1. Introduction

The computer code DYN3D developed in the Institute of Safety Research is used by research institutions, universities and regulatory bodies in Germany and other European countries for the safety assessment of nuclear reactors. According to the increasing requirements on the safety analysis, the code is undergoing a permanent development with respect to improved physical models and numerical methods. A new version of the code has been released containing an improved nodal expansion method for enhancement of the accuracy of the neutron flux calculation and so-called assembly-wise discontinuity factors for reducing the homogenisation errors. These improvements are of special importance in the case of larger and more heterogeneous fuel assemblies as well as the non-multiplying assemblies describing the radial reflector. The correct calculation of the different components of the external and feedback reactivity according to perturbation theory allows a deeper physical analysis of the feedback mechanisms being important inherent safety features. A special numerical algorithm with significantly reduced numerical diffusion based on the ‘particle-in-cell’ method was implemented for the description of boron transport. An interface has been developed to use the results of computational fluid dynamics (CFD) simulations and the semi-analytical coolant mixing model SAPR [1] for getting realistic boundary conditions for the analysis of boron dilution and overcooling transients. Several libraries of group constants different reactor types with enhanced accuracy were linked to DYN3D. Internal, external and parallel coupling of DYN3D with the system code ATHLET was performed to investigate a wide range of transients with feedback from the coolant system. The version DYN3D-MSR is under development which allows to model molten salt reactors (MSR).

2. DYN3D Model

The computer code DYN3D simulates the reactor core behaviour under steady-state and transient conditions [2]. It was developed for safety analyses of nuclear reactors after reactivity perturbations of the system, but it can be used also for fuel management calculations. The three-dimensional flux and power distributions in the reactor core, subdivided into calculational nodes, are calculated by nodal expansion methods for the solution of the neutron diffusion equation for quadratic or hexagonal fuel assembly geometry. Based on the fission power distribution, the fuel temperature distribution and heat released to the coolant are calculated from the solution of the radial heat conduction equation in fuel and cladding. The one- or two-phase coolant flow is calculated from the balance equations of momentum, mass and energy of the coolant, using the heat released to the coolant as source term. The distribution of the boron absorber in the coolant is ascertained by the solution of the convective boron transport equation. The two group constants homogenized for the core nodes are obtained from the linked neutronic data library for the given burn-up of the fuel and for the calculated state variables as fuel temperature, coolant density, coolant temperature and boron concentration. Burn-up calculations can be performed for the determination of the reactor conditions prior to the considered transient. Besides transients initiated by reactivity perturbations with characteristic times of seconds or minutes, the xenon dynamics can be investigated.
3. Nodal approximations for hexagonal fuel assemblies

The accuracy of the solution of the neutron diffusion equation can be checked by so-called mathematical benchmarks. A mathematical benchmark consists of a reference solution for a defined reactor configuration with given sets of homogenized group constants of nodes. A code solving the neutron diffusion with finite differences is mostly used for the generation of the reference solution. The reference solution is obtained by calculations with mesh sizes $h$ in the order of the diffusion length and smaller. Generally, the reference solution is the result of a calculation with sufficiently small $h$ or by extrapolation for $h$ approaching 0.

Considering the VVER-1000 reactor with the larger fuel assembly pitch of 23.6 cm, the maximum deviation of the original DYN3D neutron kinetics against the reference solution of a mathematical benchmark was in the order of 5% for the nodal powers. The deviations of the DYN3D results were caused by the nodal approximation which was based on the flux separation in radial and axial direction, nodal expansion with Bessel functions, and the coupling of nodes with the help of side averaged partial currents. Two new methods HEXNEM1 and HEXNEM2 were developed for hexagonal-z geometry to improve the accuracy. In the nodes, the transverse integration of the three-dimensional diffusion equation is used to obtain a one-dimensional equation in axial direction and a two-dimensional equation in the hexagonal plane. The two equations are coupled by the transverse leakage. Inside of the nodes, the fluxes are approximated by polynomials up to second order and exponential functions being the solutions of the homogeneous equations. The nodes are coupled by the side averaged partial currents in HEXNEM1. In HEXNEM2, in addition to the side averaged currents the nodes are coupled in the hexagonal plane by the partial currents at the corners. The comparison of the assembly powers of HEXNEM2 with the published reference solution of the AER VVER-1000 benchmark problem [3] can be seen in Fig. 1. Tab. 1 gives the deviation of $k_{\text{eff}}$, the maximum and average deviations of nodal and assembly powers for the previous DYN3D-method, HEXNEM1 and HEXNEM2. The improvement by using the HEXNEM2-method is obvious.

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**Fig. 1:** Comparison of the assembly powers of HEXNEM2 with the reference solution of the AER VVER-1000 benchmark.
Table 1: Deviations of $k_{eff}$, the nodal powers $P_i$ and the assembly powers $P_i^{ax}$ of the DYN3D models from the reference results of the AER VVER-1000 benchmark.

<table>
<thead>
<tr>
<th>Method</th>
<th>$\Delta k_{eff}$</th>
<th>$\max_i \left[ \frac{\Delta P}{P_i} \right]$</th>
<th>$\frac{1}{N_{ref}} \sum_i \left[ \frac{\Delta P}{P_i} \right]$</th>
<th>$\max_i \left[ \frac{\Delta P_i^{ax}}{P_i} \right]$</th>
<th>$\frac{1}{N_{ax}} \sum_i \left[ \frac{\Delta P_i^{ax}}{P_i} \right]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DYN3D</td>
<td>62</td>
<td>5.51</td>
<td>1.83</td>
<td>3.00</td>
<td>1.53</td>
</tr>
<tr>
<td>HEXNEM1</td>
<td>40</td>
<td>3.97</td>
<td>1.30</td>
<td>2.16</td>
<td>1.30</td>
</tr>
<tr>
<td>HEXNEM2</td>
<td>14</td>
<td>2.18</td>
<td>0.60</td>
<td>0.80</td>
<td>0.33</td>
</tr>
</tbody>
</table>

4. Assembly discontinuity factors (ADF)

Starting from the equivalence theory between the neutron diffusion equation of the original heterogeneous node and the homogeneous node the agreement between the node averaged fluxes can be improved by introduction of so-called assembly discontinuity factors (ADF) [4]. The ADF describe the ratio of the averaged fluxes at the node side $i$ of the heterogeneous and homogeneous calculations for each energy group $g$.

$$f_g^i = \frac{\Phi_{g,i}^{het}}{\Phi_{g,i}^{hom}}$$

$f_g^i = 1$ in the case of a homogeneous assembly. The more heterogeneous the assembly is, the more $f_g^i$ deviates from 1. The heterogeneities of an assembly are be caused by inserted absorber rods, different fuel pins in the assembly etc. Large heterogeneities exist in boiling water reactor nodes with inserted control rod (CR) crosses which are located in the water gaps between the fuel assemblies. Half of the water gap or the half of CR plates forming the crosses belong to the nodes. Their neutron group constants are smeared over the whole node in the homogenisation procedure. In the case of inserted CR the heterogeneous flux at the node boundary is lower than the flux of the homogenized node and $f_g^i < 1$ is obtained. By definition, the equations of the full heterogeneous problem have to be solved for the calculation of the ADF. Due to the fact that this is not possible, approximations are applied. For the fuel assemblies, approximate ADF are obtained from cell calculations with symmetrical boundary conditions. The effect of the ADF on the local power distribution in a boiling water reactor (BWR) is shown in Figures 2 and 3 [5]. The axial behaviour of the
3-dim. normalized power and void distributions of a BWR assembly with inserted CR can be seen for DYN3D calculations with and without consideration of ADF. The ADF concept can be also used in the homogenisation procedure of reflector and absorbing assemblies without fuel (VVER-440 control rods). Rather than simulating one assembly in the cell calculation with reflecting boundary conditions, the consideration of larger regions of core improves the results for the ADF [6].

5. Calculation of Dynamic Reactivities

Applying the point kinetic equations for the description of the transient behaviour of the neutrons in the reactor core the reactivity is a key core averaged parameter to understand the response of the reactor power on perturbations of the neutron multiplication. Unfortunately the point model is a too simple model for a large power reactor. A more detailed space-dependent simulation of the reactor core by solving the three-dimensional neutron diffusion equation became possible by the development of powerful computers. The changes of reactor power distributions are the response of the reactor to changes of the cross sections. First of all the eigenvalue of the steady state is calculated which is connected with the static reactivity. A dynamic reactivity during the transient can be introduced by the separation of the flux distribution \( \phi_g(r,t) \) of the neutron energy group \( g \) in an amplitude function \( N(t) \) and a shape function \( \psi_g(r,t) \) [7]:

\[
\Phi_g(r,t) = N(t) \cdot \psi_g(r,t)
\]

The dynamic reactivity \( \rho(t) \) which occurs in the generalized point kinetic equations for the amplitude function can be obtained from the flux distribution and the steady-state adjoint flux \( \Phi^*_g(r,t) \) by the perturbation theory expression:

\[
\rho(t) = \frac{\sum_x \int dV \sum_{g=1}^{g+n} \Phi^n_g(r) \left( \sum_{g'=1}^{g+n} \frac{\chi_{g'}}{k_{eff}} \sum_{g=1}^{g+n} \left( \delta \sum_{g=g'}^{g+n} \phi_g(r,t) - \Phi^*_g(r,t) \right) \Phi^*_g(r,t) \phi_g(r,t) \right)}{\sum_x \int dV \sum_{g=1}^{g+n} \Phi^n_g(r) \left( \sum_{g'=1}^{g+n} \frac{\chi_{g'}}{k_{eff}} \sum_{g=1}^{g+n} \phi_g(r,t) \phi_g^*(r,t) \phi_g(r,t) \phi_g(r,t) \right)}
\]

The changes of the diffusion coefficients \( D^*_g \) and the macroscopic cross sections \( \chi_{g,g'} \), \( \Sigma^n_{g,g'}(t) \) against their initial values occur in the numerator. \( \Sigma^n_{g,g'}(t) \) describes the negative removal cross section for \( g'=g \) and the scattering cross section for \( g\neq g \). \( V_n \) are the volumes of the nodes \( n \). Considering small changes of fuel temperature, moderator density, moderator temperature, boron concentration and control rod (CR) positions the changes of the neutron group constants can be separated by their different origins, i.e. the total change of the group constants is the sum of the changes caused by the single perturbations. The interaction of the effects cannot be neglected for larger perturbations. Fig. 4 shows the dynamic reactivities and the reactor power for the withdrawal of a control rod bank in a VVER-1000.

Fig. 4: Behaviour of nuclear power and the dynamic reactivities \( \rho \) for an assumed withdrawal of a control rod bank in a VVER-1000 reactor.
6. Boron transport

Due to different mechanisms or system failures, slugs of low borated water can accumulate in the primary cooling system of pressurized water reactors. This can happen e.g. as a consequence of a small-break-loss-of-coolant accident, when coolant circulation is interrupted and a slug of almost un-borated condensate will accumulate in the cold leg of the primary circuit. During start-up of coolant natural circulation after refilling the primary circuit with the emergency core cooling system or by switching on the first main coolant pump, this slug will be transported into the reactor core causing a significant reactivity insertion by decreasing the concentration of neutron absorber. The mixing of the unborated condensate with borated water in the reactor pressure vessel is in that case the only mitigative mechanism to prevent severe accident consequences. Realistic boundary conditions at the core inlet, that means, time-dependent boron concentration and temperature fields, will be provided by the mixing models, e.g. SAPR. Besides of mixing in the reactor pressure vessel, the description of boron transport in the core is important for the analysis of the consequences of hypothetical boron dilution events. The calculated distribution of the boron concentration in the reactor core during the transport of the slug through the core can be influenced by the numerical diffusion. Using the standard transport model of DYN3D numerical diffusion occurs, if the Courant criterion

\[
\frac{\Delta z}{\Delta t} = v
\]  

is not fulfilled (\(\Delta z\) - the thickness of axial layers, \(\Delta t\) - the time step, \(v\) - velocity of the coolant). Depending on the fast processes in the core a small time step has to be chosen, but the coolant velocity is too small to satisfy the Courant criterion. By this reason the so-called particle-in-cell (PIC) method is used in DYN3D for a more correct description of boron transport in the core. Each axial node is divided into a large number of layers. The number of boron particles in each layer is connected to the boron concentration in the node. The individual transport of the particles is calculated. Based on the number of particles in the layers the boron concentration of each axial node is calculated. Considering a 36 m³ boron free slug in one loop of a PWR and assuming pump start-up, the boron concentration at inlet and outlet of an arbitrarily fuel element 3 can be seen in Fig. 5. The inlet conditions are based on measurements at the ROCOM test facility. The time behaviour of the boron concentration

![Fig. 5: Boron concentration at inlet and outlet of channel 3 – effect of PIC-model.](image1)

![Fig. 6: Nuclear power – effect of PIC-model.](image2)
at the core outlet obtained from the PIC model is nearly the same as at the core inlet shifted by the transport time through the core. The standard model leads to unrealistic attenuation of the under-boration. This results in different reactivity insertions which are greater than $\beta_{eff}$ in any case. Fig. 6 shows the nuclear power for the two calculations. The first power peak which is limited by the Doppler feedback is nearly the same. Two additional power maximums are observed in the calculation with the PIC model, but not in the standard model. The standard model is not conservative for this type of transient. Safety limits were not exceeded even when applying the PIC model.

7. Coupling DYN3D with ATHLET

DYN3D is coupled with various thermo-hydraulic system codes (ATHLET, RELAP5) using different mathematical approaches (internal, external and parallel coupling). Attention will be focused on the coupling of DYN3D with the system code ATHLET of the Gesellschaft für Anlagen- und Reaktorsicherheit which has been developed at ISR. Besides of coupling with ATHLET, DYN3D has been coupled to the widely used code RELAP5 within scientific-technical co-operation projects with IPPE Obninsk and VUJE Trnava in an internal and a parallel manner. A wide range of transients and accidents for pressurized and boiling water reactors can be simulated by the different types of coupling. The schemes of the coupling types concerning ATHLET are shown in Fig. 7.

Depending on the considered transient a special type of coupling is preferred. If reverse flow occurs in the core e.g. during a LOCA, the internal coupling should be applied, because it cannot described by the thermal hydraulic model of DYN3D. If a large number of fuel assemblies has to be simulated in a boiling water reactor, the parallel coupling should be used by reasons of stability of calculation. Considering a larger number of fuel assemblies of a pressurized water reactor computer runs with external coupling need lower CPU-time, caused

![Diagram of DYN3D/ATHLET coupling schemes]

Fig. 7: Coupling schemes of DYN3D/ATHLET.
by the faster convergence of the thermal hydraulic model of DYN3D. There are also transients with no preference of any type of coupling. The results of all three types should be nearly the same. As an example the VVER-1000 Balakovo-4 operational transient “Switching-off of one from two working steam generator feed water pumps” was analysed by the different DYN3D/ATHLET couplings. Fig. 8 compares the nuclear power when using the three types of coupling. The thermal hydraulic models and the fuel rod models of ATHLET and DYN3D are different. In spite of this, the agreement was obtained by equal values for heat conductivity, heat capacity and gas gap conductance for fuel and cladding and the equal steady-state mass flow rates without any further tuning of models.

8. DYN3D-MSR for molten salt reactors

The nodal expansion method and the thermal-hydraulic (TH) model of the DYN3D code[2] was used as the base of a numerical code for dynamics studies of Molten Salt Reactors (MSR) which is one of the 'Generation IV' concepts. The graphite-moderated channel type MSR was selected for the numerical simulation as a representative of the reactors with liquid fuel. The DYN3D-MSR version [8] of code represents a stand-alone code and includes new routines for modelling of the liquid fuel reactor of MSR type. Two main modifications are made in the code. The model of delayed neutrons (DN) precursors includes the solution of the precursors equation with convective term. The distribution of DN is determined in the whole primary circuit. Furthermore, the heat release in the MSR is contrariwise to the classical PWRs. The energy from fission is predominantly released directly to the liquid fuel and the surrounding solid graphite is heated only with the gamma and neutrons radiation. However, the presence of heat sources in the graphite, even though they are small, causes the temperature to be higher as in the fuel which is practically cooling the graphite.

The data measured in the sixties during the Molten Salt Reactor Experiment (MSRE) in the Oak Ridge National Laboratory [9] were used to validate the MSR kinetics in 1D approach, especially the delayed neutrons model. MSRE was a 10 MWth thermal reactor with liquid
Fig. 9: Compensative reactivity inserted by control rods during the fuel pump start-up (left) and coast-down (right) transients.

molten salt fuel, moderated by graphite. It was constructed for the verification of MSR technology. The results for the zero power fuel pump start-up and the coast-down transients used to validate the code are shown in Fig. 9. In the two cases, the reactivity is changed to maintain a constant power level. Original ORNL DN data and calculated JEF DN data were used. The difference between the results is given by the different steady state loss of DN for each data set. The development of DYN3D-MSR is presently almost completed, however further extensions of the code are practicable. Because the decay of DN precursors in the fuel outside the reactor is important for the kinetics, the code should be completed by a fuel circuit model.

9. Conclusions and Outlook

Based on the improvements of the DYN3D models and on the coupling with the system codes ATHLET and RELAP5 a wide range of transients and accidents in PWR, BWR and VVER reactors can be simulated. The code version DYN3D-MSR can be used for the analysis of transients in molten salt reactors as a perspective reactor concept. Due to the extended capabilities of the code, the available developments, the validation status, and the support provided by the DYN3D development team, the code is used by research institutions and technical expert organizations in Germany and abroad, like:

- Energoproject – Nuclear Research Institute, Řež (Czech Republic)
- Scientific-Technological Centre of the NRC of Ukraine, Kiev (Ukraine)
- Institute of Physics and Power Engineering, Obninsk (Russia)
- VUJE Trnava (Slovak Republic)
- Technical University Budapest (Hungary)
- Institute of Nuclear Research and Nuclear Energy, Sofia (Bulgaria)
- ENPRO Sofia (Bulgaria)
- RWTH Aachen University (Germany)
- FRAMATOME-ANP, Erlangen (Germany)
- TÜV-Süd, München (Germany)

Several developments, validations and applications were performed in close cooperation with some of these institutions. The wide-spread use of DYN3D for VVER reactor safety analysis lead to the decision to integrate the code into the European code platform being elaborated within the European Integrated Project NURESIM coordinated by the French CEA.
References


