Development of a Coupled Multi-Physics Code System for Pebble Bed Reactor Core Modeling

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Abstract – A coupled multi-physics code system is being developed for three-dimensional full-core modeling of pebble bed reactors. Three separate modeling areas are combined in a novel way to provide detailed data of the main physical processes in the core. In the first area, discrete element method (DEM) is used to model the packing and dynamic behavior of the pebble bed. A DEM simulation provides realistic data of the randomly packed pebble bed, which is then utilized as exact pebble positions in Monte Carlo reactor physics calculations and as porosities in the calculation cells of volume averaged thermal-hydraulic calculations. The thermal-hydraulic model and the reactor physics model are coupled so that the core power and temperature fields are solved iteratively. At the current stage of the development, an open source code LIGGGHTS is used for the DEM calculations, ANSYS Fluent is used for the thermal-hydraulic calculations and the Monte Carlo code Serpent is used for the reactor physics calculations. Additional codes have been written to transfer and map data between the different codes and to control the iterative solution of the coupled thermal-hydraulics and reactor physics. In this paper, a general description of the code system is given along with a simplified demonstration calculation.

I. INTRODUCTION

Nuclear energy is converted to heat in a nuclear reactor. The heat changes the temperature of the reactor materials and the cross sections, which affect the reactor power output and thus the temperatures. Due to this interdependence the accurate estimation of the state of a reactor requires coupled solution of reactor physics and thermal-hydraulics. Heating also changes the coolant density, which affects neutron moderation. In gas-cooled reactors such as the pebble bed reactor (PBR), this effect can generally be neglected due to the minimal interaction between the helium coolant and neutrons. This feature somewhat simplifies core calculations. However, as an additional challenge, the fuel in PBRs is inside spherical elements, which form a disordered packed configuration and slowly drain through the core.

At Lappeenranta University of Technology (LUT) a code system is being developed for the multi-physics modeling of PBRs. Rather than developing entirely new software, existing codes are modified and applied for the pebble bed specific modeling tasks and coupled with an external coupling code. The reactor physics are solved with a continuous energy Monte Carlo method code, which allows the geometry to be defined in a high level of detail. Core thermal-hydraulics are solved with a computational fluid dynamics (CFD) code, which uses a porous media approach for the pebble bed. Along with reactor physics and thermal-hydraulics, the packing and dynamic behavior of the fuel pebbles is modeled using a discrete element method (DEM) code. A more realistic solution of the reactor state is expected when the packing data obtained from DEM simulations is utilized.

In this paper, the individual modeling areas and approaches are described as well as the data transfer and coupling procedures developed so far. An example calculation is performed for a simplified reactor geometry. Although the example calculation is rather crude, it is still considered sufficient to demonstrate the calculation procedure and data transfer between the different codes.
II. MODELING AREAS

Three separate physical modeling areas are combined in the calculation system as shown in Fig. 1. Information about the pebble positions in any simulated situation is obtained from calculations with the DEM code LIGGGHTS [1]. Reactor physics are solved with the Monte Carlo code Serpent [2], which has specific features for dealing with stochastic particle fuel and pebble geometries efficiently. Coolant flow and heat transfer in the core are solved with the general purpose CFD code ANSYS Fluent [3] which treats the pebble bed region as a porous media. Each of the codes can be used as stand-alone modeling tools or as a coupled code system via an external coupling interface to provide data to each other and thus yield physically more accurate results.

II.A. Discrete Element Modeling

DEM is used to model the packing and dynamic behavior of the pebbles inside the reactor core with high physical realism. DEM is a state of art computational method for solving the contact mechanics in systems consisting of individually defined particles, typically spheres [4]. Trajectories of the spheres are solved as they interact with each other when in mechanical contact. For each sphere $i$ in the system, the total contact force $F$ and torque $T$ between $n$ neighboring spheres $j$ that are in contact with $i$ are solved from

\[ F_{i,j} = \sum_{j=1}^{n} F_{ij} \]  
\[ T_{i,j} = \sum_{j=1}^{n} (R_i \times F_{ij}) \]  

where $R_i$ is the radius of the sphere and $n_j$ is the normal unit vector between the spheres $i$ and $j$. The contact force consists of a normal and tangential component for which several models exist and a selection of these is available in the LIGGGHTS DEM code. In this work, the nonlinear normal force model proposed in [5] is used. The normal force is given by

\[ F_{n} = -K_n \delta_{n} - \eta_n \dot{\delta}_{n} \left( v_{ij} \cdot n_j \right) n_j \]  
\[ F_{t} = -k_t \delta_t - \eta_t v_{ij} \]  

where the first and second term are the elastic and viscous components, respectively. In the equation, $K_n$ is the normal stiffness, $\delta_n$ is the normal overlap distance (deformation) between two spheres, $\eta_n$ is the normal damping coefficient and $v_{ij}$ is the relative velocity between the spheres. Similarly, the tangential force is given by

\[ F_{t} = -\mu \left( F_{n} \right) \]  

and

\[ T_{t} = \sum_{j=1}^{n} (R_i \times F_{ij}) \]

unless the condition

\[ \left| F_{t} \right| > \mu \left| F_{n} \right| \]  

is satisfied, in which case the tangential force is calculated as

\[ F_{t} = -\mu \left( F_{n} \right) \]  

In the above equations, $k_s$, $\delta_{ij}$ and $\eta$ are the stiffness, deformation and damping coefficient for the tangential direction, $v_{ij}$ is the slip velocity between the spheres, $t_{ij}$ is the tangential unit vector and $\mu$ is the friction factor. Values for the stiffness and damping coefficient can be estimated based on the material properties as described e.g. in [6].

After the pairwise forces have been calculated and summed up for each sphere, the translational and rotational accelerations for the spheres are calculated with Newton’s equations of motion. The DEM simulation is progressed at constant time steps where at each time step, the contacting spheres are detected and the forces are resolved. Further details of the method and a literature review of the work related to DEM modeling of pebble bed reactors are available e.g. in [7].

Basically any DEM code or even experiments can be used to provide data for the subsequent reactor physics and thermal-hydraulics calculations. The only requirement is the capability to output the pebble radii and coordinate data. In the current work the open source DEM code LIGGGHTS is used as it has rather good features, such as wall geometry input in STL (Stereo lithography) format and parallelization via MPI (message passing interface). It has efficient base algorithms as it has been built on top of the well known molecular dynamics code LAMMPS [8]. Also, the code is open source and does not require license fees.
II.B. Reactor Physics

Reactor physics are calculated with the Monte Carlo reactor physics code Serpent 2 (montecarlo.vtt.fi). The advantage of using this type of code is the possibility to define the geometries in a high detail. Although Monte Carlo method based full core calculations are rather calculation intensive, they are not impossible to perform with the computers today. Specifically in Serpent, there are some features that are especially useful for the detailed, yet efficient calculation of pebble bed geometries.

Serpent features an explicit stochastic geometry model, which allows the fuel pebbles and the fuel particles inside them to be defined explicitly in stochastic configurations. Thus, pebble coordinate data obtained from DEM simulations can be used to define the pebble locations in the reactor physics model. A high computational efficiency regardless of the number of such individual details is achieved by using a Cartesian search mesh to locate the pebbles and particles.

Another beneficial feature is the use of Woodcock delta tracking method in conjunction with the conventional ray-tracing neutron tracking routine. This provides significant speedup especially in the double heterogeneous pebble bed geometries. Further details can be found e.g. from [9].

Changing the temperatures of materials with Serpent is straightforward because of on-the-fly Doppler broadening routine. No external tools are needed during the coupled calculation and even continuous temperature distributions can be modelled.

Serpent has already been used for calculations of small pebble bed configurations as described in [10]. It is now used for calculations of full-sized reactor geometries.

II.C. Thermal-Hydraulics

Thermal-hydraulics of the reactor core in three dimensions is solved with the CFD code ANSYS Fluent by simplifying the pebble bed region as porous media. Porous media approach is used due to the huge number of pebbles in the core, which would require an enormous number of calculation cells and unfeasible computational power if the flow and temperature fields in the full reactor core would be modeled in detail even with RANS (Reynolds averaged Navier-Stokes) based turbulence models. When the porous media model is used, a coarse mesh is made for the pebble bed and the volume blockage of the spheres is presented as source terms in the fluid momentum equations.

The porous media model of Fluent is used as the base on top of which the pebble bed specific flow and heat transfer model is built via user-defined functions (UDF), i.e. additional C code utilizing specific macros available in Fluent. The porous media conservation equations for mass and momentum in Fluent are

\[ \frac{\partial}{\partial t} (\rho \phi) + \nabla \cdot (\rho \phi \mathbf{v}) = 0 \]  

(eq. 7)

and

\[ \frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\varepsilon \mathbf{v} \rho + \nabla \cdot (\rho \mathbf{v} \tau) + \varepsilon \mathbf{F} \]  

(eq. 8)

where the subscript f denotes the fluid phase and \( \varepsilon \) is the porosity, \( t \) is the time, \( \rho \) is the density, \( \mathbf{v} \) is the velocity vector, \( p \) is the pressure, \( \mathbf{\tau} \) is the stress tensor, \( \mathbf{F} \) denotes body forces (e.g. gravity) and \( \mu \) is the dynamic viscosity. The last term consists of viscous and inertial forces, for which in the case of a packed bed Ergun [11] or KTA [12] type correlations can be applied. The coefficients \( K \) and \( C \) are the permeability and the inertial loss coefficients, respectively, which are scalar quantities in the case of isotropic porosity. In the example calculation presented in this paper the Ergun equation is used so that the coefficients become

\[ K = \frac{d^2 \varepsilon^3}{150(1-\varepsilon)^2} \]  

(eq. 9)

and

\[ C = \frac{3.5(1-\varepsilon)}{d \varepsilon} \]  

(eq. 10)

where \( d \) is the pebble diameter.

Separate energy equations are solved for the solid and fluid phases in the pebble bed. They are linked together by interfacial heat transfer. In Fluent this is called the thermal non-equilibrium model. The energy equation for the fluid phase is

\[ \frac{\partial}{\partial t} (\rho \phi h) + \nabla \cdot (\rho \phi \mathbf{v} h) = \nabla \cdot (\phi \lambda \nabla T) + \phi A_s \left(T_s - T_h\right) \]  

(eq. 11)

where the subscript \( s \) denotes the solid phase and \( h \) is the specific enthalpy, \( T \) is the temperature, \( \lambda \) is the thermal conductivity, \( \alpha \) is the convective heat transfer coefficient and \( A_s \) is the specific interfacial area. The energy equation for the solid phase is

\[ \frac{\partial}{\partial t} \left[ (1-\varepsilon) \rho_s h_s \right] = \nabla \cdot \left[ \left(1-\varepsilon\right) \lambda_{eff} \nabla T \right] + \alpha A_s \left(T_s - T_s\right) + S_s \]  

(eq. 12)

where \( \lambda_{eff} \) is the effective thermal conductivity which can take into account both conduction and radiation if models such as described in [13] are used. \( S_s \) is the thermal energy source, i.e. the nuclear heating power. The interfacial heat transfer coefficient \( \alpha \) can be obtained from literature correlations. The correlation provided in [14] is used...
in this case, which estimates the Nusselt number $Nu$ as

$$Nu = 1.27 \frac{Pr^{1/3}}{\varepsilon^{1/6}} Re^{0.16} + 0.033 \frac{Pr^{1/3}}{\varepsilon^{0.5}} Re^{0.86} \quad \text{(eq. 13)}$$

where $Re$ is the Reynolds number with the pebble diameter $d$ as the characteristic length. $Pr$ is the Prandtl number. The heat transfer coefficient can then be obtained from

$$\alpha = \frac{Nu \lambda_f}{d} \quad \text{(eq. 14)}$$

The specific interfacial area $A_f$ as well as the porosity $\varepsilon$ for each calculation cell can be calculated from the DEM data of the packed pebble bed and the nuclear heat source can be obtained from reactor physics calculations.

### III. COUPLING AND DATA TRANSFER

Data between the different codes is processed and transferred via external codes. Data transfer from DEM model to the Monte Carlo model is rather straightforward as the pebbles are represented as distinct entities in both models. Data transfer to and from the thermal-hydraulic model on the contrary needs additional effort due to the continuum approach used.

#### III.A. DEM Data to Serpent

As the core geometry can be defined in full detail in Serpent including explicitly defined positions for the fuel particles and also for the pebbles, the exact pebble coordinates obtained from the DEM simulations can be used to define the pebbles inside the core. The pebble coordinates and radii are exported as a text file, which is read as an input to Serpent. An example of the pebble bed geometry in Serpent can be seen in Fig. 2 where a slice has been taken from inside the pebble bed. It also shows the individually defined fuel particles inside the pebbles.

#### III.B. DEM Data to Fluent

Because the pebble bed data obtained from the DEM simulation is discrete by nature while in the thermal-hydraulic model a continuum approach is used, the direct transfer of pebble coordinates is not possible in similar way as is done when DEM data is utilized in Serpent. A separate code has been written to utilize the pebble packing data provided by DEM also in the thermal-hydraulic model. Currently, it calculates the exact porosities and will be modified to calculate also the exact interfacial areas in each thermal-hydraulic calculation cell. This way the packing data is mapped from the discrete model to the continuum model in a way that transfers as much of the packing structure information to the coarse grid CFD model as possible.

The data mapping code reads in the pebble position and radii information and the node and cell data of the CFD mesh constructed over the pebble bed region. It then calculates the pebble volumes inside each mesh cell and calculates porosities based on the solid volume inside the cell and the total volume of the cell. The volume calculation is based on a triangulation of the partial sphere volumes. A single CFD mesh element with pebbles from a DEM simulation inside is shown in Fig. 3.

#### III.C. Fluent-Serpent Data Transfer

The power distribution calculated by Serpent is mapped to the CFD mesh in a similar way as
porosities. As Serpent provides the power produced in each pebble, the power in each CFD cell can then be calculated as the sum of the pebble powers that are fully inside the cell and as fractions of the pebble powers of the partial pebbles that are inside.

The temperature distribution calculated in Fluent is mapped to Serpent by assigning the solid temperature of each cell to the pebbles that have their centers located inside that cell. As the temperature obtained from Eq. 12 represents the surface temperature of the solid, the temperature distribution inside a pebble is estimated with Fourier’s law using the surface temperature as the boundary condition. After the surface temperatures are obtained from CFD the internal temperatures for pebbles are calculated. Currently the temperature distribution inside a pebble is accomplished by dividing it into several material layers, which are set at different temperatures. This is illustrated in Fig. 4. Once all different temperatures for all material zones are calculated the temperatures are sorted and compacted to selected amount of different temperature zones. Amount of zones are limited due to computer memory available for calculations.

The iterative solution of the reactor physics and thermal-hydraulics is handled by an external coupling code written in Perl that runs Serpent and Fluent sequentially and transfers data between them. Convergence is monitored and the iterative solution process is continued until there is no significant difference in the results between subsequent iterations.

IV. CALCULATION EXAMPLE

The data transfer methods described above are demonstrated with an example calculation with the current version of the code system. A simplified reactor core model is constructed consisting of 430,000 pebbles packed inside a cylindrical core geometry replicating that of the HTR-PM reactor [15]. The example is not a fully coupled core calculation as there is still development required especially in data transfer from Fluent to Serpent. Also, the example is not meant to be an accurate reactor simulation from which any conclusions regarding the reactor should be made. The example is merely a demonstration of the current state of the code system and the coupling methods developed so far.

IV.A. Calculation Model

A three-dimensional geometry consisting of the main core region is defined. A cylindrical cavity with a cone and an outlet pipe at the bottom is defined to accommodate the pebbles. A region of graphite surrounds the cylindrical pebble bed and in the radial direction the model ends to a layer of steel representing the pressure vessel. A gas gap between the reflector graphite and the pressure vessel wall is left. Graphite regions are defined also in the axial direction above the pebble bed and around the bottom cone to represent the top and bottom reflectors. A cross section of the geometry can be seen in Fig. 5., which also includes the thermal-hydraulic mesh. The calculation geometry built in Serpent matches that of the thermal-hydraulic model. For the DEM packing simulation, only the geometry of the core cavity is needed. A separate surface mesh consisting of triangles and exported in STL format is constructed for LIGGGHTS.

The fuel pebbles are compacted inside the cylinder in the DEM simulation by dropping them from the top of the container. Due to a long time it would take to drop them in individually, they are dropped in clusters of several pebbles at specified time intervals. The pebble column is let to stabilize into a static configuration after all pebbles have been dropped.

For the Serpent calculation model the pebble bed data is imported from the DEM simulation as coordinates and radii. The data is used directly to form the input for Serpent. However, in this example calculation only the spheres above the bottom cone are defined to contain fuel particles while the bottom spheres are defined to contain only graphite. This is done because of some simplifications also in the thermal-hydraulic model in the bottom cone.

In the thermal-hydraulic calculation the pebble bed region is defined as porous media and the models described in Sec. II. C. are applied. Temperature dependent material properties are defined and e.g. for helium those given in [16] are
used. No separate flow channels are included for the inlet flow, thus the flow enters through the top reflector and exits through the bottom reflector (and the pebble outlet tube), which are both defined as porous media. The gas gap is defined as a solid material with a low density and thermal conductivity to provide insulation between the reflector and the pressure vessel wall. All outer walls are defined as adiabatic. An operating pressure of 7 MPa is defined and the flow inlet is given a mass flow rate of 96 kg/s and temperature of 523 K. A pressure outlet with a zero gauge pressure is defined at the bottom.

**IV.B. Calculation Process**

After the DEM packing simulation in LIGGGHTS the pebble position data is exported to Serpent and mapped to the thermal-hydraulic calculation cells as described in Sec. III.B. Porosities for the calculation cells are calculated together with the information of the fractions each pebble is divided between the cells it occupies. This is done to distribute the power produced in each pebble to the correct calculation cells in the coupled thermal-hydraulics – reactor physics solution process. The pebble bed resulting from the DEM simulation, the corresponding thermal-hydraulic mesh and the calculated porosities are shown in Fig. 6. Due to the small cells in the bottom cone and outlet pipe, average porosities are calculated for regions consisting of several mesh cells.

The reactor is given a constant temperature for the first calculation in Serpent. The power produced in each pebble is obtained and by using the information of their division to the cells, the power produced in each mesh cell is calculated. In Fluent the thermal energy source is given as power density in each cell. The power data as well as the porosities in each cell are read into Fluent via specifically written UDFs. The thermal power produced in pebbles as calculated by Serpent and its division to the thermal-hydraulic mesh elements is shown in Fig. 7.

The CFD calculation uses the power data provided by Serpent. After the CFD calculation has converged, the temperatures solved from the energy equation of solid in the pebble bed cells are exported. The temperature distribution calculated by Fluent for the fuel pebble region is shown in Fig. 7. Based on the knowledge of the host cell, i.e. the cell where the pebble center is inside, the surface temperature of each pebble is given the value of its host cell. With these new temperatures, a new reactor physics calculation can then be initiated.

In a complete coupled simulation the above procedure would be repeated until reaching a pre-specified convergence criteria so that no significant change in the temperature fields and pebble powers between consecutive iterations would be observed.

**V. SUMMARY AND CONCLUSION**

Methodology used to couple DEM, Monte Carlo reactor physics and porous media CFD into a multiphysics calculation system for PBR analyses was described. The development is still in progress, although most of the base data transfer procedures
Fig. 6. Three quarters of a pebble bed produced in a packing simulation with the DEM code LIGGGHTS (left). A thermal-hydraulic mesh of the pebble bed region (middle). Mesh elements colored by their porosity (right).

Fig. 7. Produced thermal power in pebbles as calculated by Serpent (left). Power density mapped into thermal-hydraulic calculation cells (middle). Solid medium surface temperature as calculated by Fluent (right). All plots are taken from the center of the core of the fuel region of the pebble bed.
have been established. A simplified example calculation consisting of the construction of the pebble bed with LIGGGHTS, mapping the packing data to Serpent and Fluent, calculation of the reactor power, import of power data to Fluent and calculation of the reactor temperature profile was performed.

The development of the coupled code system continues with the finalization of the external data mapping and coupling interfaces. Also the possibility to migrate the thermal-hydraulic solver to a free to use, open source environment, such as OpenFOAM, will be investigated. Finally some realistic validation calculations will be performed.

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