Development of coupled systems of 3D neutronics and fluid-dynamic system codes and their application for safety analysis

S. Langenbuch[1], K. Velkov[1], S. Kliem[2], U. Rohde[2], M. Lizorkin[3], G. Hegyi[4], A. Kereszturi[4]

[1] Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, 85739 Garching
[2] Forschungszentrum Rossendorf e.V., Institut für Sicherheitsforschung, Postfach 510119, 01314 Dresden
[3] Kurchatov Institute for Atomic Energy, Kurchatov Square 1, Moskow 123 182
[4] Atomic Energy Research Institute KFKI AEKI, P.O. Box 49, 1525 Budapest 114

Abstract:

An overview is given on the development of coupled systems of 3D neutronics and fluid-dynamic system codes. In particular, the work performed in this field on the basis of the system code ATHLET developed by GRS is reported. During the last years, the coupling of different 3D neutronics codes like BIPR8 (KI), DYN3D (FRZ), KIKO-3D (KFKI) and QUABOX/CUBBOX (GRS) was implemented in order to simulate LWR, VVER and RBMK core conditions. The objectives and representative results of international activities to validate such coupled codes are described. In addition, the experiences from applications in accident analysis are summarized and further improvements are recommended.

1. INTRODUCTION

The safety analysis of NPPs is mainly based on the application of analytical simulation methods. Important fields of safety analysis are the static and transient reactor core behaviour by 3D neutronics models and the whole plant transient behaviour by fluid-dynamic system codes. In both fields the computer codes have achieved a high degree of realistic modelling. Nevertheless, the separate analysis of the reactor core by 3D neutronics models and the whole plant system using simplified neutronics models needs additional assumptions on the interfacing conditions if a strong coupling between the neutronics in the reactor core and the fluid-dynamics in the primary circuit exists. Therefore, great efforts were made to develop coupled code systems directly integrating 3D neutronics models into system codes. This presentation will describe the work performed in this field on the basis of the system code ATHLET developed by GRS. After a brief overview on the available analytical methods, the applications are described for which coupled codes can significantly improve the accuracy of simulation. The possible approaches for coupling 3D neutronics models to fluid-dynamic system codes are discussed and a report is given from recent efforts to validate such codes.

The results presented refer to international benchmark activities for code comparison like the OECD/CSNI PWR Main Steam Line Break (MSLB) Benchmark [Iva97] and to the EU Phare project SRR 1/95 [Wei00] which collected plant transient data from VVER-plants and performed analysis by coupled codes to compare with the measured data. In addition, results and experiences from further applications in safety analysis are described.

2. STATE OF ANALYTICAL METHODS AND THEIR LIMITATIONS

In the past, the calculations for the analysis of plant transients and the analysis of reactor core behaviour were performed separately. In the field of plant transient analysis the solution of thermal hydraulic equations for single-phase and two-phase flow conditions was the basis for developing system codes modelling the whole plant. Representative codes are ATHLET, CATHARE, RELAP and TRAC . In addition to the thermal hydraulics, these codes include models for describing components like coolant pumps, pressurizer and steam generator, as well as for modelling control systems and the protection system. The nuclear power generation in the reactor core is usually described by a point kinetics model and sometimes by a 1D neutronics model.

The application of the system codes needs attention to determine correctly the reactivity feedback functions for the point-kinetics model.

Detailed analysis of reactor core behaviour is based on 3D neutronics models which solve the two-energy group neutron diffusion equations including reactivity feedback effects caused by changes of coolant flow conditions and changes of the fuel rod temperatures. The efficient solution of spatial and time-dependent neutronics equations is based on coarse mesh methods or nodal functional expansion methods achieving a high accuracy even for radial nodes corresponding to the fuel assembly size.

For reactor core calculations the boundary conditions have to be defined, e.g. the mass flow and temperature distribution of the coolant at the core inlet together with the time-functions for pressure. In reality, these boundary conditions will be affected by the power generation in the reactor core. This limits the application to fast transients like a control rod ejection or transients with a weak coupling between fluid dynamics in the primary circuit and the nuclear power generation in the reactor core.

In summary, the application of these models is limited by the assumptions to consider properly the interface conditions. It may lead to very unrealistic accident conditions, if all uncertainties are taken into account by defining conservative boundary conditions. However, this is in contradiction to the actual trend of safety analysis to perform realistic best estimate analyses.

These problems of separated analysis can only be avoided by directly coupling 3D neutronics models with the system code.

3. TYPICAL APPLICATIONS OF COUPLED CODES

The analysis by coupled codes is needed for the following accident conditions, which are presently under discussion.

- The local boron dilution accident in PWR, which was identified as a potential reactivity initiated accident even in shutdown conditions when all control rods are inserted.
- The cool-down transients with strongly negative moderator temperature reactivity coefficient (MTC) in PWR. The occurrence of a recriticality during cool-down and its consequences have to be analyzed. Such high values of MTC are obtained for increased high burnup fuel or for extended use of MOX fuel.
- The results of ATWS analyses are strongly affected by feedback reactivity coefficients. The uncertainties of inherent feedback determining power production and consequently pressure increase can be strongly reduced by applying 3D neutronics models. The spatial effects are emphasized if partial failure of control rod insertion is postulated.
- Power upgrading programs generate the demand for reducing uncertainties.
- The BWR instability in plant conditions beyond the stability threshold.

For these events, the accuracy of the analyses can be improved significantly by modelling directly the interaction of the neutron kinetics and the fluid-dynamics in the coupled codes.

4. COUPLING OF THE SYSTEM CODE ATHLET WITH 3D NEUTRONICS MODELS

The AHLET code [Ler98, Tes96] is a thermo-fluid-dynamic system code for a wide range of applications comprising anticipated and abnormal plant transients, small and intermediate leaks as well as large breaks in PWRs and BWRs. The two-phase flow is described either by a 5-equation model or a full 6-equation model of both phases including models for non-condensables. The code structure is highly modular, and allows an easy implementation of different physical models. ATHLET provides a modular network approach of the primary and secondary side including all components of the plant. The ATHLET-code was developed by GRS and it is comparable to other system codes like CATHARE, RELAP or TRAC.

The coupling approach for 3D neutronics models implemented in ATHLET [Fom93, Lan96a, Lan96b] allows various options, which are also applied within other coupled code systems:

- Internal coupling
  Coupling of the 3D neutronics model to the system code ATHLET which models completely the thermal-fluid-dynamics in the primary circuit including the core region.

- External coupling

  Coupling of the 3D neutronics model including the fuel rod model and the fluid-dynamic model of the core region to the system code which models only the thermal-fluid-dynamics in the primary circuit excluding the core region.

- Parallel coupling

  The 3D neutronics model including the fuel rod model and the fluid-dynamic model represents the reactor core. The system code models the thermal-fluid-dynamics in the primary circuit and the core region in a simplified manner. The calculated boundary conditions of the system code are transferred as time-dependent boundary conditions of the more detailed core calculation performed in parallel.

These coupling approaches maintain the capabilities of the separated codes and provide the necessary exchange of main physical parameters. These are:

- The power density distribution which is the result of the neutronics calculation and which must be transferred to the fluid-dynamics.
- The distribution of fuel temperature, coolant density and coolant temperature as well as the boron concentration, which are the result of the fluid-dynamic model including the boron transport model and which must be transferred to the neutronics as feedback parameters.

The coupling of different 3D neutronics models is supported by developing a general interface in ATHLET and the specific features of the GCSM (general control simulation modul). Meanwhile, the following 3D neutronics models are coupled with ATHLET:

- QUABOX/CUBBOX from GRS [Lan77] in cartesian geometry applied for LWR and RBMK,
- BIPR-8 from Kurchatov Institute [Liz92] in hexagonal geometry applied for VVER,
- DYN3D from FZ Rossendorf [Gru93, Gru96] in cartesian and hexagonal geometry applied for LWR and VVER,
- KIKO-3D from KFKI Budapest [Ker94] also in cartesian and hexagonal geometry.

For all neutronics models the internal coupling was implemented, for DYN3D [Gru95a] also the external coupling and for KIKO-3D [Heg98] also the parallel coupling was implemented. There is a great interest to couple different neutronics models because a lot of validation and experiences exist for each model.

5. VALIDATION OF COUPLED CODES

The coupled codes will be used in safety analysis to perform more realistic analysis of accident conditions with a strong coupling between neutronics and fluid-dynamics in the primary circuit. It is therefore necessary that the validation of these coupled codes comprises the envisaged field of applications.

Certainly, the validation process is a continuation of the validation of the separated codes which has been established in the past. However, also the specific coupling approaches and their applications must be validated. Several activities were performed in international co-operations:

- The OECD/CSNI PWR core transient benchmarks [Fin91, Fin93a, Fin93b, Fra93, Fra96, Fra97, Lef94, Lef96] which have been extended for coupled codes by the PWR Main Steam Line Break (MSLB) Benchmark. This benchmark activity will be continued by analyzing a BWR Turbine Trip Benchmark that is based on measured data of a plant [Sol00].
- The EU Phare SRR 1/95 project which focussed on VVER NPPs. In a first step plant transient data from VVER-440 and VVER-1000 were collected. Then, for each plant a selected transient was analyzed by different coupled codes and the calculated results were compared with measured data of the transients.
- Relevant investigations were performed in the international association "Atomic Energy Research (AER)" which is addressing reactor physics and safety of VVER type reactors.
- Additional work was performed within the EU Phare project HU/TS/02 "Topical Issues concerning Accident Analysis: Methodologies and Management".

In the following some representative results of these efforts and experiences obtained in these studies are presented.

5.1 The PWR Main Steam Line Break (MSLB) Benchmark

The specification of this benchmark [Iva97] is based on the PWR Three Mile Island Unit 1 (TMI-1) as a reference plant. This plant has two main reactor coolant loops with once-through steam generators. The international benchmark is co-ordinated by the PennState University (PSU). The initiating event of the accident is the break of the main-steam line at one of the two steam generators at full power. At 114% nominal power, the reactor scram is actuated, postulating that the most efficient control rod fails. Further, the event sequence is determined that the non-affected steam generator will be isolated and the re-circulation pumps in both loops continue running.

For the comparison of results three phases were defined:

Phase 1: Calculation of the plant behaviour using point kinetics
Phase 2: Calculation of the 3D core behaviour with pre-defined boundary conditions
Phase 3: Calculation of the plant behaviour using 3D neutronics

Since the benchmark is structured in this way, it allows the comparison of solutions of different system codes using point kinetics (within phase 1) as well as the comparison between point kinetics and 3D neutronics solutions (comparing phase 1 and phase 3). During phase 1 it was possible to adjust the details and options of thermo-fluid-dynamic modelling in the different system codes. It confirmed also the high importance of thermo-fluiddynamic parameters and models for calculating the minimum coolant temperature in the affected coolant loop which directly determines the recriticality conditions of the reactor core. The relevant phenomena are the mass flow rate and the phase distribution of the break flow at the main steam line, the heat-transfer conditions at the steam generator tubes, details of the once-through steam generator like the recirculation flow and the steam overheating and the nodalization in the reactor vessel. The Figures 1 and 2 show the fission power using point kinetics and the cold leg coolant temperature in the affected loop from the participants of the benchmark. Initially, there is a power increase due to the cooling down of the reactor core which leads to the reactor scram at 114% nominal power. After about 60 sec, the power increases again by the cooling down of the reactor core, but mostly only a small power increase occurs. For making the comparison more easy in the following figures are shown only the results of the ATHLET-QUABOX/CUBBOX calculation. Fig. 3 shows the comparison of the fission power of ATHLET using point-kinetics and 3D neutronics. Fig. 4 shows the coolant temperatures during the cooldown of the reactor core. The minimum temperature in the cold leg is reached at about 70 sec. By discharge of the coolant at the leak, the pressure of the main steam line decreases and the steam generator is completely empty at 80 sec. Due to low water content in the steam generator, the heat transfer from the primary circuit is reduced remarkably, so the cooling down reaches its minimum.

Fig. 5 shows the reactivity state of the reactor core. It presents the contributions to reactivity by reactor scram, the positive contribution by fuel temperature or the Doppler reactivity, due to the reduced power and the corresponding decrease of the fuel temperature, as well as the positive contribution of the moderator temperature reactivity due to the continuous cooling down of the reactor core down to the minimum coolant temperature. The total reactivity of the core does not reach criticality again, but the distance is very small. The small distance causes a great sensitivity of the power transient towards model parameters and boundary conditions of the accident. In case of criticality, the power increase is higher.

A variant of the benchmark specification, the case with a more pronounced return-to-power, was used to investigate the effect of the specific number of TH channels (THC) on the accuracy of results. It is of interest to know this effect because a reduction of THC could be used to optimize the necessary computer time.

The ATHLET nodalization scheme, Fig. 6, is kept unchanged concerning the primary and secondary circuit. Three different mapping schemes have been analysed and compared. The first nodalization scheme is 1:1 modelling of the core, Fig. 7, it is the reference scheme. That means that each fuel assembly corresponds to a single THC. The total number of THC in this case is 178 (177 fuel assemblies channels and one channel for the reflector zone). In each channel the thermo-hydraulic feedback is described by a pipe and a fuel rod module of ATHLET code. No cross flows are taken into account among the THC. The second mapping scheme is the proposed one in the specification of the benchmark. It corresponds to 19 THC (one of them is a reflector channel) shown in Fig.8. The THC are located in three radial rings of the core. Each ring has 6 THC symmetrically located along the ring. The flow area of each THC in a ring is the same. This mapping scheme is proposed on the basis of the analysis done with TRAC code. To each THC is attached a heat slab describing the fuel rod with 24 equidistant nodes in axial direction. On the basis of our experience with coupled code calculations we tried to create an optimized mapping scheme. That is the scheme with 15 THC (1 for the reflector zone) presented in Fig. 9. The following model was applied:

- assemblies with control rods are united in a separate THC,
- each control rod cluster should have its own THC if it has different initial insertion depth in comparison with the other clusters or different time moment is expected or forseen to start rods movement,
- assemblies are united in separate THC if they are located around strong neutron flux disturbances (stuck rod, dropped rod, assembly with high burnup or different enrichment),
- non-controllable assemblies are grouped in one THC if they are located at one radial core ring.

The number that is put on each assembly (square) of the mapping schemes shows to which the fuel assembly THC is related. The stuck rod assembly, number one in Fig. 9, is assigned to a separate THC.

Discussion of comparisons

The total power histories for the three cases can be seen in Fig. 10. At the beginning, it increases due to the positive reactivity of the coolant temperature reduction and after reaching 114% nominal power the reactor trip is initiated. As we can see, the total power differs very slightly for the three cases. Some deviations are observed in the vicinity of the second power peak. Comparison of some average global parameters can be done on the basis of the data listed in Table 1. Deviations are observed for K_{eff} in comparisons with the reference case (177 THC). In case of the optimized scheme (14 THC) the error is smaller in comparison with the 18 THC scheme as specified in the benchmark. This tendency is valid for the mean power density, average fuel temperature and mean coolant density and remains the same for all four specific time points of the transient chosen for the comparison (steady state, time point of first power peak, time point of the second power peak and time point at the end of the transient - at100s). An even more definite tendency is observed for the maximum fuel temperature (local parameter) that can be seen in Fig. 11. At the time of the second power maximum the deviation reaches 126.9 K for the 18 THC case and only 29.8 K for the 14 THC mapping scheme.

The axial core averaged power profiles are presented in Fig. 12 (t=0 s), Fig. 13 (t= first power peak), Fig.14 (t= second power peak) and Fig. 15 (t=100s). In general the 18 THC scheme overestimates the power generation in upper core part in comparison with the 14 THC scheme and it underestimates the power in the lower core part. The differences are almost negligible at t=100s because the transient is completed and we have almost homogeneous distributions in the core. A great advantage of the 14 THC scheme in comparison with the 18 THC one, can be seen by predicting the local distributions. Axial power distributions for the THC with the stuck rod are shown in Fig.16 and 17. The profiles for 177 and 14 THC are almost full overlapping while the deviation in the upper core part for the 18 THC reaches 25 %.

The comparison of the time histories of the local and global parameters for the three cases proves that deviations from 177 THC scheme in case of the optimised mapping of 14 THC are smaller than in case of 18 THC.

This study shows that a 1 : 1 mapping of fuel assemblies and TH channels should be recommended to obtain high accuracy for the local parameter values. A model using a reduced number of TH channels is able to calculate properly averaged time-dependent behaviour, but the grouping of TH channels should be adjusted to the problem.

5.2 The validation of coupled thermohydraulics/neutron kinetics codes within SRR 1/95

The primary objective of the EU Phare project SRR 1/95 [Wei00a, Mit00] was the validation of coupled codes against collected real VVER plant transients. Organisations from seven countries participated in this project. In the first phase, plant transients data from VVER-440 and VVER-1000 were collected. The plant transient data for VVER-1000 were the following:

- In Balakovo-4 a transient with switching-off of one of two working steam generator feed water pumps at full power,
- In Zaporoshye-6 a transient with a disconnection of the generator from the electric grid, i.e. the degradation of the turbo-generator power from 1000 MW electric power down to the house load level of 50 MW.
- In Kozloduy-6 at 90% nominal power, two neighbouring main coolant pumps were switched off.

In addition, transients from VVER-440 plants were collected, namely

- In Loviisa-1 a transient was initiated by the load drop of one turbo-generator, i.e. the electric power output of the plant was suddenly reduced by half.
- In Dukovany-2 a test was carried out during the start-up of the unit at 55% nominal power, whereby 3 out of 6 working main coolant pumps were simultaneously switched off.

Within this project all relevant plant data and the available measured parameters were collected and documented for future analysis. For each VVER type, one transient has been chosen to be analysed by the coupled codes.

In the following, the results of the analysis of the Balakovo transient are reported as an example. The initiating event for the transient was the switching-off of one of the two working steam generator feed water pumps at full power. Two seconds after the pump failure, the power control system responded by inserting the first control rod group from core top to bottom within four seconds. Group No. 10, that had been at the axial position of 275 cm, started moving in at the rate of 2 cm/s. As a result of dropping group No. 1, the neutron power decreased to about 63 % of the nominal value within 10 seconds. The slow insertion of group No. 10 down to a position of 140 cm resulted in a power decrease to about 45 %. The reactor power was stabilised at this level by the automatic power controller. In the secondary circuit, the flow rate through the second feed water pump that was still in operation, was increased by some 50 % within 16 seconds after the failure of the first pump, in order to partly compensate the deficient feed water flow. In the following, the flow rate of the second pump was reduced again to match the decreasing thermal power of the primary circuit. During the whole transient, the water level in the steam generators was always kept well above the heater tubes.

The Balakovo transient was analysed by using the coupled code complexes HEXTRAN-SMABRE [Kyr95a, Mie98] and ATHLET coupled with the 3D core models DYN3D [Gru95a, Gru95b] and BIPR-8 [Fom93]. HEXTRAN-SMABRE calculations were performed by VTT, ATHLET/BIPR-8 calculations by KI Moscow and ATHLET/DYN3D calculations by FZR, INRNE Sofia and STC-NRS Kiev. In all cases, the nuclear data libraries and codes that have been used for the burn-up calculations are consistent with the libraries and neutronic codes applied in the transient analyses.

To obtain the reactor state before the transient, burn-up calculations were carried out by all participants over the first 152 full-power days of the first fuel cycle, using the operation history provided by KI. The maximum burn-up deviations of 4 % between the codes occur in assemblies near the core boundary. The measured critical boric acid concentration was 3.00 g/kg, the calculated values were between 2.74 g/kg and 3.41 g/kg. The main reason for the differences between the calculations was found in the different nuclear data used. Three-dimensional core power distributions derived from self-powered neutron detector measurements in the stationary states before and after the transient were compared with the values calculated by the different codes. The maximum deviation is about 5.4 % in an assembly at the core boundary.

The control rod group positions as functions of time were provided as input to all transient calculations. Fig. 18 (upper part) shows the positions of the control rod group 10. The measured pressure in the main steam header (MSH) was applied as a boundary condition in the ATHLET calculations (Fig. 18, lower part). The regulation of the calculated steam mass flow was modelled by a controller, which guarantees that the pressure in the calculation follows the data in the table. The measured feed water mass flow rate was also used as a boundary condition. The modelling of the feed water collector and the feed water pumps is included in the SMABRE model. The control of the feed water valves is based on the collapsed water level values. The feed water flow does not affect the primary circuit behaviour, as long as the steam generator heater tubes are totally covered by water. This behaviour was reproduced by both the ATHLET and

SMABRE calculations for the whole transient, although different water levels in the steam generators were computed.

The behaviour of the calculated and measured reactor power and the cold leg temperature is shown in Fig. 19. The power is controlled for the most part by the control rod movements, but there is also an effect of fuel and coolant temperature on reactivity and power. The cold leg temperature decreases with falling power, but it is influenced by the pressure in the secondary circuit, too. A rising steam header pressure means an increasing saturation temperature, which leads to a decreasing heat transfer in the steam generator. The result is a rising cold leg temperature, and vice versa.

In the first seconds of the transient, the power decreases very fast as a result of dropping the first control rod group. The minimum is reached at t = 6 s, when the group is fully inserted. The power rise observed in the next few seconds, is mainly caused by a positive reactivity due to fuel temperature decrease. The measured power increase after the end of the insertion of control rod group K1 is about 200 MW. The calculated values are between 190 and 300 MW. The deviations between the calculations are caused by different temperature dependencies of the nuclear cross sections and different assumptions on the thermal properties of the fuel rods. Detailed investigations have shown that the change of the heat transfer coefficient (HTC) in the gas gap during the transient is relevant. With dropping fuel temperatures, the gap width increases, which leads to a decreasing HTC. This reduces the fuel temperature decrease. Comparing the results of DYN3D/ATHLET calculations with constant and changing HTC in the gap, performed by FZR, has shown that the difference in the power level of the final state (caused by this effect) is about 150 MW.

In the time interval between t = 10 s and t = 60 s, the power is mainly controlled by constantly inserting control rod group K10 at the speed of 2 cm/s. But the cold leg temperature decrease between 10 s and 20 s causes a reactivity increase (moderator density feedback), which for the most part compensates the reactivity effect of group 10, so that the power does not drop much in this short interval. After stopping the insertion of group 10 at t = 60 s, power and temperatures are stabilised. In the time interval between t = 115 s and t = 185 s, further control rod movements occur initiated by the power regulator. When approaching a new stationary state (t > 250 s), the differences between calculated and measured power are mostly within the accuracy of the neutron power measurement of ± 2 %.

Generally, the physical behaviour of the NPPs, especially of the core and the primary circuit is well described by the coupled codes used. A good agreement between calculated and measured safety-relevant parameters has been achieved for both the VVER-440 and the VVER-1000 reactor transient. In both transients, a main effect was the fission power decrease due to control rod group insertion. Differences in the nuclear data used in the calculations are the cause of different control rod efficiencies leading to differences in power levels. The fuel temperature feedback on reactivity also influences the power. Both effects can hardly be separated.

For separately studying the control rod efficiencies, the neutronic codes including the applied nuclear data bases should additionally be validated against measurements in zero-power research reactors.

The results of kinetic experiments carried out in the V-1000 facility of the Kurchatov Institute, Moscow, would be very suitable for this purpose. As for the calculated fuel temperature, the present investigations have revealed that it is very sensitive to the modelling of the gas gap between fuel pellets and rod cladding. A dynamic modelling of the gap width is necessary.

In addition, transients for the Kozloduy-6 and the Zaporoshye-6 units have been analysed in the frame of bilateral projects on scientific-technical co-operation [Gru00a, Gru00b]. For the analysis of a transient with coast-down of two from four working main coolant pumps in the NPP Kozloduy, different approaches were applied for a preliminary analysis of cross flow effects in the core, e.g. an ATHLET model with 10 coolant channels interconnected by cross flow objects has been developed [Gru00b].

Altogether, it was shown that the coupled neutron kinetic / thermal hydraulic codes under consideration are capable of simulating typical VVER plant transients. Hence the work contributes to increase the confidence in the results of the code systems. In the future, some more details of the automatic control systems should be included in the thermal hydraulic system models. The remaining transients, measured in VVER-1000 and VVER-440 plants, that were documented for the SRR1/95 project can be used for further validation work.

5.3 AER benchmark activities

A systematic benchmark work on reactor dynamics has been performed in the last years in the framework of the international association “Atomic Energy Research” (AER) on reactor physics and safety of VVER type reactors. Concerning reactor dynamics, 5 benchmark problems have been considered up to now. The complexity of these benchmarks has been increased systematically, so that the influence of various models, like neutron kinetics methods, nuclear cross sections and thermal hydraulics can be studied separately. The first three benchmarks dealt with the ejection of an asymmetrically situated control rod at hot zero power in a VVER-440 type reactor. In the fourth dynamic benchmark, a boron dilution scenario was studied. In the first benchmark, only neutron kinetics without feedback was considered. In the second benchmark, a simple modelling of the Doppler feedback was included. The third and fourth dynamic benchmark included a full thermo-hydraulic model of the reactor core. While in the first and second benchmark the macroscopic cross sections were given, in the further benchmarks each participant had to use their own cross section libraries. The results of these benchmarks have been published, e.g. in [Tel93, Gru94, Kyr95b, Kyr96, Kyr97, Kyr98] and will be compiled in an AER benchmark book.

This benchmark book, besides the dynamic benchmarks, contains also various benchmark exercises on problems like isotope contents of burned fuel, burn-up credit, fuel cycle calculations and other reactor-physics problems and is scheduled to be released to OECD for general use.

The fifth dynamic benchmark of AER was the first benchmark problem for coupled 3D neutron kinetics/thermo-hydraulic system codes. It has been defined by FZR to analyse a steam leak scenario for a VVER-440 type reactor [Kli97]. A double end break of the main steam collector (MSCB) was assumed to produce a homogeneously distributed overcooling without consideration of coolant mixing effects. In the initial state, the reactor was assumed to be at sub-critical state at the end of the first fuel cycle. The burn-up distribution at the end of the cycle had to be calculated by the participants. Each participant had to use their own macroscopic cross section sets. The main task of the benchmark was to analyse the re-criticality of the scrammed reactor due to overcooling. The power excursion in the case of re-criticality is terminated by the injection of highly borated water after activation of the high pressure ECC system.

Fig. 20 shows the behaviour of the reactor power calculated by different participants [Kli98]. Differences in the time of re-criticality and the height of the power peak between various solutions of the AER benchmark can be explained by the use of different cross section data. The re-criticality temperatures obtained by steady-state calculations using the different codes and cross section libraries varied in the range from 218.3 ^{o}C to 228.2 ^{o}C, while e.g. the mass losses from the leak agreed very well (see Fig. 21). The time of power increase after re-criticality varies in the different calculations between 62 s and 123 s, the maximum of the power peak differs between 534 MW and 686 MW. These differences are caused by the different rates of reactivity insertion due to the overcooling, which are caused first of all by the differences in the moderator feedback coefficients. Significant differences in the thermohydraulic parameters (coolant temperature, pressure) occurred only at the late stage of the transient during the emergency injection of highly borated water. The rate of ECC water injection depends significantly on the primary circuit pressure behaviour. Differences in the pressure behaviour lead to different amounts of highly borated ECC water injected until the end of the transient. In every case, the amount of injected boric acid is sufficient for achieving sub-criticality.

As a continuation of the AER benchmark efforts for VVER-440 type reactors, recently the 6th AER dynamic benchmark has been defined [Kli00]. It comprises the double end break of one main steam line at full power conditions. Additional new features include effects of coolant mixing in the reactor vessel, asymmetric operation of the feed water system and the definition of a fixed isothermal re-criticality temperature for normalising the nuclear data.

5.4 Accident analysis performed within EU Phare project HU/TS/02

In the project EU Phare HU/TS/02 [Hop99] two accident conditions were studied for VVER-440/213: a steam-line break and a boron dilution transient. The following codes were used by the participants:

- KIKO-3D - ATHLET (KFKI)
- HEXTRAN - SMABRE (VTT)
- DYN3D - ATHLET (FZR), only for steam-line break

- BIPR-8 - ATHLET (KI)

For both cases different assumptions on the mixing before the reactor core inlet were postulated.

The main conclusions were the following:

For the steam-line break the analysis showed that differences in the temperature dependence of nuclear cross-sections led to large differences in the solutions. It was found that this was at least as important as uncertainties in the thermal hydraulic modelling.

In the analysis of the boron dilution calculations it was observed that the numerical diffusion caused strong additional mixing during the transport in the loops.

6. SUMMARY

Generally, the physical behaviour of the NPPs in the reactor core and the primary circuit is well described by the coupled codes. The 3D neutronics models allow to achieve a consistent treatment of static nuclear design analysis and accident analysis because power density distributions and changes of reactivity are determined in the same manner taking into account the specific core loading and the fuel assembly design.

The benchmark activities in the OECD/CSNI framework for LWR and as well as in the AER group for VVER contribute very much to the experience in the application of coupled codes. These activities stimulate the international information exchange and identify directions of further improvement. The effort within the EU Phare project SRR 1/95 was a great step forward in validating coupled codes against plant transient data. The collection of measured data from VVER plant transients was a successful effort and made available several documented plant transient data for future analysis. The results achieved by analysis of two of these transients increased the confidence in the capability of coupled code systems. It would be worth while to undertake such an initiative also for LWRs in the frame of the EU research programme. An international approach would promote the practical application of coupled codes in safety analysis.

The analysis of results using independently calculated nuclear cross-sections by lattice-cell codes revealed differences of these data, in particular for the worth of control rods and for core states with coolant temperatures below nominal conditions.

The experience obtained by the code applications also identified some remaining limitations. The most relevant issue is the lack of efficient and sufficiently accurate mixing models within coupled codes. Today, the mixing phenomena are still analyzed by experimental investigations and growing experience is obtained by CFD analysis. It is not appropriate to integrate CFD into coupled codes, but reliable simplified models with an acceptable range of application should be developed. For calculating local values of safety parameters with high accuracy, it will be necessary to implement pin-by-pin power reconstruction features and flow-models including cross-flow effects as they are already available in some codes. In the applications it was observed that the modelling of the fuel rod, e.g. variable gap heat resistance and burnup-dependent effects, need refinements in the models.

In summary, the development of coupled codes, which fully integrate 3D neutronics into system codes, is an important step towards realistic and accurate analysis of accident conditions in NPPs.

7. ACKNOWLEDGEMENT

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8. REFERENCES

[Fin91] H. Finnemann, A. Galati: NEACRP 3D LWR Core Transient Benchmark, Final Specifications; NEACRP-L-335 (Rev.1), Oct. 1991 (Jan. 1992)

[Fin93a] H. Finnemann, H. Bauer, A. Galati, R. Martinelli: Results of LWR Core Transient Benchmarks; NEA/NS/DO(93)25, Oct. 1993

[Fin93b] H. Finnemann, H. Bauer, A. Galati, R. Martinelli: Results of LWR Core Transient Benchmarks, Proc. of Joint International Conference on Mathematical Methods and Supercomputing in Nuclear Applications. Karlsruhe, 19-23 April 1993

[Fom93] P. Fomitchenko, M. Lizorkin, L. Gilvanov et al. (1993), Coupling of the thermal- hydraulic system code ATHLET and the 3D-neutronics model BIPR8, RRC KI Moscow, GRS Garching (Germany), Interim report

[Fra93] R. Fraikin, H. Finnemann: NEA-NSC 3-D/1-D PWR Core Transient Benchmark: Uncontrolled Withdrawal of Control Rods at Zero Power - Final Specifications; OECD Nuclear Energy Agency, NEA/NSC/DOC(93), Sept. 1993

[Fra96] R. Fraikin: Review of a NEA-NSC PWR Benchmark on Uncontrolled Withdrawal of Control Rods at Zero Power; Physor 1996, Mito, Japan, pp J-99/108, Sept. 1996

[Fra97] R. Fraikin: PWR Benchmark on Uncontrolled Rods Withdrawal at Zero Power, Final Report; NEA/NSC/DOC(96)20, Sept. 1997

[Gru93] U. Grundmann, U. Rohde: DYN3D/M2 - A Code for the Calculation of Reactivity Transients in Cores with Hexagonal Geometry; Report FZR 93-01, Rossendorf, January 1993

[Gru94] U. Grundmann: „Results of the Second Kinetic AER Benchmark“, *Proc. 4th Symposium of AER*, pp. 397, KFKI Atomic Energy Research Institute, Budapest (1994)

[Gru95a] U. Grundmann, D. Lucas, S. Mittag, U.Rohde: Weiterentwicklung und Verifikation eines dreidimensionalen Kernmodells für Reaktoren vom Typ WWER und seine Ankopplung an den Störfallanalysecode ATHLET, *Report FZR-84,* Rossendorf, April 1995

[Gru95b] U. Grundmann, D. Lucas; U. Rohde: Coupling of the Thermohydraulic Code ATHLET with the Neutron Kinetic Core Model DYN3D*, Int. Conf. on Mathematics and Computations, Reactor Physics and Environmental Analysis*, Portland, Oregon (USA), April 30 - May 5, 1995, Proc. Vol. 1, pp. 257-263.

[Gru96] U. Grundmann, U. Rohde: DYN3D - A 3-dimensional Core Model for Steady State and Transient Analysis of Thermal Reactors; Int. Conf. on Physics of Reactors, Mito (Japan), Sept. 16 - 20, 1996

[Gru00a] U. Grundmann, S. Kliem, U. Rohde, A. Seidel, V. Khalimonchuk, A. Kuchin: Beiträge zur Validierung fortgeschrittener Störfallanalysecodes mit 3D Neutronenkinetik – WTZ mit der Ukraine, *Report FZR-301*, Rossendorf, Oktober 2000

[Gru00b] U. Grundmann, S. Kliem, U. Rohde, A. Seidel, D. Panayotov, B. Ilieva (2000): Adaption, Validierung und Anwendung fortgeschrittener Störfallanalysecodes mit 3D Neutronenkinetik – WTZ mit Bulgarien, *to be published as FZR report*

[Heg98] G. Hegyi, A. Kereszturi, I. Trosztel, S. Langenbuch, W. Horche, K. Velkov: Improvement of Plant Transient Analysis for VVER by Coupling KIKO3D with ATHLET, ICONE-6, San Diego, CA, USA, May 10-14, 1998

[Heg99] G. Hegyi, A. Kereszturi, I. Trosztel: Simulation of Some Plant Transient by the Coupled-Code System ATHLET/KIKO3D; Proc. of the 9th Symp. Of AER, Demänovska Dolina Slovakia, 4-8, October 1999

[Hop99] G. Höppner: Final Report Phare/Hu/TJ/02, Topical Issues concerning Accident Analysis: Methodologies and Management Riskaudit Report no 345, December 1999

[Iva97] K.N. Ivanov, T. Beam and A. Baratta, PWR MSLB BENCHMARK, Final Specification, October 1997, US NRC, OECD NEA.

[Iva00] K.N. Ivanov et al.: PWR MSLB Benchmark, VOL. 2: Summary of Results 1 (Point kinetics); NEA/NSC/DOC, Draft, Oct. 2000

[Ker94] A. Kereszturi: KIKO3D - A three dimensional kinetics code for VVER-440. Transactions of the ANS Winter Meeting, Washington, 1994

[Kli97] S. Kliem: „Definition of the Fifth Dynamic AER Benchmark Problem - a Benchmark for Coupled Thermohydraulic System/ Three-Dimensional Hexagonal Neutron Kinetic Core Models“, *Proc. 7th Symposium of AER*, pp. 429-438, KFKI Atomic Energy Research Institute, Budapest (1997)

[Kli98] S. Kliem: „Comparison of the Results of the Fifth Dynamic AER Benchmark - A Benchmark for Coupled Thermohydraulic System/3D Hexagonal Neutron Kinetic Core Models“, *Proc. 8th Symposium of AER*, pp. 429-469, KFKI Atomic Energy Research Institute, Budapest (1998)

[Kli00] S. Kliem, A. Seidel, U. Grundmann: Definition of the 6th dynamic AER benchmark – main steam line break in a NPP with VVER-440, *X. Symposium on VVER Reactor Physics and Reactor Safety,* Moscow (Russia), September 18-22, 2000 (proceedings to be published)

[Kyr95a] R. Kyrki-Rajamäki (1995), Three-dimensional reactor dynamics code for VVER type nuclear reactors, Espoo (Finland), VTT Publications 246

[Kyr95b] R. Kyrki-Rajamäki and E. Kaloinen: „Results of the Third Three-Dimensional Hexagonal Dynamic AER Benchmark Problem Including Thermal Hydraulics Calculations in the Core and a Hot Channel“, *Proc. 5th Symposium of AER*, pp. 255, KFKI Atomic Energy Research Institute, Budapest (1995)

[Kyr96] R. Kyrki-Rajamäki, U. Grundmann and A. Kereszturi: „Results of Three-Dimensional Hexagonal Dynamic Benchmark Problems for VVER Type Reactors“, *Proc. Int. Conf. on the Physics of Reactors PHYSOR96*, pp. J-229 - J-238, Mito, Japan (1996)

[Kyr97] R. Kyrki-Rajamäki: „Comparison of the First Results of the 4th Hexagonal Dynamic AER Benchmark, Boron Dilution in the Core“, *Proc. 7th Symposium of AER*, pp. 321, KFKI Atomic Energy Research Institute, Budapest (1997)

[Kyr98] R. Kyrki-Rajamäki: „Results of a 3D Reactor Dynamics Benchmark Problem on Boron Dilution in the Core“, *Proc. International Conference on the Physics of Nuclear Science and Technology*, v. 2, pp. 1537-1544, ANS, La Grange Park, IL (1998)

[Lan77] S. Langenbuch, W. Maurer, W. Werner, Coarse Mesh Flux Expansion Method for the Analysis of Space-Time Effects in Large LWR Cores, Nuclear Science and Engineering, 63, 437-356, 1977

[Lan96a] S. Langenbuch, M. Lizorkin, U. Rohde, K. Velkov, 3D Neutronic Codes coupled with Thermal-Hydraulic System Codes for PWR, BWR and VVER Reactors. OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements, Annapolis, Md., U.S.A., November 5-8, 1996

[Lan96b] S. Langenbuch, H. Austregesilo, P. Fomitchenko, U. Rohde, K. Velkov, Interface Requirements to Couple Thermal-Hydraulic Codes to 3D Neutronic Codes. OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements, Annapolis, Md., U.S.A., November 5-8, 1996

[Lan99] S. Langenbuch, K.-D- Schmidt, K. Velkov: The Coupled Codes System ATHLET - QUABOX/CUBBOX, Model Features and Results for the Core Transients of the OECD PWR MSLB Benchmark; Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications, Vol. 1, Madrid, Spain, Sept. 1999

[Lan00] S. Langenbuch, K.-D. Schmidt, K. Velkov: Analysis of Different Mapping Schemes of Thermo-Hydraulic Channels for the OECD PWR Main Steam Line Breac Benchmark Phase 3; Proc. of ICONE 8, April 2-6, 2000, Baltimore, USA

[Lef94] T. Lefvert: OECD/NEA Nuclear Science Committee BWR Stability Benchmark, Final Report; NEA/NSC/DOC)94)15, March 1994

[Lef96] T. Lefvert: Ringhals 1 Stability Benchmark, Final Report; NEA/NSC/DOC(96)22, Nov. 1996

[Ler98] G.Lerchl, H.Austregesilo, ATHLET Mod 1.2 Cycle A, User's Manual, March 1998, GRS-P-1/Vol.1,Rev.1

[Liz92] M.P. Lizorkin, V. N. Semenov, V.S. Ionov, V.I. Lebedev: Time dependent spatial neutron kinetic algorithm for BIPR8 and ist verification; Proceedings of the 2nd Symposium of AER (Atomic Energy Research) for Investigating Neutron Physics and Thermohydraulics Problems of Reactor Safety, Paks, Hungary, Sept. 21 -26, 1992, Budapest, KFKI, 1992, pp389-408

[Mie98] J. Miettinen (1998), SMABRE Code Manual, Volume 1: SMABRE System Models and Numerical Methods, Espoo (Finland), Interim report

[Mit00a] S. Mittag, S. Kliem, F.-P. Weiss, R. Kyrki-Rajamäki, A. Hämäläinen, S. Langenbuch, S. Danilin, J. Hadek, G. Hegyi, A. Kuchin, D. Panayotov (2000): Validation of Coupled Neutron-Kinetic / Thermal Hydraulic Codes for VVER, *CSNI Workshop on Advanced TH/Neutronics Codes,* Barcelona (Spain), April 10-13, 2000

[Mit00b] S. Mittag, S. Kliem, F.P. Weiss, R. Kyrki-Rajamöki, A. Hämäläinen, S. Langenbuch, S. Danilin, J. Hadek, G. Hegyi: Validation of coupled neutron kinetic/thermmal-hydraulic codes, Part 2: Analysis of a VVER-440 transient (Loviisa-1); Annals of Nuclear Energy, send to be published.

[Sol00] J. Solis, K.N. Ivanov, B. Sarikaya: BWR Turbine Trip (TT) Benchmark, VOL. 1: Specifications; NEA/NSC/DOC, Draft, Oct. 2000

[Tel93] M. Telbisz and A. Kereszturi: „Results of a Three-Dimensional Hexagonal Kinetic Benchmark Problem“, *Proc. 3th Symposium of AER*, pp. 217, KFKI Atomic Energy Research Institute, Budapest (1993)

[Tes96] V. Teschendorff, H. Austregesilo, G. Lerchl: Methodology, Status and Plans for Development and Assessment of the Code ATHLET; Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements, Annapolis, Nov. 5-8, 1996

[Wei00a] F.-P. Weiss, S. Mittag (2000): Validation of Coupled neutron kinetic / thermal hydraulic codes against transients measured in VVER reactors, *Final Technical Report FZR/SRR195/FIN2.1*, Rossendorf, March 2000

[Wei00b] F.P. Weiss, U. Rohde, U. Grundmann, V. Teschendorff, B. Bwitak: Aufgabenstellung - Validierung - Anwendung von gekoppelten 3D-Kernmodellen und Systemcodes; Atomwirtschaft (ATW) 45 Jg. Heft 6, Juni 2000

Table 1. Comparison of results for the three studied cases of the PWR MSLB Benchmark using different numbers of TH channels

		14 TH	**18 TH**	**177 TH**
K_{eff}		1.00354	1.00439	1.00291
t = 0				
Power Density	[W/cm^3]	91.237	91.254	91.232
Average Fuel Temperature	[K]	838.6	837.4	839.5
Hot Spot Fuel Temperature	[K]	968.8	946.6	979.1
Mean Coolant Density	[g/cm^3]	0.711	0.712	0.711
Time of first Power Peak	[s]	7.420	7.4196	7.4201
t = peak 1				
Power Density	[W/cm^3]	106.375	106.935	105.830
Average Fuel Temperature	[K]	847.9	847.1	848.6
Hot Spot Fuel Temperature	[K]	978.6	961.0	992.3
Mean Coolant Density	[g/cm^3]	0.714	0.714	0.714
Time of second Power Peak	[s]	67.345	67.892	67.24
t = peak 2				
Power Density	[W/cm^3]	22.120	22.841	21.708
Average Fuel Temperature	[K]	585.4	586.6	584.4
Hot Spot Fuel Temperature	[K]	1017.7	861.0	987.9
Mean Coolant Density	[g/cm^3]	0.752	0.753	0.752
t = 100 s				
Power Density	[W/cm^3]	7.457	7.215	7.655
Average Fuel Temperature	[K]	562.0	561.7	562.3
Hot Spot Fuel Temperature	[K]	654.4	616.3	654.5
Mean Coolant Density	[g/cm^3]	0.768	0.768	0.768