FORSCHUNGSZENTRUM ROSSENDORF FZR

WISSENSCHAFTLICH-TECHNISCHE BERICHTE
FZR-248
Januar 1999
ISSN 1437-322X

Ulrich Grundmann, Siegfried Mittag, Ulrich Rohde

The 3-Dimensional Core Model DYN3D

Herausgeber:
FORSCHUNGSZENTRUM ROSSENDORF
Postfach 51 01 19
D-01314 Dresden
Telefon +49 351 26 00
Telefax +49 351 2 69 04 61
http://www.fz-rossendorf.de/

Als Manuskript gedruckt

FORSCHUNGSZENTRUM ROSSENDORF

WISSENSCHAFTLICH-TECHNISCHE BERICHTE

FZR-248

Januar 1999

Ulrich Grundmann, Siegfried Mittag, Ulrich Rohde

E-mail:
U.Grundmann@fz-rossendorf.de
S.Mittag@fz-rossendorf.de
U.Rohde@fz-rossendorf.de

The 3-Dimensional Core Model DYN3D

Obninsk 98' Information Exchange Forum on Safety Analysis for NPP's

Obninsk, October 26 - 30, 1998

Abstract

Analyzing the safety margins in transients and accidents of nuclear reactors 3-dimensional models of the core were used to avoid conservative assumptions needed for point kinetics or 1-dimensional models. Therefore the 3D code DYN3D has been developed for the analysis of reactivity initiated accidents (RIA) in thermal nuclear reactors. The power distributions are calculated with the help of nodal expansion methods (NEM) for hexagonal and Cartesian geometry. The fuel rod model and the thermohydraulic part provide fuel temperatures, coolant temperatures and densities as well as boron concentrations for the calculation of feedback effects on the basis of cross section libraries generated by cell codes. Safety relevant parameters like maximum fuel and cladding temperatures, critical heat flux and degree of cladding oxidation are estimated.

DYN3D can analyze RIA initiated by moved control rods and/or perturbations of the coolant flow. Stationary and transient boundary conditions for the coolant flow, the core inlet temperatures and boron concentrations at the core inlet have to be given. For analyzing more complex transients the code DYN3D is coupled with the plant model ATHLET of the GRS. The extensive validation work accomplished for DYN3D is presented in several examples. Some applications of the code are described.

Kurzfassung

Die Verwendung 3-dimensionaler Kernmodelle zur Untersuchung der Sicherheitsreserven bei Übergangsprozessen und Störfällen in Kernreaktoren vermeidet konservative Annahmen, die bei der Benutzung des Punktmodells oder 1-dimensionaler Modelle erforderlich sind. Aus diesen Gründen wurde das 3-dimensionale Rechenprogramm DYN3D für die Untersuchung von Reaktivitätsstörfällen in thermischen Reaktoren entwickelt. Die Leistungsverteilung wird mit nodalen Methoden für hexagonale oder kartesische Geometrie berechnet. Das Brennstabmodell und der thermohydraulische Teil von DYN3D liefert die Brennstofftemperaturen, Kühlmitteltemperaturen, - dichten und Borkonzentrationen zur Berücksichtigung der Rückkopplung auf der Grundlage von Wirkungsquerschnittsbibliotheken, die mit Hilfe von Zellcodes erstellt wurden. Es werden sicherheitsrelevante Parameter wie maximale Brennstoff- und Hüllrohrtemperaturen, kritische Wärmestromdichten und Hüllrohroxidschichtdicke berechnet.

DYN3D kann Reaktivitätsstörfälle untersuchen, die durch Bewegungen der Regelstäbe oder Störungen der Kühlmittelströmung hervorgerufen werden. Die stationären und zeitabhängigen Randbedingungen für die Kühlmittelströmung, die Kühlmitteleintrittstemperaturen und Borkonzentrationen müssen am Kerneintritt vorgegeben werden. Zur Untersuchung komplexer Störfälle wurde DYN3D mit dem thermohydraulischen Anlagenmodell ATHLET der GRS gekoppelt. Die umfangreichen Arbeiten zur Verifizierung und Validierung von DYN3D werden an Beispielen beschrieben. Einige Anwendungen des Rechenprogramms werden dargestellt.

The 3-Dimensional Core Model DYN3D

U. Grundmann, S. Mittag and U. Rohde
FZ Rossendorf
Institute of Safety Research

1. Introduction

Analyzing the safety margins in transients and accidents of nuclear reactors 3-dimensional models of the core were used to avoid conservative assumptions needed for point kinetics or 1-dimensional models. Therefore the 3D code DYN3D has been developed for the analysis of reactivity initiated accidents (RIA) in thermal nuclear reactors [1]. The power distributions are calculated with the help of nodal expansion methods (NEM) for hexagonal and Cartesian geometry which is shortly described in section 2.1. Section 2.2 gives a description of the fuel rod model and the thermohydraulic part providing fuel temperatures, coolant temperatures and densities as well as boron concentrations for the calculation of feedback effects on the basis of cross section libraries generated by cell codes.

DYN3D can analyze RIA initiated by moved control rods and/or perturbations of the coolant flow. Stationary and transient boundary conditions for the coolant flow, the core inlet temperatures and boron concentrations for each fuel assembly have to be given. For analyzing more complex transients the code DYN3D is coupled with the plant model ATHLET of the GRS. The two different types of coupling realized are described in section 2.3 Some examples of the extensive validation work for the hexagonal version are described in chapter 3. Chapter 4 presents results of the Cartesian version compared with benchmarks. The validation of the fuel rod and heat transfer model is described in chapter 5. Some examples of application of the code are shown in chapter 6. Chapter 7 gives an short overview of the present and future activities concerning the code DYN3D.

2. The Models of DYN3D

Fig. 1 shows an overview of the models used in the code. The models are described in the following sections.

2.1 Neutron Kinetic Model

The core model DYN3D was firstly developed for VVER-type reactors with hexagonal fuel assemblies required for safety assessment of the operating VVER-440 reactors at the nuclear power station near Greifswald. The 3D neutron kinetic model is based on the solution of the 3-dimensional 2-group neutron diffusion equation by a nodal expansion method which is specific for the geometry of fuel assemblies [2]. It is assumed that the macroscopic cross sections are spatially constant in a node

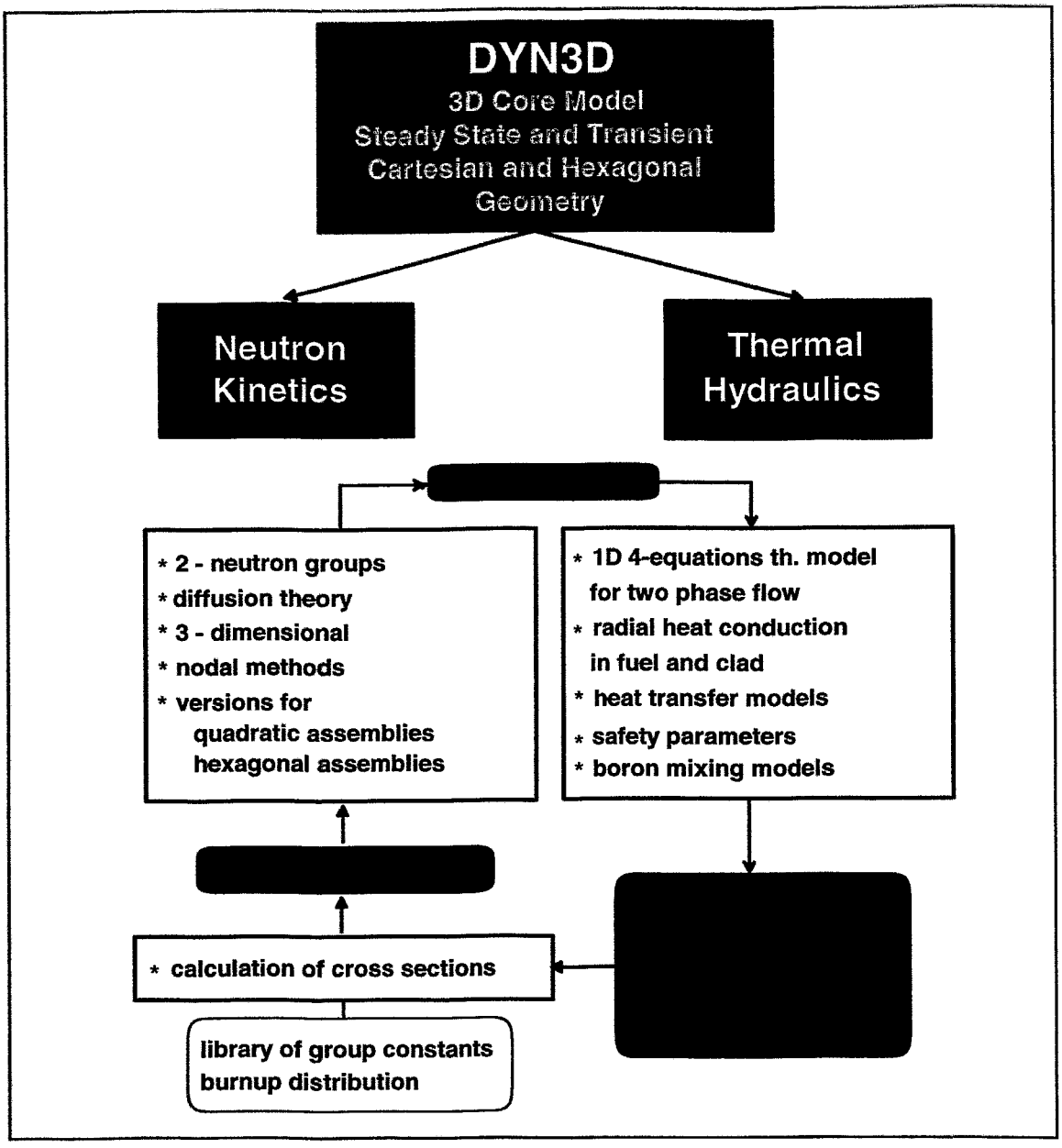

Fig. 1: Scheme of the code DYN3D

being a part of the hexagonal fuel assembly. The stationary diffusion equation in the node is solved by factorizing the space dependency of neutron fluxes in the radial plane and the axial direction. A 2-dimensional diffusion equation in the radial plane and a 1-dimensional equation in axial direction are obtained. The two equations are coupled by the transversal bucklings. In the hexagonal plane the fluxes are expanded by using Bessel functions being the solutions of the Helmholtz equation. The low order coefficients are expressed by the node averaged fluxes and the incoming partial currents averaged over the interface of the hexagon. In this way, the

outgoing partial currents at the interfaces are given by the node fluxes and the incoming partial currents. The matrix elements of these relations depend on the tranversal buckling and the eigenvalue k_{eff}. The 1-dimensional equation in axial direction is solved by a polynomial expansion up to the fourth order. The outgoing partial currents in axial direction are given by the averaged fluxes, incoming partial currents and higher order coefficients. The equations for the 3rd and 4th order polynomials are obtained by Galerkin weighting. The outgoing partial currents at a node interface are the incoming currents in the neighbouring nodes. The steady state diffusion equation is solved by an inner and outer iteration process. The outer iterations are the fission source iterations accelerated by a Chebychev extrapolation scheme. A small number of inner iterations (3 - 5) are sufficient for the convergency. During the outer iteration process the matrix elements are recalculated few times (3-5).

In the case of Cartesian geometry, the 3-dimensional diffusion equation of each node is transformed into 1-dimensional equations in each direction x,y,z by transversal integrations [3]. This method is applied in many nodal techniques published in literature [4,5]. The equations are coupled by the transversal leakage term. The 1-dimensional equations are solved with the help of flux expansions in polynomials up to 2nd order and exponential functions being the solutions of the homogeneous equation. The fission source in the fast group and the scattering source in the thermal group as well as the leakage terms are approximated by the polynomials. The outgoing partial currents are expressed by the incoming partial currents and the polynomial coefficients of the flux expansion. The iteration technique is similar to that applied for the hexagonal geometry.

Concerning the time integration over the neutronic time step an implicite difference scheme with exponential transformation is used. The exponents in each node are calculated from the previous time step or during the iteration process. For the calculation of matrix elements describing the relation between partial currents and averaged fluxes it is assumed that the time behaviour of the neutron fluxes in the nodes is exponential and the local variation of the source of delayed neutrons is proportional to the source of prompt neutrons. These assumptions allow the same treatment of diffusion equation in the nodes as in the steady state. In the iteration process we have to solve an inhomogeneous problem. Similar methods as used for the steady state are applied.

If a transient at a given time within the burnup cycle has to be investigated, a cross section library for this state is required. In order to enable DYN3D users to independently calculate three-dimensional burnup distributions for all possible states occuring during a reactor cycle, a burnup version of the code has been developed. Essentially, the extension of DYN3D to a burnup version is done by putting a burnup loop around the stationary kernel of the code. Starting point of the loop is a given material and burnup distribution reflecting the reactor core operational history which may include previous fuel cycles. For the given state, the code firstly generates the actual burnup-specific nodal group data using a macroscopic neutron group data library. The following steady-state iteration includes temperature feedback as well as the calculation of the critical boron acid concentration. The resulting stationary nodal

power densities are assumed to be constant for a certain time interval, in which the nodal burnup values increase only little, compared to their increase during a whole reactor cycle. For the actual burnup time-step interval, DYN3D calculates a burnup growth which is used to generate the nodal group data for the next step.

In this way the burnup calculation proceeds by quasi-stationary time steps until the end of cycle or the interesting burnup state is reached, which then can be studied by dynamic DYN3D calculations. During the whole operation period of a reactor, the material distribution within the core is often modified, for example by changing the positions of partially burnt-out fuel elements, by putting in new ones, and also by control rod movements. All these manipulations as well as changes in total power, coolant inlet temperature and mass flow are modelled.

2.2 The Thermohydraulic Model of DYN3D

The thermohydraulic model of the reactor core and the fuel rod model are implemented in the module FLOCAL [6] being a part of DYN3D. The reactor core is modelled by parallel cooling channels which can describe one or more fuel elements. The parallel channels are coupled hydraulically by the condition of equal pressure drop over all core channels. Additionally, so- called hot channels can be considered for the investigation of hot spots and uncertainties in power density, coolant temperature or mass flow rate. Thermohydraulic boundary conditions for the core like coolant inlet temperature, pressure, coolant mass flow rate or pressure drop must be given as input for DYN3D. Applying the coupled DYN3D - ATHLET code they are provided by the ATHLET code.

Mixing of coolant from different loops before entering the core can be modelled by applying several options. Homogeneous mixing can be assumed for each reactor type and number of loops. For VVER-440 type reactors, an analytical mixing model for the downcomer and the lower plenum is implemented in the code. The model is based on the analytical solution of the Navier-Stokes equations in the potential flow approximation in three-dimensional cylindrical geometry and the diffusion equation for heat transport or soluble poison. Turbulent Peclet numbers for the downcomer and the lower plenum are parameters of the model, which are used for a best fit adaptation to experimental results. The mixing model represents an interface between the cold legs of the primary loop and the core inlet.

The module FLOCAL comprises

- a one- or two-phase coolant flow model on the basis of four differential balance equations for mass, energy and momentum of the two-phase mixture and the mass balance for the vapour phase allowing the description of thermodynamic non-equilibrium between the phases,

- a heat transfer regime map from one-phase liquid up to post-critical heat transfer regimes and superheated steam,

- a fuel rod model for the calculation of fuel and cladding temperatures and the determination of some parameters for fuel rod failure estimation.

The two-phase flow model is closed by constitutive laws for heat mass and momentum transfer, e.g. vapour generation at the heated walls, condensation in the subcooled liquid, phase slip ratio, pressure drop at single flow resistance's and due to friction along the flow channels as well as heat transfer correlations. Different packages of water and steam thermophysical properties presentation can be used [6].

The heat transfer regime map which is implemented in FLOCAL ranges from one-phase liquid convection up to superheated steam. The occurrence of heat transfer crisis is stated by different correlation's for the critical heat flux. The transient boiling region is described by the KIRCHNER and GRIFFITH interpolation for the heat flux. In the stable post-crisis region for inverted annular or dispersed flow the GROENEVELD - DELORME or a modified BROMLEY correlation's are used. After full evaporation of coolant, heat transfer to superheated steam is estimated by a forced convection correlation [6].

Special emphasis is put on adopting the model to the conditions of RIA accidents where a combination of high heat fluxes with high degree of coolant subcooling is typical and thermodynamic non-equilibrium effects are important. A correlation for the Leidenfrost or minimum stable film boiling point T_{MSFB} takes into account the influence of fluid subcooling. In the post-crisis region, a special non-equilibrium correction to the heat transfer coefficient due to subcooled liquid is used, too.

For the estimation of fuel and cladding temperatures the heat conduction equation in one-dimensional radial geometry is solved. In the gas gap between fuel and cladding the heat transfer components due to conduction in the gas, radiation and fuel-cladding contact are considered. The modelling of these heat transfer components is similar as in typical fuel rod behaviour codes i.e. GAPCON-THERMAL. The idea of the model is that the parameters for the stationary reference state (geometrical gap width , gas pressure and composition) are given and have to be obtained from detailed fuel rod behaviour codes. The changes during the instationary process are estimated by the model.

A thermomechanical model of the fuel and cladding behaviour is implemented into the code. The aim of this model is the estimation of gas gap conductance behaviour for a realistic temperature calculation. This is important again especially for RIA calculations. The thermomechanical model is based on following assumptions:

- one-dimensional modelling of mechanics in radial direction,

- simple superposition of radial thermal, elastic and plastic deformations without axial coupling,

- elastic deformation of the fuel is only taken into account in the case of fuel-cladding contact, plastic deformations of the fuel are not considered,

- cladding is described in the thin shell approximation.

A deterministic model of fuel rod failure during accidents is not included in FLOCAL , but some parameters for the diagnostic of possible fuel rod failure are given, that is:

- fuel enthalpy for each axial node of the rod,

- cladding oxide thickness,

- signalization of possible cladding rupture, when the cladding stress is positive (inner pressure is larger than outer pressure) and exceeds the yield point.

For testing and validation of the fuel rod and heat transfer model in the code FLOCAL experiments on fuel rod behaviour under RIA conditions were calculated. These investigations demonstrated the relevance of detailed gas gap modelling and heat transfer estimation under high subcooling conditions [7,8].

2.3 Coupling of ATHLET and DYN3D

For analyzing more complex transients where the coolant flow conditions are influenced by the core behaviour DYN3D was coupled with the ATHLET code. The code ATHLET has been developed by the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS). An overview on the capabilities of ATHLET is given in [9]. It can be applied to the whole spectrum of operational and accident transients, small and intermediate leaks up to large breaks of coolant loops or steam lines at PWRs and BWRs. The code includes basic modules for thermohydraulics, heat transfer and heat conduction, neutron kinetics (point kinetics and 1D neutron kinetics) and balance of plant simulation. Within the General Control and Simulation Module (GCSM) a general interface is available, that allows to couple other independent modules to ATHLET without changes of the code architecture. The fluiddynamics is described by a five-equation model, with separate conservation equations for liquid and vapour mass and energy, and a mixture momentum equation, accounting for thermal and mechanical non-equilibrium, and including a mixture level tracking capability. Recently, a six equations version is available. In the code the 1D thermohydraulics is used.

In accomplishing the coupling of ATHLET and DYN3D two basically different ways were pursued [10, 11, 12]. The first one uses only the neutron kinetic part of DYN3D and integrates it into the heat transfer and heat conduction model of ATHLET. This is a very close coupling, the data have to be exchanged between all core nodes of the single models (internal coupling). For this reason a great number of data have to be transferred. This version demands extensive additional programming.

In the second way of coupling the whole core is cut out of the ATHLET plant model (external coupling). The core is completely modelled by DYN3D. The thermohydraulics is split into two parts: the FLOCAL model of DYN3D describes the thermohydraulics of the core, the ATHLET code models the coolant system. As a consequence of this local cut it is easy to define the interfaces. They are located at the bottom and at the top of the core. The pressures, mass flow rates, enthalpies and concentrations of boron acid at these interfaces have to be transferred. So the external coupling needs only a few parameters to be exchanged between the codes and is therefore easy to be implemented. It is effectively supported by the above mentioned GCSM of the ATHLET code. For this reason almost no changes of the single programs are necessary and the two codes can be developed independently. This is an important advantage of the external coupling.

Depending on the application each of the two versions of coupling has its advantages and disadvantages:

Internal coupling:

- solution of the thermohydraulic equation system in the ATHLET code
- description of reverse flow is possible
- mixture levels in the core can be described
- longer CPU times by using a larger number of coolant channels in the core

External coupling:

- whole core simulation with a large number of coolant channels possible
- integration of mixing models
- more detailed fuel rod model of DYN3D available
- no reverse flow in the core
- no mixture level in the core

3. Validation of the Hexagonal Version of DYN3D

Comprehensive validation work for the two versions of the code DYN3D/H and DYN3D/R has been accomplished. DYN3D has been verified by comparisons of results with experimental data and by benchmarks. As there are no experiments available for accident scenarios, the comparisons with other codes and benchmarking are important steps of code validation.

The steady state calculation of the hexagonal version was compared with benchmarks. The neutron kinetics was validated in cooperation with the Czech Nuclear Research Institute (NRI) by kinetic experiments at the LR-0 zero power reactor. Comparisons with different codes for hexagonal fuel assemblies were carried out in the frame of Working Group D "VVER Safety Analysis" of the Atomic Energy Research (AER) association, a forum for co-operation in the field of VVER reactor physics research. The burnup option of DYN3D has also been validated by calculating several burnup cycles and control rod worths in the corresponding burnup states of a Hungarian VVER 440 and by comparisons between calculated and measured reactivity coefficients and critical boron concentrations from NPP's Zaporoshye, Dukovany and Greifswald.

Some examples of the validation work can be shown will be shown in the following.

3.1 Steady State Benchmark for VVER-440

The so-called Seidel Benchmark was created for the verification of the steady state flux calculation in a VVER-440. In the last years two benchmark solutions were constructed by using the DIF3D code [13,14]. The two group cross sections for the different types of fuel, absorber and reflector in a fresh core of a VVER-440 are given. The bank with the regulating rods is half inserted in the reactor. Comparisons of the two reference solutions give differences with can be neglected. Fig. 2 shows the comparison of the DYN3D assembly powers with the values of reference [14].

One can see in fig. 2 that the deviation of the eigenvalue k_{eff} is 40 pcm and the maximum deviation of assembly powers is 1.13%. Considering the nodal powers P_i which are not shown here the maximum deviation is $\Delta P/P=2.75\%$.The achieved accuracy of the 3D calcuation is sufficient for analyses of the reactor VVER-440. The diameter of the fuel assemblies at the VVER-440 is 14.7 cm. It is assumed that the deviations are higher for the VVER-1000 with the assembly diameter of 23.6 cm.

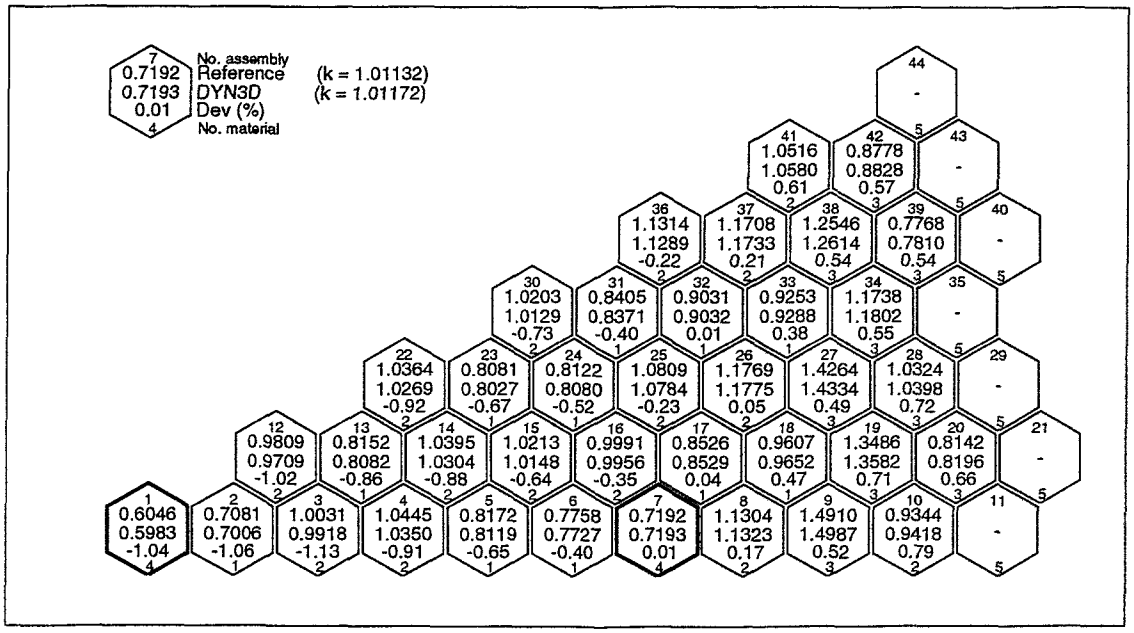

Fig. 2: Seidel Benchmark for VVER-440: Comaparison of eigenvalue k_{eff} and the normalized assembly powers with the reference solution

3.2 Calculations to the LR-0 Kinetic Experiments

Kinetic experiments at the LR-0 reactor of the NRI in Rez consisting of VVER-1000 assemblies with the shorter length of 125 cm were carried out for the code validation [15]. A control rod were moved down and back to its original position or were inserted in the core. Two types of core configuration with 31 and 55 fuel assemblies were used in three stages of experiments. Micro fission chambers were situated in the central tubes in different axial positions of several assemblies. The stability of the detectors was not sufficient for the comparison of steady state distributions, but relative detector rates $R_i(t)/R_i(0)$ sampled by a series of identical experiments show a time behaviour which can be used for the validation of the code.

Fig. 3 shows the comparison of calculation and measurement for 3 detector positions for an experiment where a peripheral rod was moved down in 8.4 s over a distance of 24 cm. After staying at this position for 11.6 s the control rod was shifted to its original position. The lower curve in fig. 3 represent the comparison for the detector in the fuel assembly with the moved cluster rod. Here the detector became surrounded during the insertion of the rod by the absorber fingers which cause a local depression of the flux at the detector position. It is not exactly described by the homogeneous cross sections used in the nodal calculation. Therefore a linear correction of the nodal results with the help of fine mesh calculations was carried out. The node averaged flux was used for the comparisons with the measurement at the other detector positions. The DYN3D calculations for the rest of the measurements show similar agreement [16].

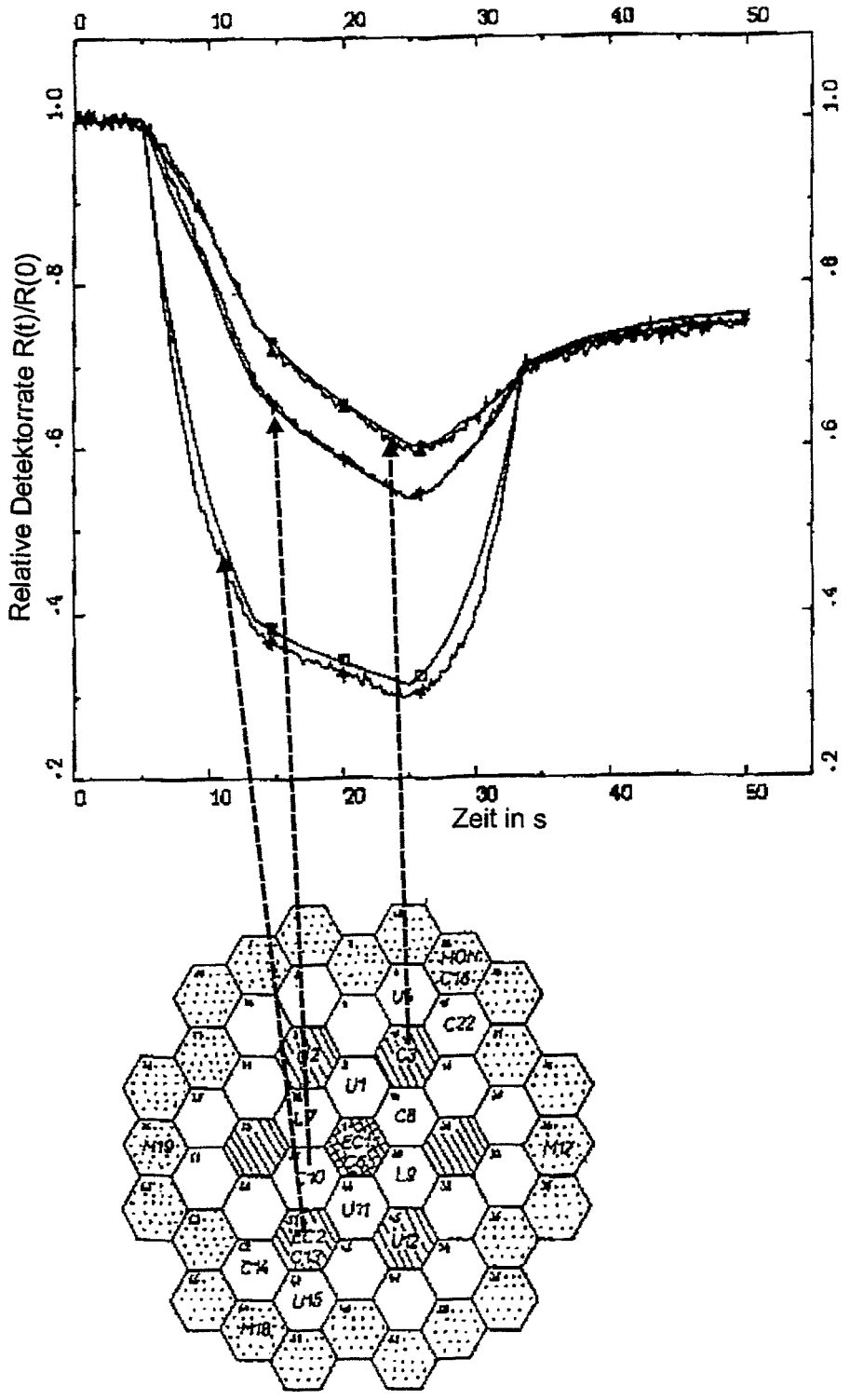

Fig. 3: Kinetic experiment at the reactor LR-0: Comparisons between relative detector rates at 3 positions and the results of DYN3D calculation

3.3 Third AER Benchmark on control rod ejection in a VVER-440

The results of different codes for rod ejections in a VVER-440 were compared in the frame of Working Group D "VVER Safety Analysis" of the Atomic Energy Research (AER) association [17]. The first two comparisons of the implemented neutronic models were based on given cross sections data. The ejection of a peripheral rod of the bank K6 in a VVER-440 with successive scram was considered in the first benchmark. The second problem was similar to the first one, but the ejected control rod worth was 2β (β is the part of delayed neutrons) which results in a sharp and high power peak connected with large deformations of flux. The Doppler effect as the main feedback effect for this type of transients was considered as the only feedback.

It was concluded from the second benchmark that the differences in total power release and maximum fuel temperature are mainly caused by the different models for the description of the black absorbers in the codes. Therefore the cross sections and the rod worth were given in the 3rd benchmark for comparing the models of coolant flow and fuel rod on the basis of given thermophysical properties. The super prompt critical power excursion starting from hot zero power leads to a strong increase of maximum fuel temperatures. Results of five different research institutes calculated with four different code systems were compared:

- KFKI AEKI Budapest (KIKO3D)
- NRI Rez (DYN3D)
- RC Rossendorf (DYN3D)
- RRC Kurtchatov Institute, Moscow (BIPR8-ATHLET)
- VVT Energy, Helsinki (HEXTRAN)

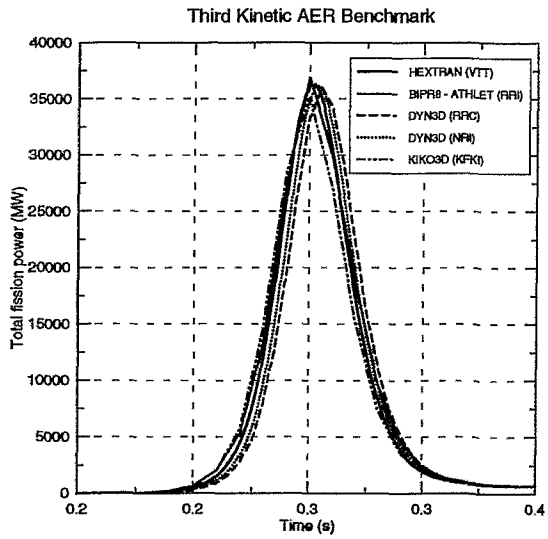

Fig. 4: Comparison of power peak

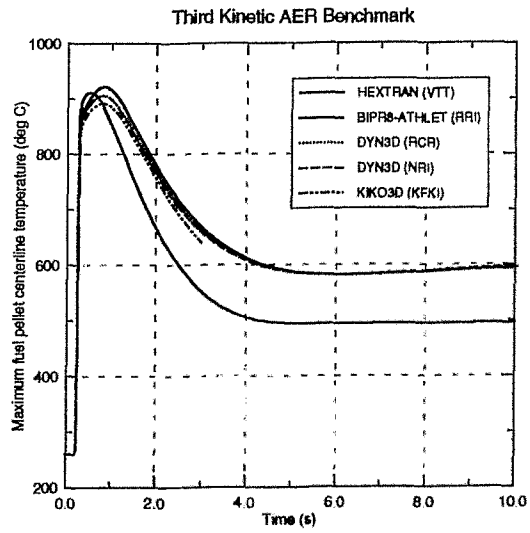

Fig. 5: Comparison of maximum fuel pellet centerline temperature

Fig. 4 shows the comparisons of power peaks which is very sensitive in such benchmarks. The results for the behaviour of maximum fuel pellet centerline temperatures is seen in Fig. 5. It shows a good agreement in the range of temperature increase. A possible explanation of the deviations of BIPR8-ATHLET results after the temperature maximum might be the different heat transfer model selected for this application in the ATHLET code.

3.4 Validation of the burnup version

The burnup version was validated by calculating several fuel cycles of Paks unit 2 (Hungary)[18]. A starting burnup distribution was given for the end of the 3rd cycle of the Paks VVER-440. Starting from this point, the burnup progress had to be calcu-

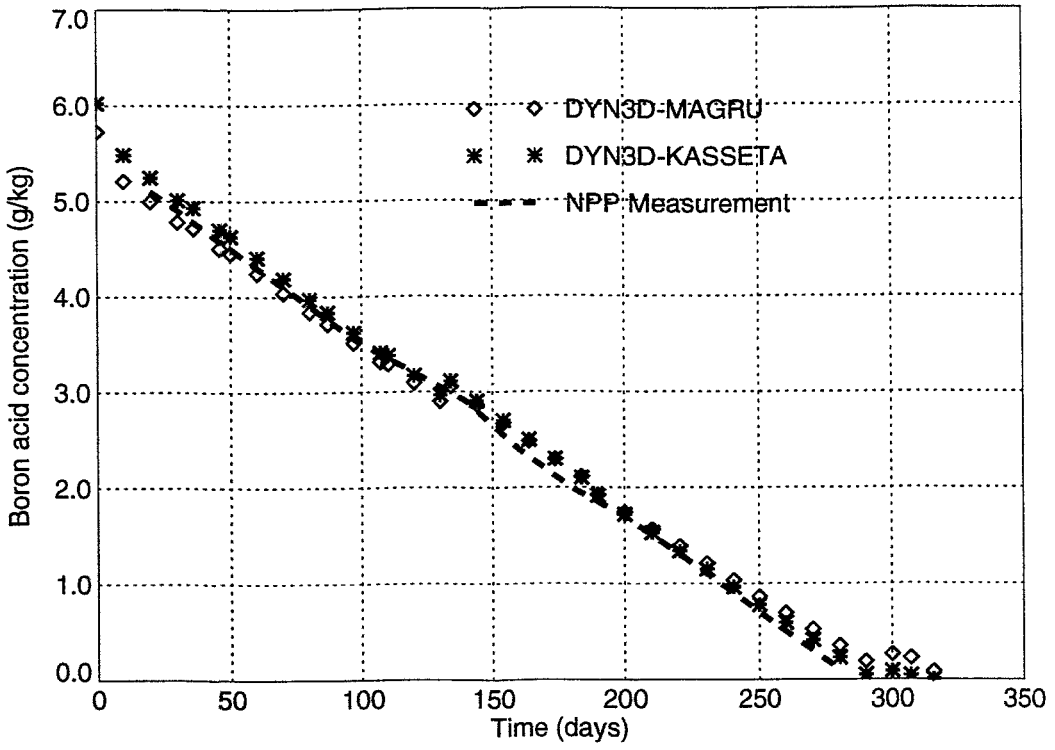

Fig. 6: Critical boron acid concentration during cycle 5, Paks-2.

lated through the cycles 4 to 7 using the corresponding shuffle schemes (reloading of fuel elements) and operational histories provided by the utility.

Fig. 6 shows an example of a boron let-down over one of the cycles modelled. The DYN3D calculations were carried out by using two different neutron group data libraries: MAGRU-440 [19] and KASSETA-440 [20]. Both calculations show a good agreement to the values measured in the Paks utility [21]. The burnup distribution obtained

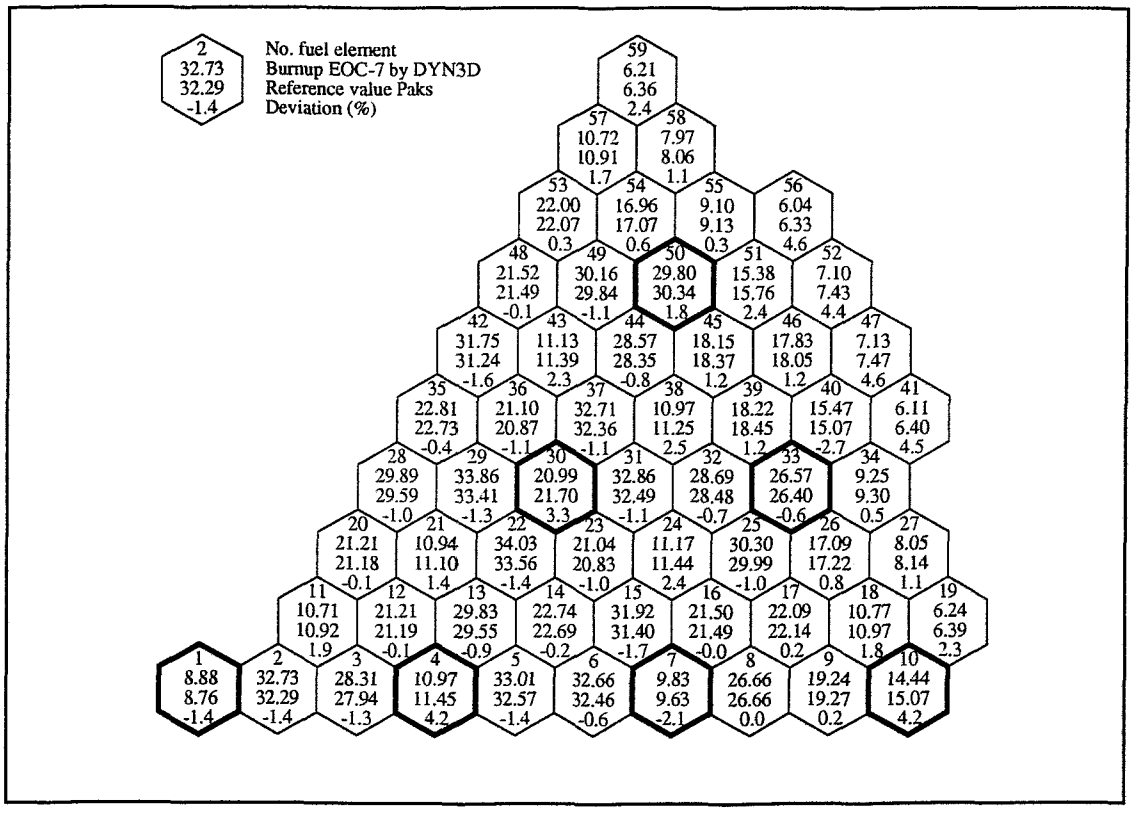

Fig. 7: Burnup distribution of Paks-2, end of cycle 7.

by DYN3D for the end of cycle 7 was compared with reference results provided by Paks NPP [22]. The maximum relative deviations in burnup are less then 5 %, absolute differences are not greater then some 0.5 MWd/kgU. Fig. 7 shows the comparison of fuel element burnup values at the end of the cycle for a 60-degree symmetry sector of the core. The greatest relative deviations are observed at the core boundaries, which may be caused by different boundary treatment in DYN3D and the burnup code used in Paks.

4. Validation of the Cartesian Version of DYN3D

The version for Cartesian geometry was compared with the 3D IAEA benchmark (steady state), the NEACRP benchmarks for control rod ejections in a standard PWR and the NEA-NSC Benchmark on Uncontrolled Withdrawal of Control Rods at Zero Power.

4.1 Three-Dimensional IAEA Benchmark

Calculations for the 3D steady state IAEA benchmark [23] were carried out. The DYN3DR eigenvalue and assembly powers compared with the reference values are shown in Fig. 8. The deviation of the eigenvalue k_{eff} is 3 pcm and the maximum deviation of assembly powers is 1.4 % in assembly no. 35 near to the reflector.

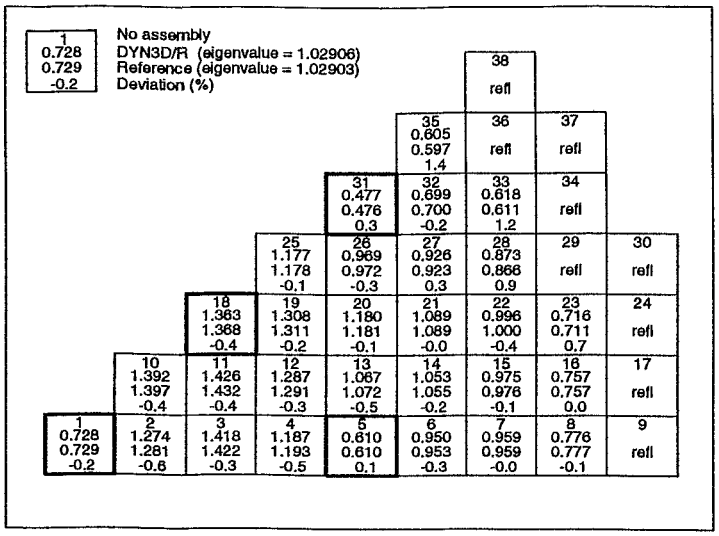

Fig. 8: 3D IAEA Benchmark: Comparison of DYN3D/R results with the refence

4.2 NEACRP PWR Benchmarks on Rod Ejections

The PWR rod ejection problems [24, 25] at hot zero power (HZP) and full power (FP) were calculated by DYN3DR and the obtained results were compared with the published reference solutions. The six problems are ejection of the central rod at HZP and full power (A1 and A2), ejection of a peripheral rod in octant geometry at HZP and FP (B1 and B2) and ejection of one peripheral rod at

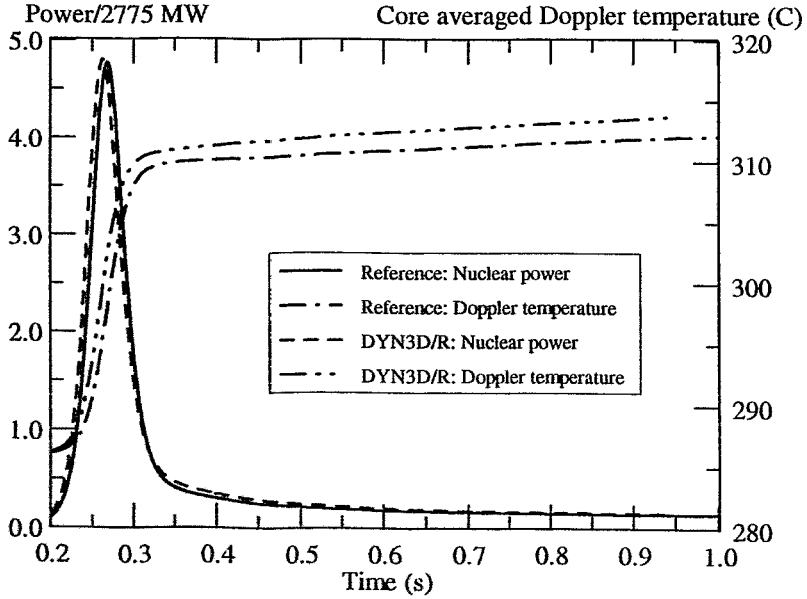

Fig. 9: NEACRP Benchmark C1: Comparison of DYN3D/R results with reference solutions

HZP and FP (C1 and C2). The nominal power of the reactor is 2775 MW. In all cases the ejection time of rods is 0.1 s. The transient was calculated until t = 5.0 s. The comparison of power and core averaged Doppler temperature for problem C1, which is one of the most interesting cases, can be seen in Fig. 9. The reference solution was generated by the PANTHER code using 4 nodes per assembly in one layer. A good agreement of the DYN3DR results with the reference solutions was obtained for all six cases.

4.3 NEA-NSC Benchmark: Withdrawal of Control Rods

Transients initiated by an uncontrolled withdrawal of control rods at HZP were defined for the reference PWR considered in the previous benchmarks [26]. The DYN3D results were compared with the reference solutions [27] in [28]. Some results are presented for the case D describing the withdrawal of banks A and B. The banks C and D are fully inserted and bank S is withdrawn at the initial state. Fig. 10 shows the an octant of core configuration which is symmetrical. All rods begin to fall 0.6 s after fission power reached 35% of nominal power. The critical boron concentration of DYN3D/R is 796.11 ppm. The deviation to the reference

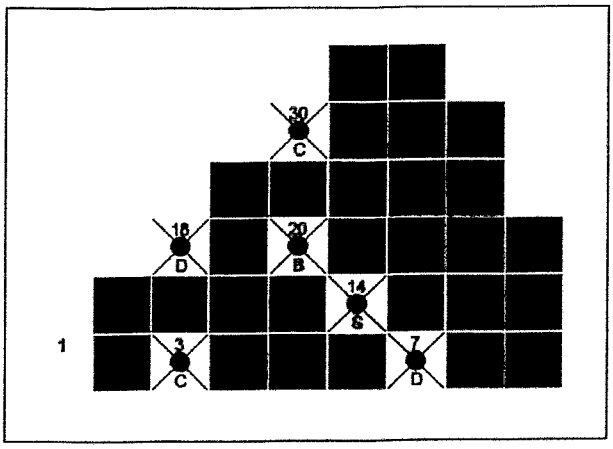

Fig.10: NEA-NSC Benchmark: Core configuration with control rod positions.

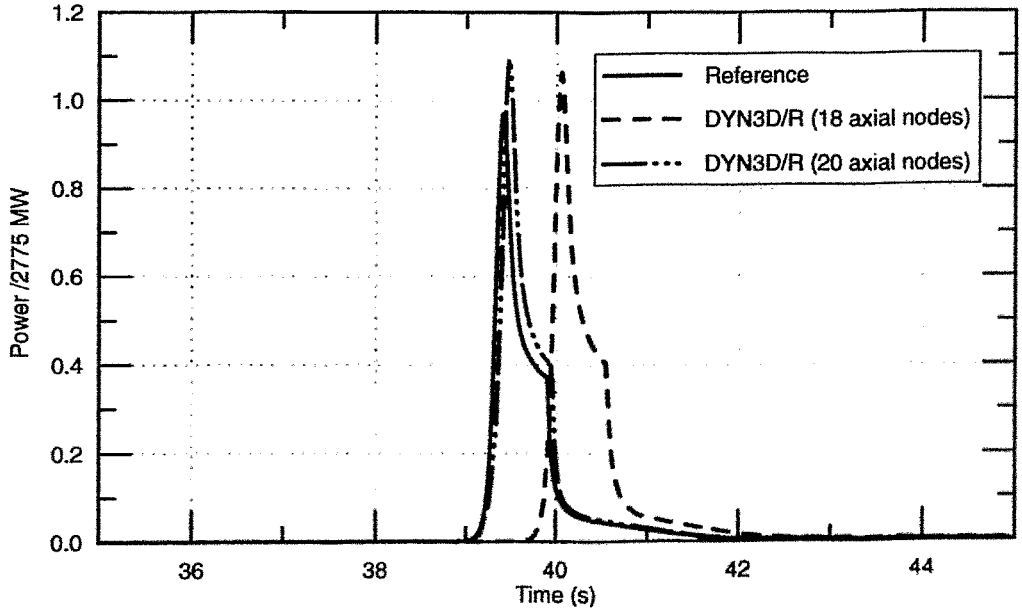

Fig. 11: NEA-NSC Benchmark - Case D: Behaviour of nuclear power of DYN3D calcualtions with different axial mesh

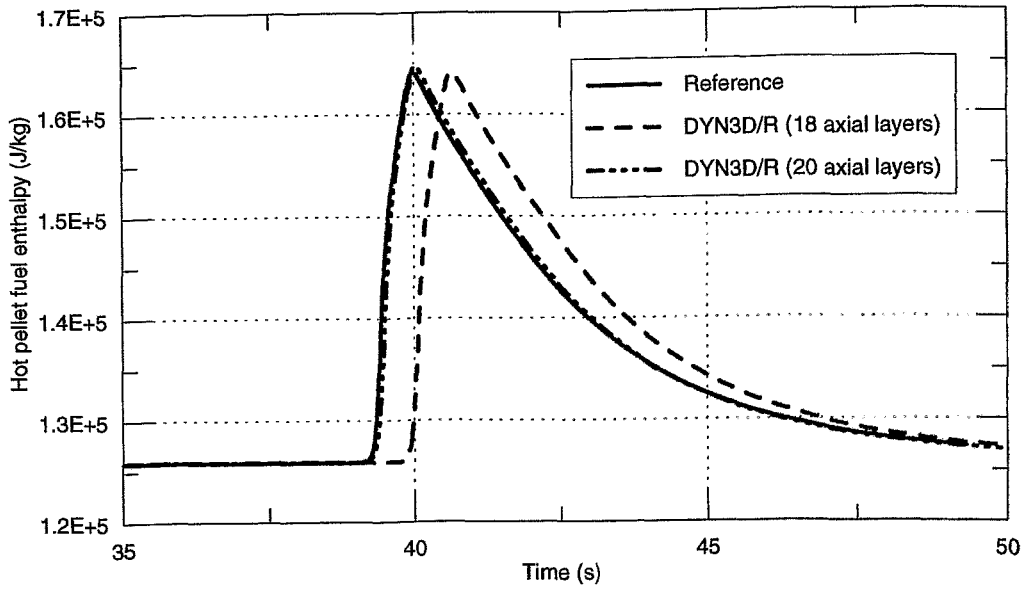

Fig. 12: NEA-NSC Benchmark - Case D: Behaviour of fuel enthalpy of DYN3D calculations with different axial mesh

value is 2.5 ppm. A standard axial mesh of 18 layers was given for this benchmark, but other meshes could be chosen by the code users. Firstly, the DYN3D/R calculation was carried out with this standard mesh. When the reactivity insertion is larger than prompt critical we observe a power excursion which is limited by the Doppler effect before the control rods are inserted by the scram. Fig. 11 shows the time behaviour of fission power in comparison to the reference. We see that the power peak of the DYN3D calculation occurs nearly 0.7 s later. This deviation seems to be caused by differences of the reactivity insertion. The position of the power peak at the time scale is very sensitive to the time when the reactor becomes prompt critical. If the lower end of a control is located inside an axial layer, the so-called cusping effect occurs as a result of using a geometrical nodal weighting of cross sections. In DYN3D a flux weighting is applied, but the cusping effect is not completely removed. A better agreement of the position of the power peak is obtained by the following approach. Each of the two axial layers, in which the lower control rod ends are moved just before reaching the prompt critical state (until the begin of scram) is split into two layers. Thus the total number of core layers is increased from 18 to 20. It can be seen from fig. 11 that this approach leads to an improvement. A very interesting parameter during a transient like this is the energy release in the fuel. Fig. 12 shows that the maximum of the hot pellet fuel enthalpy is in good agreement with the reference value. The calculation with the standard mesh shows a shift of the peak similar to that in fig. 11 which does not occur by using the finer mesh.

5. Validation of the Fuel Rod and Heat Transfer Model of DYN3D

In reactivity transient analysis, the heat transfer from fuel to coolant plays an important role. This heat transfer is affected significantly by the behaviour of the gas gap between fuel and cladding, but also by the heat transfer conditions at the cladding surface. It affects, on the one hand, the fuel temperature, being a significant safety and neutron kinetics feedback parameter. On the other hand, a heat transfer crisis can occur at the cladding surface leading to wall superheating, which can result in cladding destruction. The heat transfer through the gas gap is affected by the behaviour of fuel and cladding, because it depends on the gap width, gas composition and gas pressure in the gap, as well as on possible mechanical contact pressure between fuel and cladding. For this reason the validation of the fuel rod and heat transfer model in the code DYN3D was performed by comparison of calculated results with experimental results from the literature. A detailed description of the fuel rod and heat transfer model in DYN3D as well as of the validation calculations is given in [6, 29]. Experiments on the fuel behaviour during large power pulses were carried out e. g. in the Japanese Nuclear Safety Research Reactor (NSRR), in the Russian research reactors IGR and GIDRA and in the frame of the French CABRI experimental programme [30, 31, 32]. The NSRR is a modified TRIGA reactor with a small power pulse half width of a few milliseconds. The Russian GIDRA reactor is of water - solution - enriched type producing narrow power pulses, while the IGR recator is a graphite moderated one with a higher pulse half - width reaching from 0,5s to a few seconds. Experimental results for tests where shortened probes of fresh fuel rods were inserted into a water or air-filled capsule are provided in [33, 34, 35]. In all tests, the water was at atmospheric pressure. An overview of the experiments calculated by use of the DYN3D fuel rod model is given in Table 1.

ΔE is the energy release in the fuel probe, τ – the power pulse half-width, ΔT - the coolant subcooling, $h_{f,max}$ - the energy deposition in the fuel (calculated), T_{clad} - the maximum cladding temperature, t_{rewet} - the time until rewetting after heat transfer crisis, δ_{ox} - the oxide layer thickness due to cladding oxidation. The calculated results are printed bold.

In general, a good agreement is reached between the calculations and the experiments, which were carried out in very different conditions (pulse half width, coolant subcooling, energy release). Fig. 13 shows the results for the IGR experiments No. 6 from table 1. In the experiment, a cladding surface overheating was observed for a short time. Measured and calculated temperature curves for this experiment are also provided in [36].

Remarkable differences can be seen between the NSRR and the IGR experiments. In the NSRR experiments, the energy release in the burst was lower than in IGR experiments with water cooling, but much higher cladding temperatures are reached. This is due to the very small pulse width which leads to an almost adiabatic heating of the fuel rod during the burst. In the NSRR experiments considered, the effect of coolant subcooling was investigated while the other conditions (energy release, pulse width) were fixed. This allows to adjust the heat transfer model by

	NSRR Experiments			IGR Experiments				
Exp. No.	1	2	3	4	5	6	7	8
$\Delta E[cal/g]$	190	190	190	207	284	326	360	93
$\tau[ms]$	7	7	7	1050	650	500	800	4300
$\Delta T[K]$	10	40	80	80	80	80	80	air
$h_{f,max}[cal/g]$	**187**	**185,5**	**183,5**	**123**	**179**	**216**	**~200**	**?**
T_{clad}[deg C]	1500	1330	1000	141	177	967	940	1200
	1447	**1278**	**1177**	**153**	**167**	**891**	**1040**	**1320**
$t_{rewet}[s]$	38	15	10	-	-	6,3	11	-
	41	**20**	**7,2**	**-**	**-**	**6,6**	**12,5**	**-**
$\delta_{ox}[\mu m]$	12	8	5	-	-	?	?	?
	29	**13**	**7**	**-**	**-**	**-**	**-**	**-**

Table 1: Overview on RIA experiments calculated with the DYN3D fuel rod model - experimental and calculated results

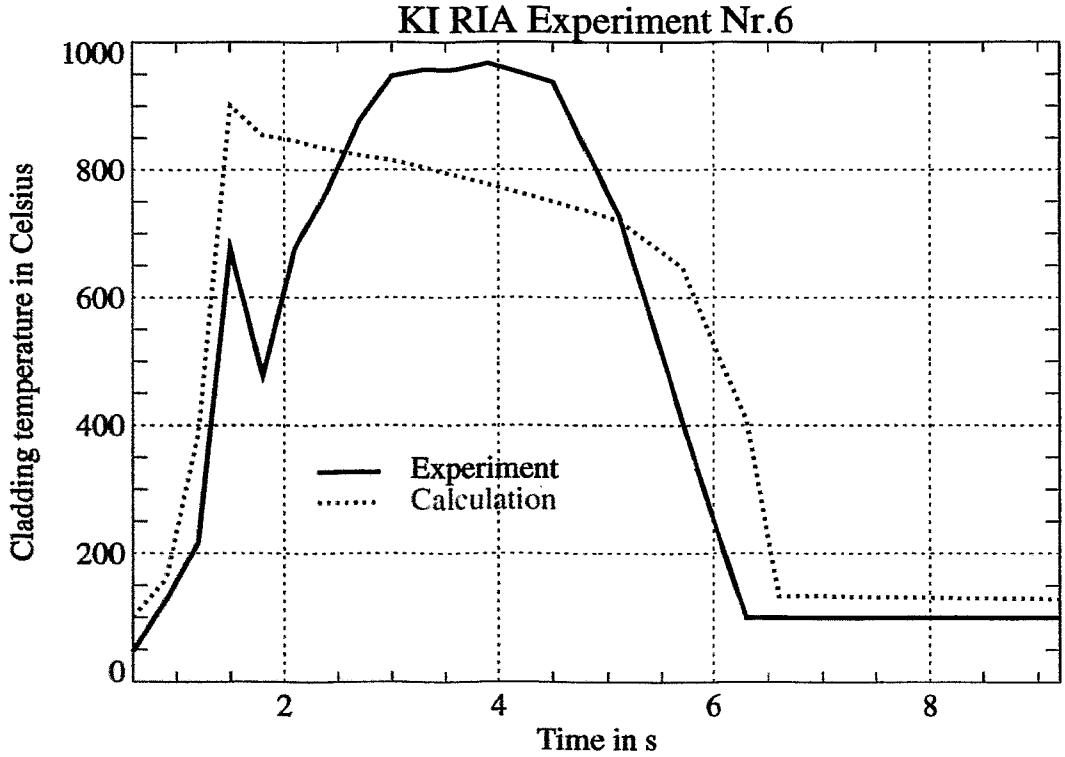

Fig 13: Comparison between calculation and measurement for RIA -experiment no. 6.

introducing non-equlibrium corrections for the minimum stable film boiling temperature and the film boiling heat transfer coefficient (see section 2.2).

However, the experiments compiled in Table 1 are carried out under stagnant flow conditions at low coolant pressure. RIA in nuclear power reactors during power operation are characterized by high pressure and coolant mass flow rates.

Experiments at higher pressures and mass flow rates at NSRR, IGR and CABRI reactors are reported about, but data are not available. Therefore, sensitivity studies were performed for a hypothetical test case, which represents an idealized power pulse at VVER-440 conditions (nominal pressure and mass flow rate) with variation of the energy release and at different burn-up values. Burn-up dependent input data for the normal conditions reference states of the gas gap, which are used as input data for the fuel rod model, were obtained from calculations with the detailed fuel rod behaviour code STOFFEL [37].

It was found from the calculation results, that the relevant mechanism of fresh fuel failure is melting, the fuel enthalpy at failure is about 230 cal/g. This is consistent with data from literature. For burned-up fuel, cladding failure is possible due to high mechanical stress at much lower fuel enthalpy values (about 125 cal/g for burn-up of 25000 MWd/t). This corresponds also to results reported in the literature [38]. However, the DYN3D fuel rod model needs improvements in the description of burned fuel, where much more complicated phenomena in gap behaviour and fuel - cladding mechanical interaction are more relevant than for fresh fuel.

From the calculations of RIA experiments in research reactors and numerical investigations for a test case corresponding to power reactor conditions, the following conclusions can be drawn:

- The DYN3D fuel rod model is able to reproduce experimental results on fuel rod behaviour during large power bursts and even to provide a rough estimation of fuel failure onset conditions.

- A mechanistic description of gas gap behaviour, including at least a simple thermo-mechanical model, is relevant for realistic fuel rod behaviour estimation in the frame of a reactor dynamic code.

- The model does not properly take into account complicated effects in high burn-up fuel. However, a rough estimation of burned fuel with medium burn-up seems to be possible.

6. Application of DYN3D for Accident Analysis

The hexagonal version of the code DYN3D was developed for 3-dimensional safety analyses of the VVER-reactors of the former GDR. After the political changes the Greifswald power station with five VVER-440 reactors was shut down. In the frame of an IAEA regional project the code DYN3D was made available for institutions of countries with operating VVER reactors. Meanwhile the code is used for safety analyses by the Nuclear Research Institute in Rez and Energoproject Prague (Czech Republic), the State Scientific and Technical Centre for Nuclear and Radiation Safety in Kiev (Ukraine), by the Nuclear Regulatory Authority of Slovak Republic and the institute VUJE Trnava (Slovakia) and the Institute of Nuclear Research and Nuclear Energy in Sofia (Bulgaria). In the frame of the scientific technological cooperation DYN3D was transferred to the IPPE Obninsk and to the Technical University Budapest. The IPPE plans to couple DYN3D with the RELAP code. The code was applied for a lot of calculations in these institutions. In the Czech Republic the code is licensed by the Nuclear Authority for safety analysis. In the following two examples for code application in the FZ Rossendorf are presented.

6.1 Boron Dilution Transient in a VVER-440 by Using Different Mixing Models

An incorrect startup of a pump in an isolated loop containing a plug of diluted absorber can initiate a reactivity accident in a VVER-440. It is assumed that the main gate valve is opened after starting the main coolant pump. At beginning of the transient, the VVER-440 reactor is operating at 1210 MW (88% of nominal power). The control rod bank K6 is 75 cm inserted in the core. The mass flow rate after start of pump is 8667 kg/s (nominal value). The boron concentration in the considered loop was reduced from the critical value of 5.34 g H_3BO_3/kg (934 ppm) to 2.82 g H_3BO_3/kg (494 ppm). The plug reaches the core inlet at t = 0.0 s. A ramp-like transition time of 0.1 s is assumed before the boron dilution at the core inlet has its maximum value. The transport time through the core amounts to 0.8 s, i. e. after 0.8 s the inserted reactivity reaches its maximum. Within 3 s the boron concentration returns to its initial value at the core inlet. The transient was analyzed over a time of 10 s. The failure of the shut down system was considered. The pressure was assumed to be constant during the transient. Three cases of boron mixing were investigated:

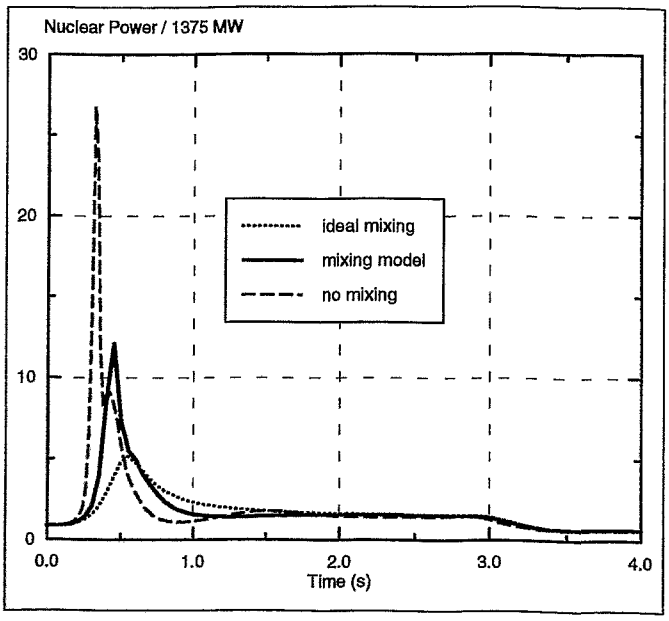

Fig. 14: DYN3D: Nuclear power versus time for 3 different mixing models

- no mixing, i. e. the boron concentration is reduced only in one sixth of core which belongs to the loop with the plug,
- application of the mixing model implemented in DYN3D,
- ideal mixing.

Depending on the mixing model different deformations of the neutron flux distribution can be expected which influences the inserted reactivity. Fig. 14 shows the behaviour of nulcear power for the 3 different models. Some safety relevant parameters are given in Table 2. The investigation were described in more detail in [39, 40]. The investigations show that the assumption of ideal mixing is not conservative and the other unrealistic case without mixing leads to serious consequences.

parameter	ideal mixing	mixing model	no mixing
maximum reactivity (β_{eff})	0,794	0,986	1,243
Peak power (MW)	7092	16655	37071
Max. fuel temperature (°C) of hot channel	2186	>2800	>2800
Min. critical power ratio of hot channel	0,98	0,73	0,68
Max. cladding temperature (°C) of hot channel	850	1542	>1800
number of fuel elements with metal water reaction	-	4	36

Table 2: Safety related parameters of boron dilution transien

6.2 Investigation of a Boron Dilution Transient in a PWR

The initial event is a small break LOCA in a PWR. The reactor is shut down. By evaporation and condensation in the loop with the leak a plug of coolant with low concentration of boron occurs. After re-start of natural circulation it is transported with low coolant velocity ($v \sim 5 cm/s$) into the core. Based on safety analyses with the code RELAP5 and experiments in a test loop the time behaviour and the distribution of boron concentration and coolant temperature at the core inlet were given for the worst case [41]. The core inlet was divided into four radial zones with different conditions which can be seen for a quarter of core in fig. 15. Fig. 16 and 17 show the variation of the boron concentration and the coolant temperature at the core inlet for the four radial zones and the average value in time. The two cases of heterogeneous distribution and the homogeneous distribution with the average value were investigated.

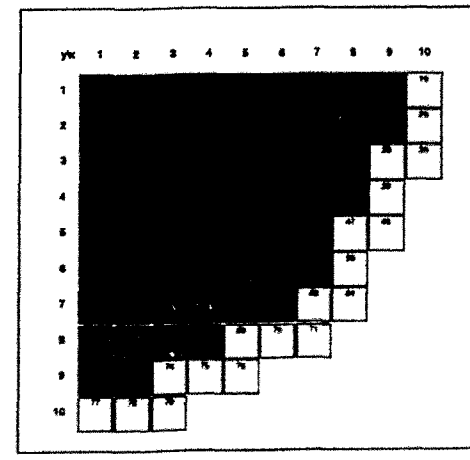

Fig.15: Boron Dilution Transient: Radial zones with different inlet conditions

The transient was calculated by applying a „particle in cell" - method, developed for the simulation of transport processes in chemical reactors, to the boron transport. During the process the reactor became critical and nearly

prompt critical (0.9 ß) by the decrease of boron concentration in the core. Fig. 18 shows the reactivity and nuclear power versus time. The curves show that the assumption of homogeneous distribution is not conservative. Therefore a realistic

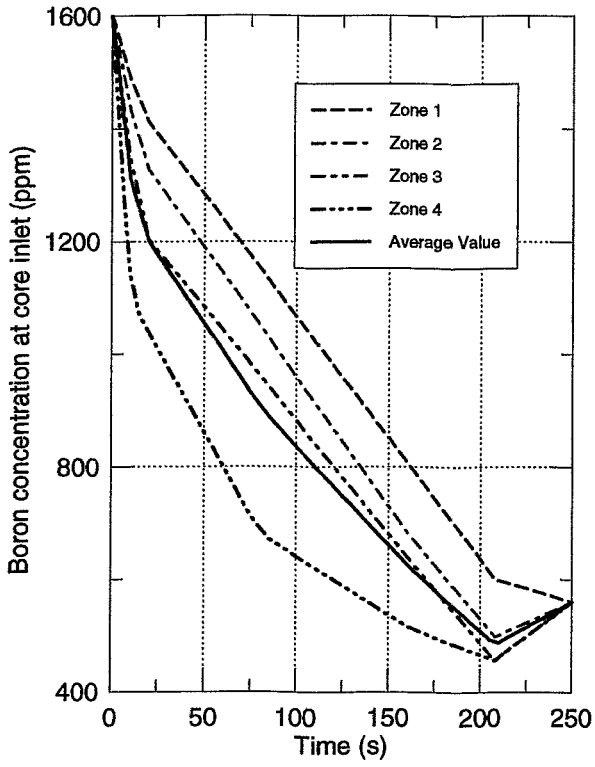

Fig.16: Behavior of boron concentration at the core inlet for the 4 radial zones

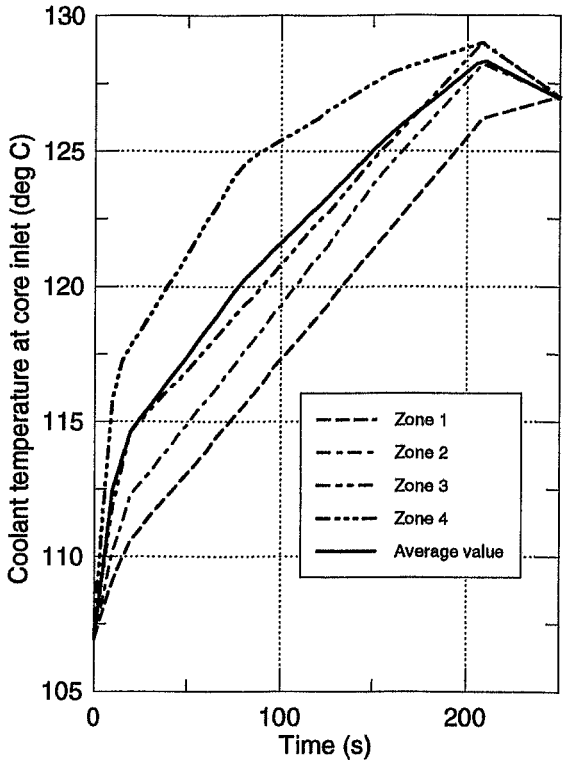

Fig.17: Behavior of coolant temperature at the core inlet for the 4 radial zones

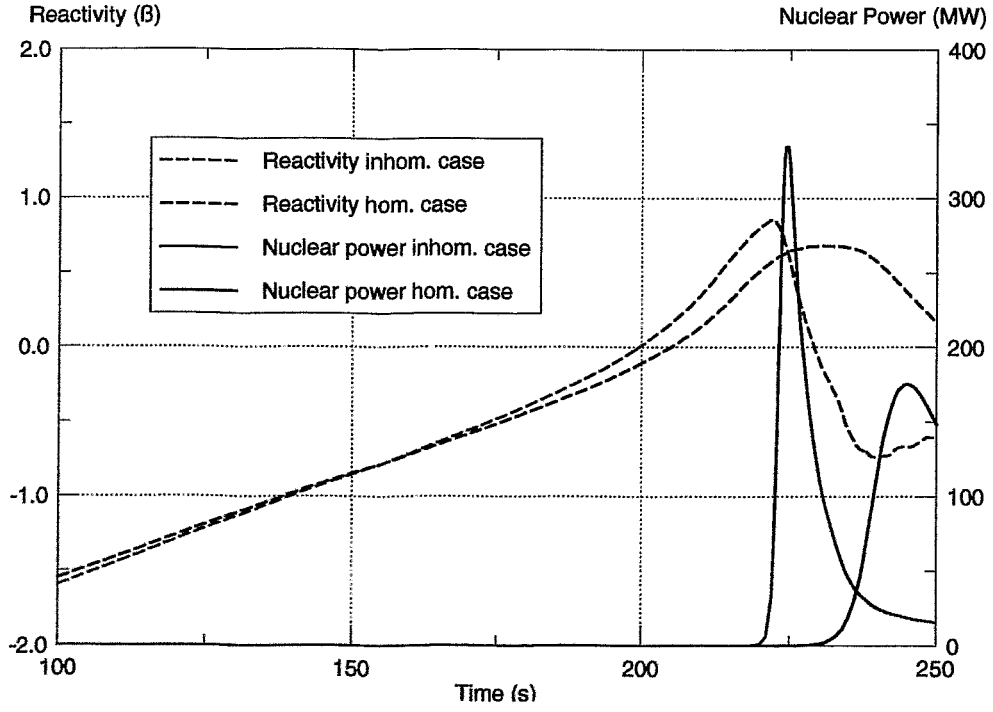

Fig.18: Reactivity and nuclear power for inhomogeneous and homogeneous boron dilution

description of the mixing processes in the reactor vessel is very important for safety considerations of such type of transients.

7. Present and Future Activities

Future activities are divided to further improvement of the code by implementing additional models, enhanced accuracy of neutronics and development of a 3D coolant flow model for the core. Validation activities are continued by comparison of calculated results with measurements from NPPs.
If we consider the accuracy of the nodal method for the larger fuel assemblies of the VVER-1000 an improvement of the nodal method is required. A method taking into account not only the fluxes and currents at the interfaces of the hexagon but also the corner values is under development. First calculations show an improvement of results for benchmark problems.

A flux reconstruction method was developed for the 2-dimensional inner nodal flux reconstruction in the hexagonal assemblies. The method is based on the fluxes at the interfaces of the hexagon and the corner fluxes. The integration of the method in the DYN3D code for the calculation of the hot channels is also part of the future work.

Improved cross section data libraries generated with the help of WIMS and HELIOS codes are under development and to be connected to DYN3D.

If there are inhomogeneities of the coolant flow in the reactor core leading to driving forces perpendicular to the direction of the main stream a three dimensional thermohydraulic model is needed for the description of the coolant flow in the core. Different models are in discussion.

References

[1] U. GRUNDMANN and U. ROHDE, "DYN3D/M2 - a Code for Calculation of ReactivityTransients in Cores with Hexagonal Geometry", Proc. of IAEA Technical Committee Meeting on Reactivity Initiated Accidents, Wien (1989) or Rep. FZR 93-01, Research Center Rossendorf (1993)

[2] U. GRUNDMANN, "A NEM for Solving Time-Dependent 3-Dimensional Diffusion Equation for Hexagonal Geometry", Proc. International Conference on the Physics of Reactors PHYSOR'90, Marseille (1990)

[3] U. GRUNDMANN, "The Code DYN3DR for Steady-State and Transient Analyses of Light Water reactor Cores with Cartesian Geometry", Rep. FZR 114, Research Center Rossendorf (1995)

[4] M. R. WAGNER, "Three-Dimensional Nodal Diffusion and Transport Methods for Hexagonal Geometry", Nucl. Sci. Engng. 103, 377 (1989)

[5] H. L. RAJIC and A. M. OUGOUAG, "ILLICO: A Nodal Neutron Diffusion Method for Modern Computer Architectures", Nucl. Sci. Engng., 103, 392 (1989)

[6] U. ROHDE, "Modelling of Fuel Rod Behaviour and Heat Transfer in the Code FLOCAL for Reacrtivity Accident Analysis of Reactor Cores", 1st Baltic Heat Transfer Conference, Göteborg, (1991), published in: Transport Processes in Engineering, 2: Elsevier Publ., Amsterdam, (1992)

[7] N. OHNISHI, K. ISHIJIMA and S. TANZAWA, "A Study of Subcooled Film-Boiling Heat Transfer under Reactivity Initiated Accident Conditions in Light Water Reactors", Nucl. Sci. Engng., 30, 331 (1984)

[8] V. G. ASMOLOV et. al, "Rechnerische und experimentelle Untersuchungen des Verhaltens eines einzelnen Brennelementes bei großen Leistungsexkursionen", Kernenergie, 30, 299 (1987)

[9] M. J. BURWELL, G. LERCHL, J. MIRO, V. TESCHENDORFF and K. WOLFERT, "The Thermalhydraulic Code ATHLET for Analysis of PWR and BWR Systems", in Proc. of Fourth Int. Topical Meeting on Nuclear Reactor Thermal Hydraulics, Karlsruhe, (1989), p. 1234

[10] U. GRUNDMANN, U. ROHDE, S. MITTAG, D. LUCAS, "Weiterentwicklung und Verifikation eines dreidimensionalen Kernmodells für Reaktoren vom Typ WWER und seine Ankopplung an den Störfallcode ATHLET", Report FZR-84, 95p., FZ Rossendorf (1995).

[11] U. GRUNDMANN, D. LUCAS and U. ROHDE, "Coupling of the Thermohydraulic Code ATHLET with the Neutron Kinetic Core Model DYN3D", in Proc. Int. Conf. on Mathematics and Computations, Reactor Physics, and Environmental Analyses, Portland, (1995), p. 257

[12] U. GRUNDMANN, D. LUCAS, U. ROHDE, "Coupling of the Advanced Thermohydraulic Code ATHLET with the 3D Core Model DYN3D", *Int.Topical Meeting on VVER Safety*, p. 197, ENS, Prague (1995).

[13] Y. A. CHAO and Y. A. SHATILLA, „Conformal Mapping and Hexagonal Methods - II: Implementation in the ANC-H Code", Nucl. Sci. Engng., 121, 210 (1995)

[14] CS. MARACZY,"A Solution of Seidel's 3D Benchmark for VVER-440 with the DIF3D-FD Code", 5th Symposium of AER, Dobogokö (Hungary), 1995. Proceedings, p. 287.

[15] V. RYPAR, J RACEK, K.-H. FÄHRMANN, U. GRUNDMANN and D. ZIEGENBEIN, "Neutron Kinetic Investigations at the LR-0 Zero-Power Reactor", Nucl. Sci. Engng., 105, 218 (1990)

[16] GRUNDMANN, U.; HÁDEK, J.; "Calculations of Neutron Kinetics Experiments on the LR-0 Reactor with the Three - Dimensional Code DYN3D/M1", Kernenergie , 34 (1991) 12.

[17] R. KYRKI-RAJAMÄKI, U. GRUNDMANN and A. KERESTURI, "Results of Three-Dimensional Dynamic Benchmark Problems for VVER Type Reactors", *Proceedings of the Int. Conf. on the Physics of Reactors PHYSOR96*, pp. J-229 - J-238, Mito, Japan (1996).

[18] S. MITTAG,"Burnup and Rod Worth Calculations for Paks-2 Using the Code DYN3D with two Different Group Data Libraries", 6th Symposium of AER, Kirkkonummi (Finland), 1996. Proceedings, p. 499.

[19] G. AGTHE, H.-J. KRETZSCHMAR,"Zur automatisierten Bereitstellung neutronenphysikalischer Weniggruppenparameter für die makroskopische Berechnung von Spaltzonen thermischer Reaktoren",Kernenergie, 33 (1990), p. 165-170 (Teil 1), 214-218 (Teil 2).

[20] I. TINKA," VVER Diffusion Data Libraries Prepared by the KASSETA Code", 3rd Symposium of AER, Piestany (Slovak Rep.), 1993. Proceedings, p. 42.

[21] L. KORPAS: Private Communication, 1996.

[22] L. KORPAS et al., "AER Benchmark Problem for Calculation of Control Rod Worth of VVER-440 Reactor", Working Group B Meeting of AER, Piestany (Slovak Republik), 1992.

[23] "Argonne Code Center: Benchmark Problem Book", Rep. ANL-7416, Suppl. 2, Argonne National Laboratory, (1977)

[24] H. FINNEMANN and A. GALATI, "NEACRP 3-D LWR Core Transient Benchmark", Report NEACRP-L-335, Rome, (1992)

[25] H. FINNEMANN, H. BAUER, A. GALATI and R. MARTINELLI, "Results of LWR Core Transient Benchmarks", Rep. NEA/NSC/DOC(93) 25, OECD NEA, (1993)

[26] R. FRAIKIN and H. FINNEMANN, "NEA-NSC 3-D/1-D PWR Core Transient Benchmark Uncontrolled Withdrawal of Control Rods at Zero Power", Rep. NEA/NSC/(93) 9, Paris, (1993)

[27] R. FRAIKIN,"PWR Benchmarks on Uncontrolled Rods Withdrawal at Zero Power", NEA/NSC/DOC(96)20, Septemer 1997

[28] U. GRUNDMANN AND u: ROHDE,"Verification of the Code DYN3D/R with the Help of International Benchmarks", Rep. FZR 195, Research Center Rossendorf (1997)

[29] U. ROHDE : „The modeling of fuel rod behaviour under RIA conditions in the code DYN3D", 8th Symposium of AER, Bystrice nad Pernstejnem/Czech Republic, 21.-25.9.1998, Proc. to be published

[30] J. PAPIN et al.: „French Studies on High-Burnup Fuel Transient Behaviour Under RIA Conditions", Nucl. Safety , 37 (4) pp. 289 - 327

[31] FUKETA, T. et al. : „NSRR/RIA Experiments with High-Burnup PWR Fuels", Nucl. Safety, 37 (4) pp. 328 - 342

[32] ASMOLOV, V., L. YEGOROVA: „The Russian Research Program: Motivation, Definition, Execution, and Results", Nucl. Safety 37 (4) pp. 343 - 352

[33] OHNISHI,N.,K.ISHIJIMA,S.TANZAWA, Nucl. Sci. Eng. 88 (1984) , p.331-341

[34] ASMOLOV,V.G. et al., Kernenergie, 30 (1987) , p.299-304

[35] BURMISTROV, E., S. BASHKIRZEV, U. ROHDE: „Validation Experience for FLOCAL, ESCES, MAIVA, SCDAP/RELAP Codes on the Basis of Post-Test Calculations for Russian and Japanese RIA Experiments", internal report, Research Centre Rossendorf, 1993

[36] BASHKIRZEV, S., V. KUZNETSOV, V. PROSELKOV: „The Calculation Analysis of the VVER-440 Fuel Behaviour in Design Reactivity Initiated Accidents", 7th Symposium of AER, Althörnitz (Germany), September 23 - 26, 1997, Proc. Vol. 2, pp. 759 - 780

[37] REINFRIED, D.: „Zur mathematischen Modellierung des Bestrahlungsverhaltens von Druckwasserreaktorbrennstäben", PhD Thesis, Rossendorf , 1985

[38] COURTRIGHT,E.L.: „A Survey of Potential Light Water Reactor Fuel Rod Failure Mechanisms and Damage Limits", NUREG/CR-1132 (PNL - 2787) , July 1979

[39] GRUNDMANN, U.; ROHDE, U.; "Investigations on a Boron Dilution Accident for a VVER-440 Type Reactor by the Help of the Code DYN3D", Proceedings of the 1994 Topical Meeting on Advances In Reactor Physics, Vol. III, pp. 464-471, Knoxville, TN(USA), April 11-15, 1994.

[40] GRUNDMANN, U.; ROHDE, U.; "3-Dimensional Analysis of a Boron Dilution Accident by Using the Code DYN3D/M2", Jahrestagung Kerntechnik '94, Stuttgart, 17. - 19. Mai, 1994.

[41] TIETSCH, W.; TISCHER, J.; "Analysis of Boron Dilution during Small Break LOCA in a 2x4 Loop B&W Type PWR", paper will be presented at Jahrestagung Kerntechnik '99, Karlsruhe, 18. - 20. Mai, 1999.