core extremely well.

4.2. Neutron flux and power

The total neutron flux and power density are calculated by MCNP for HTR-PAP20 core, and the results are shown in Fig. 8. The active core height is considered to be 88.182 cm (nine layers, each 9.798 cm high) in order to avoid fractional fuel pebbles. This critical core height is also used for thermal hydraulic analysis of HTR-PAP20. The \( k_{\text{eff}} \) value for this core height is found to be 1.02197. The maximum neutron flux and power density are found to be \( 1.3434 \times 10^{14} \text{n/cm}^2 \text{s} \) and \( 4.3117 \text{MW/m}^3 \), respectively, which are observed in the bottom layer of the core.

4.3. Burnup and refuelling

The burnup analysis is performed by MCNP-ORIGEN codes for HTR-PAP20 under continuous full power operation. The critical core height is set to 107.778 cm (11 layers) to provide sufficient excess reactivity to analyze the initial burnup with 10% enriched fuel in the core. The \( k_{\text{eff}} \) value at this critical core height is found to be 1.08083. The change in \( k_{\text{eff}} \) and depletion of \( ^{235} \text{U} \) as a function of burnup are shown in Fig. 9. The change in \( k_{\text{eff}} \) is found to be 6.577%, whereas the depletion of \( ^{235} \text{U} \) is 14.37% after 7300 MWd burnup.

The technique of batch at constant reactor power is applied during reloading of fuel in the core. Each time a complete axial mesh is filled with 20% enriched \( ^{235} \text{U} \) fuel. Three layers of fuel are introduced in the core to make the reactor supercritical. The \( k_{\text{eff}} \) is found to be 1.09231 for the core height of 137.172 cm. The depletion of \( ^{235} \text{U} \) for old (already burnt) and new fuels as a function of burnup is shown in Fig. 10 along with the change in \( k_{\text{eff}} \) value. It is found that after 14,600 MWd of burnup the depletion of \( ^{235} \text{U} \) for old and new fuels is 23.71% and 18.665%, respectively. Therefore, from initial loading to the following this scheme, the approximate core lifetime becomes 2 years and 11 months \( (k_{\text{eff}} = 1.0) \). Following this scheme, one should be able to calculate the total lifetime of a reactor for any particular core height. The batches can also be subdivided into smaller sub-batches which stand for continuous fuelling. The combination of MCNP and ORIGEN is also useful for predicting isotopic concentrations of any daughter nuclide and fission products as a function of burnup which is very important for any proliferation study.
4.4. Kinetic parameters

The kinetic parameters play a significant role during reactor transients. The Monte Carlo technique is applied to evaluate these parameters. The MCNP and ORIGEN codes are used to calculate the xenon reactivity worth. The calculated point kinetic parameter values are tabulated in Table 4. No approximation is required to evaluate the kinetic parameters by Monte Carlo technique. The
accuracy greatly depends on the developed models and techniques. The newly developed advanced models for different HTRs during this study will encourage the use of transport theory in determining kinetic parameters for those reactors.

4.5. Steady state temperature

The fuel pebble and helium gas temperatures in the HTR-PAP20 core are calculated by the RELAP5/Mod 4.0 code under steady state normal operating condition at full power. The RELAP5 code calculates the total power produced in each layer of the active core (88.182 cm) based on the normalized power density distribution calculated by MCNP (Fig. 8). The results are plotted in Fig. 11. It is observed that 18.59 MW power is produced from the fission and 1.41 MW is gamma ray power. The maximum fuel pebble centreline and helium gas temperatures in the active core are found to be 1171 K and 1028 K, respectively. The reference values calculated by PANTHERMIX and VSOP codes for the fuel pebble centreline temperatures are 1116 K and 1184 K, respectively, and the maximum helium gas temperatures are 1042 K and 1035 K, respectively (Kuijper et al., 1996; Oppe et al., 1996; Teuchert et al., 1994). These excellent agreements justify the use of RELAP5 for steady state thermal hydraulic analysis of pebble bed type gas cooled reactors. It also shows that the developed models and

![Figure 8](image.png)

**Fig. 8.** Axial neutron flux and power density distribution inside the HTR-PAP20 core.

![Figure 9](image.png)

**Fig. 9.** Change in $k_{\text{eff}}$ and depletion of $^{235}\text{U}$ as a function of burnup after the initial loading of 10% enriched fuel in HTR-PAP20 core.
necessary modifications make it possible to use this widely used LWR analysis code for HTR analysis.

4.6. Reactor transients

To demonstrate further capabilities of RELAP5 code, two transient calculations are performed on the basis of benchmark specifications for a Loss of Flow Accident (LOFA) and a Loss of Coolant Accident (LOCA) (Kuijper et al., 1996). The initial condition is the beginning of life at full power reactor operation with Xe-equilibrium.

Table 4

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neutron lifetime (s)</td>
<td>1.3333 × 10^{-6}</td>
</tr>
<tr>
<td>Effective delayed neutron fraction</td>
<td>0.00779</td>
</tr>
<tr>
<td>Doppler coefficient (Δk/k°C)</td>
<td>-3.479 × 10^{-5}</td>
</tr>
<tr>
<td>Fuel</td>
<td>-2.340 × 10^{-5}</td>
</tr>
<tr>
<td>Moderator</td>
<td>-3.45</td>
</tr>
</tbody>
</table>

Fig. 10. Change in $k_{eff}$ and depletion of $^{235}U$ as a function of burnup after refuelling the HTR-PAP20 core using 20% enriched fuel.

Fig. 11. Total power distribution and fuel pebble centreline temperature calculated by RELAP5 during steady state full power operation of HTR-PAP20.
4.6.1. Loss of flow accident

The loss of flow accident presupposes a halted mass flow rate (from 18.7 kg/s to 0.01 kg/s in 30 s), while the helium pressure of 5.0 MPa remains unchanged. In reality, a LOFA will occur when the rotational speed of the shaft becomes zero. The helium flows from the core into the gas turbine that drives the shaft connected to the gas compressor and generator. A possible reason might be that the power demand becomes too high which decelerates the shaft. Another possible reason is a turbine trip which constitutes a loss of driving power for the compressor and generator, causing a rapid deceleration of the shaft.

For the reference core the incident has been calculated by RELAP5 code. Fig. 12 shows the total (fission + decay) reactor power and the maximum fuel temperature as a function of time. From the figure, it follows that the reactor reaches recriticality after 8.5 h. Prior to that point the reactor power consisted of decay heat with only a tiny fraction of spontaneous or prompt fission. Two effects bring the reactor back to criticality: firstly, the gradual decrease in decay power results in a cooler reactor thereby increasing reactivity and secondly, the xenon concentration decreases which also introduces a positive reactivity. The time-averaged power and time-averaged maximum fuel temperature

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**Fig. 12.** Calculation of total power and fuel pebble centreline temperature by RELAP5 as a function of time after the occurrence of LOFA in HTR-PAP20.

**Fig. 13.** Calculation of total power and fuel pebble centreline temperature by RELAP5 as a function of time after the occurrence of LOCA in HTR-PAP20.
increases after the recriticality. The maximum fuel temperature reaches its highest value of 1741 K after 90 h. The heat transfer from the core to the ambient takes place by radiation, natural convection within and above the core, and conduction in the radial direction to earthen wall. The high temperature characteristics of the graphite reflector allow sufficient temperature gradient to move the heat.

4.6.2. Loss of coolant accident

The loss of coolant accident also presupposes a depressurization scenario along with the loss of flow (mass flow decreases from 18.7 kg/s to 0.01 kg/s and the pressure drops from 5.0 MPa to 1.0 MPa in 10 s). Such a scheme could occur in reality as a result of a rupture (guillotine break) in the cooling circuit of the reactor. Helium will flow out of the containment into the reactor building until the pressure becomes stabilized at 1.0 MPa. For a loss of cooling accident, the prompt fission power will rapidly decrease and after a few minutes become negligible compared to the decay power. Passive cooling processes have to transport the decay heat from the core to the pressure vessel steel wall where it can be transferred to the environment by free convection. It is a slow process, and it takes days before equilibrium is reached. It may be mentioned that no human intervention is needed to control the incident and to limit the consequences.

Fig. 13 shows the total reactor power and the maximum fuel temperature after the incident. Almost similar pattern in the plot is observed like the loss of flow incident. The main difference between the LOCA and LOFA is the enhanced effect of free convection in the pebble bed plus cavity in the case of LOFA. A lower pebble bed temperature is the result and, as the xenon worth is nearly identical, a similar point of recriticality is observed. The reactor reaches recriticality after 8.25 h, and the maximum fuel temperature of 1855 K is observed after 87 h. The heat transfer from the core to the ambient mainly takes place by radiation and conduction. For the reference core, the maximum fuel temperature still remains below the limiting fuel temperature of 1873 K for TRISO coated particles with SiC layer (Nabielek et al., 1990).

5. Conclusions

This study presents an integrated effort to analyze the pebble bed type HTRs using general purpose computer codes. In order to perform the analysis, the chain of MCNP-ORIGEN-RELAP5 codes is used to generate new models and techniques that couple the core neutronics with the thermal hydraulics. This coupling has been developed in order to come to a more detailed and realistic simulation of the entire system. For the neutronics part of the core, new advanced models are developed using Monte Carlo technique. The evaluated $k_{eff}$ values are in good agreement with those of experimental evaluations and also with the predictions of MVP/GMVP. The burnup and refuelling scheme is generated by MCNP-ORIGEN codes. For the thermal hydraulics part of the core, the RELAP5 code is used to develop realistic model and implementation of appropriate correlations. Combinations of these different parts made it possible to assess what detail is required for the HTR calculations. The study demonstrates that the combination of MCNP-ORIGEN-RELAP5 codes is quite suitable for performing neutronics, burnup and thermal hydraulics of pebble bed HTRs. Application of the coupled MCNP-ORIGEN-RELAP5 codes will certainly promote the design and development study of the pebble bed type gas cooled reactors.

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