Coupled neutronics / thermal hydraulics calculations for High Temperature Reactors with the DALTON - THERMIX code system

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Abstract

A code system for the simulation of steady state and transient behavior of High Temperature Pebble-Bed type Reactors was developed. To this end a new time-dependent (3D) diffusion code DALTON was coupled to an existing thermal-hydraulics code THERMIX.

In order to validate the code system, simulations of the Pebble Bed Modular Reactor (PBMR) design and the Arbeitsgemeinschaft Versuchsreaktor (AVR) were performed for steady state and transient conditions. Special attention has gone to the coupled calculation methodology for the various types of transients.

Both the PBMR simulations and a comparison of the calculation results with experimental data of the AVR were satisfactory. The code system provides a key element in the development and optimization of (Very) High Temperature Reactor designs in the framework of the RAPHAEL project.

1 Introduction

In this paper the methodology and validation of a code system for coupled neutronic and thermal-hydraulic analysis of High Temperature pebble-bed reactors is presented. This code system provides a key element in the development of future Very High Temperature Reactor (VHTR) designs in the framework of the RAPHAEL project (D. Hittner, 2006). For the development of this code system a new 3D time-dependent diffusion code DALTON was coupled to an existing thermal hydraulics code THERMIX (Struth, 1995).

Models of the PBMR-400 design and the AVR were made and steady state and transient calculations were performed. In this paper the calculation methods and results of the simulations are discussed.

2 Coupled neutronics / thermal hydraulics code system

2.1 Calculation scheme

In Fig. 1 a schematic overview of the coupled code system is presented. The coupled code system consists of the codes DALTON and THERMIX that are described in Sect 2.2 and 2.3 respectively, and several other codes and scripts. A description of the tasks of each component of the code system is given below:

DALTON DALTON calculates a 2D zone averaged power profile using neutron cross sections that are corrected for the local temperature and Xenon concentration.

THERMIX The new power profile is used in THERMIX to calculate the temperature profile in the reactor at the new time point. For the
core region, a two-dimensional moderator temperature profile is augmented with a one-dimensional calculation for the temperature profile in the pebbles.

**XS library** Before the thermal hydraulic and neutronic calculations are started, a neutron cross section (XS) library is created as a function of the fuel and moderator temperatures and the Xenon concentration. In the case of the PBMR-400 benchmark the cross sections were supplied as part of the benchmark description and also depend on the local fast and thermal buckling.

**Xenon** The Xenon concentration is determined using the simplified depletion chains for Xenon and Iodine.

**MIXER** An in-house perl script (MIXER) updates for each calculation step the neutron cross sections by linear interpolation using several routines of the SCALE code system (SCALE-5, 2005).

**MASTER** Depending on the type of transient the MASTER program, which is an in-house perl script, decides how often data is exchanged between the different codes and what the calculation mode type of the codes has to be, i.e. steady state (eigenvalue) or transient mode.

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**2.2 DALTON**

The DALTON code can solve the 3D multi-group diffusion equations on structured grids (xyz or rzθ coordinates). The code’s capabilities include both the fundamental and higher lambda modes and time-eigenvalues through the Arnoldi method by linking with the ARPACK package (Lehoucq et al., 1997). Transient analysis in forward and adjoint mode is possible with or without precursors. Spatial discretization is performed using a second order accurate finite volume method.

The precursor concentration at the new time level is eliminated from the flux equation (Pautz and Birkhofer, 2003). Effectively the system can then be solved in a decoupled manner by solving for the multi-group flux first and subsequently for the precursor groups. DALTON uses an adaptive time-stepping algorithm that is based on the use of the second order time-accurate Backward-2 scheme. This scheme is fully implicit and unconditionally stable.

Whether a time step is accepted or not depends on the maximum allowed absolute error, atol, and relative error, rtol, as supplied by the user.

\[
\sqrt{\frac{1}{N} \sum_{i=1}^{N} \left( \frac{LTE_i}{atol + rtol \times \phi_i} \right)^2} \leq 1
\]  

where LTE is the local truncation error of the Backward-2 scheme. For prediction of the time step to be used in the next step, a similar procedure is adopted. The linear systems arising from discretization are solved using preconditioned CG where the preconditioner is based on an incomplete factorization. In the multi-group case, acceleration of the Gauss-Seidel group by group solution procedure is obtained by the techniques introduced in references (Morel and McGhee, 1994; Adams and Morel, 1993). Another option available is to use a GCR Krylov acceleration technique where the preconditioner consists of the Gauss-Seidel procedure.

**2.3 THERMIX**

THERMIX (Struth, 1995) is a 2D thermal hydraulics code. The code consists of the two modules THERMIX (heat conduction and thermal radiation) and DIREKT (convection). In THERMIX the energy conservation equation is solved for steady state or time dependent cases with the help of several libraries for heat conductivity, heat capacity and heat transfer. In DIREKT the conservation equations for continuity, momentum and energy are solved. The temperature and pressure of gases and liquids (without phase transition) can be calculated. An implicit calculation scheme is used for the solution of the equations in transient calculations.
2.4 Time step control and calculation mode

For transient calculations DALTON and THERMIX are used consecutively without performing additional iterations. The time step control within the codes is done independently of each other.

A (global) time step control algorithm was tested for the "Cold Helium Inlet" transient in Sec. 3.3. The control algorithm ensures convergence and stability of the coupled calculation result, similar to the time step control in DALTON described in Sec. 2.2 (Eq. 1). However, a vector $y$ containing $N$ state variables is used to check the 'global' time step and predict the new step size, instead of the neutron flux $\phi_i$ that is used in Eq. 1. A restart of the coupled code system from the previous time point is required if the criterion is not met. The vector $y$ contains the following variables: the average temperatures of the helium, fuel and moderator and the total reactor power.

The calculation mode type can be adjusted for certain transient simulations, such as a Loss Of Forced Cooling Accident, in which the reactor is in a sub-critical condition for a long period and the fission power is negligible. In these cases, the calculation procedure is switched to a THERMIX standalone calculation combined with an eigenvalue calculation in DALTON up to the point of re-criticality. At this point the calculation mode is switched back to fully coupled dynamics and the flux and precursor levels are re-initiated, starting from a low power level (1 W).

3 PBMR-400 benchmark

The Pebble Bed Modular Reactor (PBMR) is a 400 MW HTR that is currently under development (see Fig. 2). Steady state and transient benchmark exercises for this design are organized by the Nuclear Energy Agency (NEA). Steady state results of the benchmark calculated with DALTON-THERMIX can be found in (P. Mkhabela, 2006) and are omitted here for the sake of brevity. Pressurized and Depressurized Loss Of Forced Cooling (PLOFC and DLOFC) transient simulations as well as a Cold Helium Inlet transient case have been performed.

Fig. 2: Schematic overview of the PBMR-400 design containing an annular pebble bed and a fixed inner reflector.

3.1 Depressurized Loss Of Forced Cooling

In the Depressurized Loss Of Forced Cooling (DLOFC) without SCRAM the mass flow is reduced from 192.7 kg/s to a trickle flow of 0.2 kg/s and the pressure is reduced from 90 to 1 bar during the first 13 seconds of the transient. A simulation in which the mass flow is reduced to 0 kg/s is also performed. In a second case a SCRAM is executed after 13 seconds in which the control rods are fully inserted within 3 seconds.

The response of the reactor power for both cases (with or without SCRAM) of the DALTON-THERMIX calculation during the first 300 seconds is presented in Fig. 3. The temperature feedback causes a reduction in the fission power of the reactor. In the case that a reactor SCRAM is included, the fission power is reduced rapidly and the total reactor power is determined by the decay heat within seconds after the SCRAM.

In the case that no SCRAM has been executed, the reactor becomes critical again after it has sufficiently cooled down. The point of re-criticality occurs in the DALTON-THERMIX calculation after 42.7 h.

Fig. 3: Effect of a SCRAM on the Power during the first 300 seconds of a DLOFC transient.
which is close to the results of others. After several oscillations in power and temperature the fission power reaches a quasi-steady state (see Fig. 4), while both the temperature in the pebble bed and the reflectors increase.

The results of the average and maximum fuel temperature in the pebble bed during the DLOFC without SCRAM is shown in Fig. 5. The presence of the trickle flow cools the core, which results in a smaller (negative) reactivity feedback from the fuel. Therefore the reactor becomes re-critical at an earlier stage and the final fuel temperature is higher. The fuel temperature histories for the DLOFC with SCRAM (no trickle flow) are presented in Fig. 6. The faster reduction in reactor power in the beginning of the transient makes only a small difference on the temperatures compared to the case without SCRAM. However, the SCRAM prevents the reactor from reaching (re-)criticality in a later stage in the transient.

Note that in the calculation of this transient the period between 500 seconds and the point of re-criticality has been performed with a THERMIX stand-alone to reduce calculation time. The total CPU time for this transient was 110 hours.

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seconds of the transient and the mass flow is reduced to 0 kg/s. After the pressure reduction it is assumed that the helium inventory in the reactor remains constant, allowing the pressure to vary over time depending on the helium temperature.

The natural convection in the reactor increases the ability of the reactor to remove the decay heat, resulting in much lower temperatures. In Fig. 7 the temperature profiles in the reactor are shown after 100 hours in the DLOFC transient and after 50 hours in the PLOFC transient. It can be seen that for the PLOFC, which includes natural convection, the heat is transported to the top region of the core and the temperatures are much lower than for the DLOFC case.

3.3 Cold Helium inlet transient

The Cold Helium Inlet case simulates a bypass valve opening, which allows "cold" Helium to enter the core inlet plenum. A temperature ramp reduction of 50 °C is applied over 10 seconds, while all other input parameters remain constant. It is assumed that the reactor protection system would cause the valve to close after 300 seconds, which would bring the helium inlet temperature back to 500 °C.

The results of the reactor power and the change in the maximum fuel, moderator (average over the pebble radius) and helium temperature during a Cold Helium Inlet transient are presented in Fig. 8. The reduction in helium inlet temperature at the beginning of the transient results in a temperature decrease of the reflector, surrounding the flow paths of the helium riser, the inlet plenum and the temperature of the pebble bed. The decrease of the reflector temperature and the corresponding negative reactivity effect is almost immediately overruled by a more important positive reactivity effect caused by the feedback of the fuel temperature. This results in an increase of the reactor power and a corresponding rise in fuel temperatures, which in turn slows down the rise in reactor power. A large reduction in power from t = 310 seconds can be identified which is caused by the increase in helium inlet temperature.

The adaptive global time step routine was tested for this transient case. Besides the general behavior of the reactor power described above, small oscillations in reactor power causes large fluctuations in the time step size. On a number of occasions the time step routine decided to recalculate a certain time interval with reduced time step size. An overall reduction of the total calculation time of 10 % was achieved when compared to the case with a fixed global time step.

4 Simulation of the AVR

The AVR reactor had 21 years of successful power operation and was used as a test bed for various fuel and refueling strategies in Jülich, Germany (R. Bäumer et al., 1990). A coupled steady state and a Loss Of Coolant Accident (LOCA) transient case have been simulated.

4.1 Description of the AVR

A schematic overview of the reactor is shown in Fig. 9 and a horizontal cross section at the axial center of the core is shown in Fig. 10.
An important characteristic of the AVR is the location of the steam generators and the blowers inside the inner Reactor Pressure Vessel (RPV) (Fig. 9). The helium flows through the reactor core from the bottom to the top, where it is cooled in the steam generator.

Fig. 10: Horizontal section of the AVR core (Krüger (1989)) showing the reflector noses and the positions of the thermocouples with letter “A” through “D”.

Another important feature of the AVR is that it has four so called 'reflector noses' stretching into the pebble bed, which are made of graphite. Each reflector nose has a guiding tube for movement of control rods (Fig. 10).

4.2 Description of the Loss Of Coolant Accident experiment

The LOCA experiment was designed to simulate the reactor losing forced cooling and system pressure in full load condition. However, a fast depressurization could not be performed for practical reasons. Alternatively, the helium was pumped into the storage vessel by the gas purification system in three days. The reactor was operated for some days at low power level (4 MW) until the full load (46 MW) temperature distribution was obtained. The temperatures of the main components are shown in the second column of Table 1.

The LOCA transient was initiated by a shut down of the blowers, whereby forced cooling of the reactor was stopped. The decay heat curve for full load conditions (46 MW thermal power) was simulated with the fission power by moving the control rods. The steam generator operated at about 50 percent of full mass flow during the entire LOCA experiment and the water inlet temperature decreased from 130 °C to 60 °C.

Table 1: Steady state temperatures of the AVR before the transient

<table>
<thead>
<tr>
<th>Locations</th>
<th>Experiment (° C)</th>
<th>Calculation (° C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Side reflector: Inner (A)</td>
<td>555</td>
<td>562</td>
</tr>
<tr>
<td>Middle (B)</td>
<td>545</td>
<td>552</td>
</tr>
<tr>
<td>Outside (C)</td>
<td>535</td>
<td>528</td>
</tr>
<tr>
<td>Reflector nose (D)</td>
<td>608</td>
<td>592</td>
</tr>
<tr>
<td>Bottom reflector</td>
<td>207</td>
<td>209</td>
</tr>
<tr>
<td>Reactor barrel</td>
<td>276</td>
<td>276</td>
</tr>
<tr>
<td>Inner RPV, Middle of reactor</td>
<td>189</td>
<td>180</td>
</tr>
<tr>
<td>Top of reactor</td>
<td>196</td>
<td>192</td>
</tr>
<tr>
<td>Discharge tube</td>
<td>198</td>
<td>188</td>
</tr>
</tbody>
</table>

4.3 Coupled steady state calculation

The steady state of the reactor at 4 MW was calculated by performing a coupled neutronics/thermal hydraulics calculation with DALTON-THERMIX.

DALTON has been used in 3D mode (9 energy groups) to calculate the 3D flux and power profile, which is averaged in the azimuthal direction to generate a 2D profile (Fig. 11) for the use in THERMIX. The power peak appears in the top-right of the core, rather than in the center. The main reasons for this are the presence of the reflectors and noses near the outer region and the use of different fuel pebbles for the center region and the outer region of the core.

Fig. 12 shows the temperature distribution of the reactor at the beginning of the transient. The position of the maximum temperature appears on the top, outside of the core. It is determined by the corresponding power density and the mass flow distribution in the reactor.

Fig. 11: 2D power density profile of the reactor core
The third column in Table 1 gives the calculated temperatures of the reactor, which are in good agreement with the experimental results shown in the second column of the table.

4.4 Simulation of the LOCA

After the reactor reached a full load temperature distribution, the transient of the LOCA experiment was started. The blowers were shut down and the mass flow of the primary loop reduced to zero.

After the forced convection stopped, the conduction, radiation and local natural convection all contributed to the heat transfer between the reactor core and the steam generator. Although it is commonly considered as unimportant in a low pressure system, natural convection did contribute to the heat transfer in the AVR during the LOCA experiment (Krüger, 1989). It was found that the natural convection was underestimated in the 2D THERMIX model, since the complex 3D geometry of the top region of the core could not be modeled explicitly. In order to simulate this local natural circulation, a very small artificial mass flow of 0.02 kg/s is applied.

Figure 14 illustrates the temperature of the side reflector at the axial center of the reactor core. For the sake of brevity only point B (see Fig. 10) has been shown. Temperatures of points A and C show similar behavior. The temperatures of the side reflectors increase at the beginning of the transient because of the absence of forced cooling and the consequent accumulation of the decay heat. The side reflectors reach the maximum temperature after about 16-22 hours according to the experimental data. The corresponding calculated results reach the maximum 1-2 hours later.
than the experiment. Then, the reactor gradually cools down, discharging the heat to the steam generator and the outer reactor pressure vessel by conduction, radiation and natural circulation.

The reflector noses stretch into the reactor core and therefore the temperature of the tip of the nose is close to the temperature of the pebbles at this radial position (see Table 1 point D). Figure 15 shows the surface temperature of a pebble at the axial center of core and the same radial position as the tip of the reflector nose. The measured temperature of the reflector nose is also shown in this figure. They change synchronously at the beginning of the transient. Similar to temperatures in the side reflector, the measured temperature of the reflector nose reduces faster than the calculated value after \( \sim 15 \) hours. Despite of the differences, the temperatures show a similar trend.

Figure 13 illustrates the temperature distributions of the reactor after 50 hours. When compared with Fig. 12 it can be concluded that heat is transferred from the top to the bottom of the core in the beginning of the transient. This phenomenon of temperature rearrangement dominates the behavior of the reactor in this stage of the transient. The process lasts about 30 hours according to the calculation. After this period the heat transfer to the steam generator and RPV determine the shape of the temperature profile of the reactor. The maximum temperature of the core moves from outside-top to the center-middle of the core, which is in accordance with the measurements.

5 Conclusion

In this paper the code system DALTON-THERMIX for modeling coupled neutronics and thermal-hydraulics of High Temperature Reactor was presented. Both the PBMR simulations and a comparison of the calculation results with experimental data of the AVR were satisfactory. The code system will be used in the future for the design and optimization of High Temperature Reactors.

Acknowledgments

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References


