A Time-Dependent Neutron Transport Code Coupled with the Thermal-Hydraulics Code ATHLET

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ABSTRACT

We introduce a new neutron transport code for transient analyses of nuclear systems. The code system is based on the well-known Discrete Ordinates code DORT, which solves the steady-state transport equation for an arbitrary number of energy groups and standard 2D geometries. To minimise the errors due to temporal discretisation, an unconditionally stable, fully implicit time integration scheme has been employed. This requires various modifications to the transport code, the extensive use of elaborated acceleration techniques and substantially tightened convergence criteria for fluxes and fission densities. To perform coupled accident analyses, an interface to the thermal hydraulic system code ATHLET has been developed. Nodal power densities from the transport code are passed to ATHLET to calculate thermal-hydraulic system parameters, e.g. fuel and coolant temperatures. These are in turn used to generate DORT-compatible nuclear cross sections by interpolation from pre-calculated data sets for each time step. Finally, to demonstrate the transient capabilities of the coupled code system, the research reactor FRM-II has been analysed. Several design basis accidents were modelled, like the loss of offsite power and the unintended control rod withdrawl.

1. INTRODUCTION

Routine transient analyses for large nuclear power plants are nowadays mainly performed employing nodal coarse-mesh diffusion methods coupled to thermal hydraulic system codes like ATHLET. Although these calculations have been sufficient for many accident scenarios and are applicable to numerous reactor types, the results from few-group 3D-diffusion calculations are sometimes questionable and could clearly be improved by applying neutron transport theory instead. While both deterministic and Monte-Carlo transport codes are used extensively for steady-state analysis, there have hardly been attempts to also consider such methods in the framework of coupled reactor safety studies, mainly due to the excessive CPU times expected.

In this paper we demonstrate the possibility to perform coupled time-dependent analyses for realistic nuclear systems using the transport theory approach. For this purpose we employed a fully implicit, unconditionally stable time integration scheme and the classical Discrete Ordinates method, as it is implemented in the well-known S_N-code DORT [1]. In the following sections we will comment on the

theoretical background of the new transport code, the necessary changes to DORT to implement the time-dependent option and some efficient acceleration techniques. We introduce the coupling of neutronics and the thermal hydraulics code ATHLET and its application to the research reactor FRM-II in Garching (Germany). Some transient studies are performed, namely a loss of coolant accident and the withdrawl of a control rod.

2. THEORY

The time-dependent neutron transport equation (all symbols and abbreviations are well-known and standard in the literature):

$$\underbrace{\frac{1}{v(E)}\frac{\partial}{\partial t}\psi(\vec{r},\vec{\Omega},E,t)}_{\text{Temporal Change}} = \underbrace{-\vec{\Omega}\cdot\nabla\psi(\vec{r},\vec{\Omega},E,t)}_{\text{Leakage Term}} \underbrace{-\Sigma_t(\vec{r},E)\psi(\vec{r},\vec{\Omega},E,t)}_{\text{Interaction Term}}$$

$$+\underbrace{q_{\text{extern}}(\vec{r},\vec{\Omega},E,t)}_{\text{External Source}} + \underbrace{\int dE' \int_{4\pi} d\vec{\Omega}'\Sigma_s(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega})\psi(\vec{r},\vec{\Omega}',E',t)}_{\text{Scattering Term}} \tag{1}$$

$$+\underbrace{\chi_p(\vec{r},E)(1-\beta)\int dE'\nu\Sigma_f(\vec{r},E')}_{\text{Prompt Fission}}\phi(\vec{r},E',t) + \underbrace{\sum_{l=1}^{6}\chi_d^l(\vec{r},E)\lambda_l C_l(\vec{r},E)}_{\text{Delayed Fission}}$$

together with the usually six precursor equations:

$$\frac{\partial}{\partial t}C_l(\vec{r},t) = -\lambda_l C_l(\vec{r},t) + \beta_l \int_0^{\infty} dE'\nu\Sigma_f(\vec{r},E')\phi(\vec{r},E',t) \tag{2}$$

constitutes a system of partial differential equations, which describes the behaviour of any nuclear system. (In the equations above, we have tacitly assumed, that cross sections may be explicit function of time or may be implicitly time-dependent due to the influence of thermal hydraulic system properties). However, the vast majority of transport codes can only handle the simpler steady-state equation:

$$\underbrace{\vec{\Omega}\cdot\nabla\psi(\vec{r},\vec{\Omega},E)}_{\text{Leakage Term}} + \underbrace{\Sigma_t(\vec{r},E)\psi(\vec{r},\vec{\Omega},E)}_{\text{Interaction Term}} = \underbrace{\int dE' \int_{4\pi} d\vec{\Omega}'\Sigma_s(\vec{r},E'\to E,\vec{\Omega}'\to\vec{\Omega})\psi(\vec{r},\vec{\Omega}',E')}_{\text{Source Term}}$$

$$+\underbrace{\frac{1}{k_{\text{eff}}}\chi_p(\vec{r},E)\int dE'\nu\Sigma_f(\vec{r},E')\phi(\vec{r},E')}_{\text{Fission Term}} + \underbrace{q_{\text{extern}}(\vec{r},\vec{\Omega},E)}_{\text{External Source}} \tag{3}$$

where all time-dependencies have been omitted and a separate treatment of the neutron precursors is no longer necessary. In what follows we will show, that the solution of the time-dependent equations 1 and 2 can be reduced to a series of solutions of the simpler steady-state type equation 3.

We impose the fully implicit discretisation scheme and approximate the time derivative in equation 1 as follows (*H* denotes the full transport operator):

$$\frac{1}{\mathrm{v}}\frac{\partial}{\partial t}\psi\left(\vec{r},\vec{\Omega},E,t\right) \approx \frac{\psi(t+\Delta t)-\psi(t)}{\mathrm{v}\,\Delta t} =: \frac{\psi^{(n+1)}-\psi^{(n)}}{\mathrm{v}\,\Delta t} = H^{(n+1)}\psi^{(n+1)}. \tag{4}$$

A similar relation holds for the six precursor equations. Inserting these expressions in equations 1 and 2 and sorting by indices *n* and *n*+1 yields:

$$\begin{aligned} &-\vec{\Omega}\cdot\nabla\psi^{(n+1)}\left(\vec{r},\vec{\Omega},E\right)+\underbrace{\left(\Sigma_t+\frac{1}{\mathrm{v}\Delta t}\right)}_{\Sigma_t'}\psi^{(n+1)}\left(\vec{r},\vec{\Omega},E\right)=\int dE'\int_{4\pi}d\vec{\Omega}'\Sigma_s\left(\vec{r},E'\to E,\vec{\Omega}'\to\vec{\Omega}\right)\psi^{(n+1)}\left(\vec{r},\vec{\Omega}',E'\right)+\\ &\underbrace{\left[\chi_p(E)(1-\beta)+\sum_{l=1}^{6}\chi_d^l\lambda_l\gamma_l\beta_l\right]}_{\chi'(E)}\int dE'\nu\Sigma_f\left(\vec{r},E'\right)\phi^{(n+1)}\left(\vec{r},E'\right)+\underbrace{\sum_{l=1}^{6}\chi_d^l\lambda_l\gamma_l\frac{1}{\Delta t}C_l^{(n)}(\vec{r})+\frac{1}{\mathrm{v}\Delta t}\psi^{(n)}\left(\vec{r},\vec{\Omega},E\right)}_{q'}. \end{aligned} \tag{5}$$

This is nothing else but the steady-state transport equation for the fluxes $\psi^{(n+1)}$ with a modified total cross section, a modified fission spectrum and a "time source" term, which comprises of the fluxes and precursors of time step *n*. These quantities have already been calculated in the previous time step and are thus known at time step *n*+1.

Therefore, the transient extension of a steady-state code is rather straightforward. In principle, the only changes are to build a fixed-source term for each time step, to modify total cross section and fission spectrum appropriately and to call the transport code for each time step over and over again. Feedback effects can be accounted for by varying the cross sections at each time step, corresponding to the thermal hydraulics of the system. The main drawback of this implicit scheme is the fact, that each time step requires a CPU time comparable to a criticality calculation. If already the steady-state equation of the system is difficult to solve, a transient with possibly thousands of time steps would be completely unfeasible.

3. IMPLEMENTATION OF THE CODE DORT IN A TIME-DEPENDENT SCHEME

After having analysed several available steady-state transport codes, we finally chose the well-known S_N-code DORT as the most promising candidate for the time-dependent extension. This code has been successfully applied in many distinct areas and provides us with an excellent performance, especially for systems with large scattering ratio and a significant amount of upscatter. We give a short summary of DORT's main features:

- Arbitrary S_N-order, arbitrary P_N-scattering expansion, arbitrary number of energy groups
- Standard 2D-geometries available: x-y, r-θ, r-z
- Acceleration of inner iterations by the Coarse-Mesh-Rebalance method (CMR)
- Error mode extrapolation for acceleration of outer iterations
- Broad parameter choice to optimise the iteration strategy

The code DORT was implemented as a subroutine into an existing 2D-diffusion code. This was advantageous, since large parts of input- and postprocessing routines, the thermal hydraulics interface to the GRS code ATHLET and several other useful procedures could directly be taken over to DORT.

To achieve higher accuracy and better convergence, DORT was also adapted to 64-bit architectures and is now running in double precision mode on a large variety of UNIX-platforms, including IBM-AIX, COMPAQ/Digital-Unix and Linux.

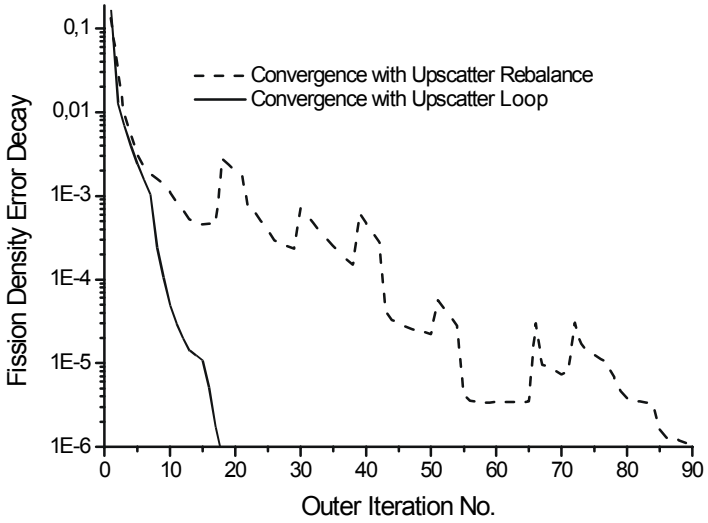

Figure 1: Effectiveness of upscatter loop compared to the upscatter rebalance scheme as included in DORT. We show the error decay for a typical research reactor calculation in 13 energy groups.

As already mentioned above, the time-dependent application of DORT requires several modifications to cross sections and source terms, which have to be performed for each single time step. The modifications of total cross section and fission spectrum are easily implemented and can be done in external modules. To build an appropriate "time source" term turned out to be more complicated. In DORT, a fixed distributed source must be passed in a specific moment expansion. This is sufficient for the isotropic precursor terms in q' (equation 5); the flux values of the previous time step, however, must be passed in their explicit angular representation to the next timestep (cf. equation 5). This option had to be added to the DORT source code.

To improve the convergence rate of the outer iterations, several actions had to be taken. First of all, the rather ineffective upscatter rebalance scheme in DORT was replaced by an upscatter "cycle". Instead of inverting the group transport operator only once per energy group and per outer iteration, a loop over all thermal groups is executed within one outer iteration. This ensures, that all groups receiving upscatter are properly converged. Without this change, a clean error decay in systems with a pronounced thermal spectrum cannot be guaranteed. However, a clean error decay is an essential requirement for an effective acceleration of the outer iteration cycle and is hence vital to the performance of the code. This is demonstrated in Fig. 1, where the error decay of the fission density in a steady-state calculation for a a typical research reactor system (13 energy groups, four of which receive upscatter) is shown. The standard DORT code required almost 100 outer iterations to converge the fission density to better than 10^{-6}. Although only 4 thermal groups were used here, the overall-convergence of the problem is very bad. The application of our upscatter cycle reduces the number of outer iterations to less than 20.

To further enhance the convergence properties of the code, advantage was taken from the use of Chebyshev polynomials to perform a fission density extrapolation. The corresponding routine can optionally replace the error mode extrapolation, as it is implemented in standard DORT. The effec-

tiveness of the Chebyshev scheme strongly depends on the so called dominance ratio of the system under consideration, i.e. the ratio of the two largest eigenvalues. Two examples are shown in Fig. 2 for systems with dominance ratios of 0.712 and 0.983 respectively. In the left picture we compare both Chebyshev and error mode extrapolation with the unaccelerated case, i.e. the power iteration. Due to the rather small dominance ratio, the error decays quite quickly and attains an asymptotic rate for the power iteration. The acceleration achieved by extrapolation techniques is modest and amounts roughly to a factor of 2-3, with the Chebyshev method being slightly favourable over the simple error mode extrapolation. In contrast, for a system with large dominance ratio (Fig. 2, right), Chebyshev extrapolation is extremely effective, as can be seen from the massive error reduction compared to the unaccelerated power iteration.

Despite the use of effective acceleration schemes for inner and outer iterations, solving for a single timestep is still expensive. However, one can benefit from the fact, that the solution of timestep n is in general a quite good approximation to the fluxes to be calculated for timestep n+1, and can be used as an excellent starting guess for the iterative solver. The guess may still be improved by doing a time-like extrapolation. By constructing "inverse reactor periods" from timestep n-1 and n, which are resolved in space as well as in angle and energy:

$$\omega^{(n)}\left(\vec{r},\vec{\Omega},E,t_n\right)=\frac{1}{\Delta t_n}\ln\left(\frac{\psi^{(n)}\left(\vec{r},\vec{\Omega},E,t_n\right)}{\psi^{(n-1)}\left(\vec{r},\vec{\Omega},E,t_{n-1}\right)}\right) \tag{6}$$

one can construct estimates for the angular fluxes $\tilde{\psi}^{(n+1)}$:

$$\tilde{\psi}^{(n+1)}=\psi^{(n)}\cdot\exp\left(\omega^{(n)}\,\Delta t_{n+1}\right) \tag{7}$$

Though this scheme is rather simple, it is extremely efficient. This is demonstrated in Fig. 3, where a comparison is shown for the convergence rate in a typical research reactor problem. On the left hand side, we have used the unextrapolated fluxes as a starting guess for solving the next timestep.

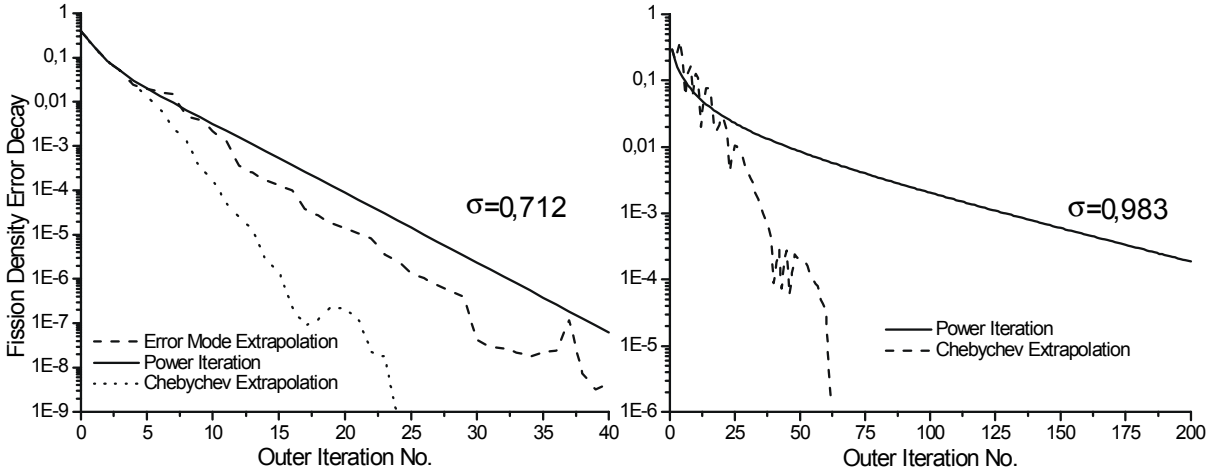

Figure 2: Comparison of extrapolation techniques. The left picture shows the convergence for Chebyshev and error mode extrapolation as compared to the usual power iteration for a system with dominance ratio 0.712, the right picture the same quantities for a dominance ratio close to unity.

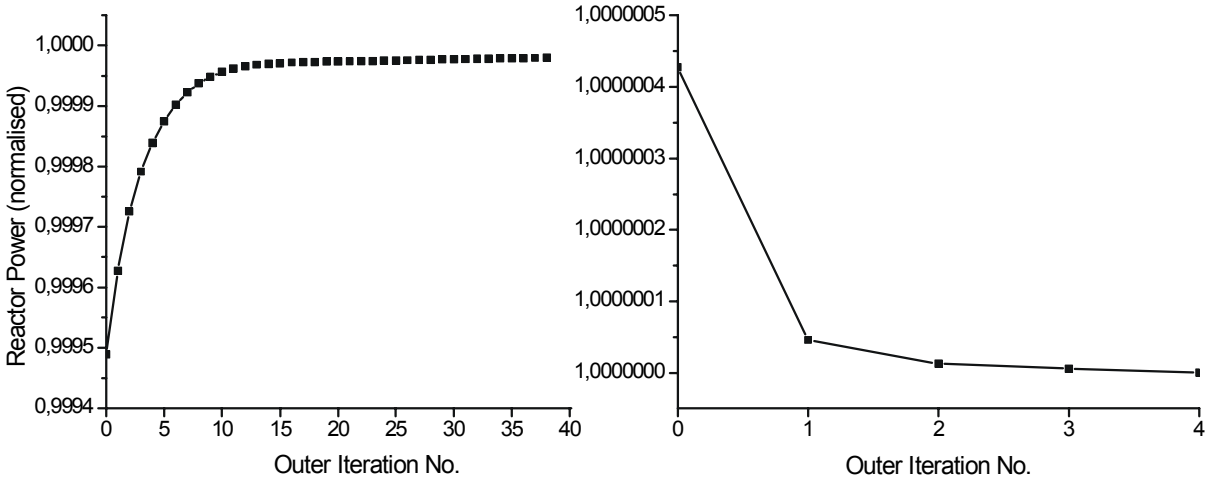

Figure 3: Outer iteration convergence for one time step in a typical research reactor calculation. Shown are the convergence without (left) and with temporal flux extrapolation technique.

Although the power values corresponding to timestep n and n+1 differ only by approximately $5 \cdot 10^{-4}$, roughly 40 iterations are necessary to obtain new fluxes and fission densities converged to better than 10^{-7}. If one uses the time-extrapolated fluxes instead, convergence is dramatically improved: the power value estimated from the flux guess ("zeroth iteration") is already quite close to the true value and it takes only a few more iterations to obtain very accurate fluxes and power densities.

The phase-space resolved reactor periods additionally serve for adapting the maximum time step size. By comparing the temporal flux change with a simple exponential, a rough, conservative estimate of the numerical truncation error can be obtained. Another problem is due to the iterative solution method: the longer the time step, the worse is the convergence within the outer iterations. This may actually pose much tighter restrictions on the advisable maximum time step size than the numerical truncation error.

The extensive use of Chebyshev acceleration, upscatter cyle and time-like extrapolation methods within the transient code system reduces the computing time needed for a single time step by more than an order of magnitude as compared to a criticality problem, although the numerical effort is formally identical.

4. COUPLING OF TRANSPORT CODE AND ATHLET

The transport code has finally been coupled to the well-known thermal hydraulic system code ATHLET [2], which is under development at GRS (Gesellschaft für Anlagen- und Reaktorsicherheit mbH, Germany). The coupling of ATHLET to multidimensional neutron kinetics has been successfully carried out for several codes like QUABOX/CUBBOX, BIPR-8 and DYN3D and is described elsewhere [3].

In Fig. 4 we depict the cooperation of all computer codes participating in the new coupled code system. Besides ATHLET and DORT, a third program for evaluating cross sections is necessary to

complete the cycle. To account for feedback effects, this part has to receive thermal hydraulic parameters from ATHLET as spatially resolved quantities for user-specified "feedback zones" .

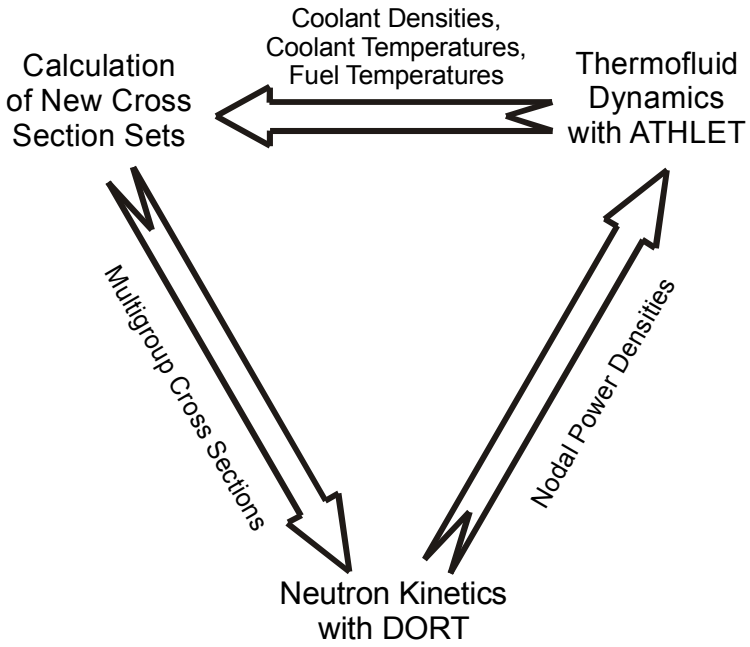

Figure 4: Overview of all codes participating in the coupled neutron transport/ATHLET model and the data exchange between the different modules

For each of these zones, an individual nuclear cross section set is generated and assigned to. The generation of nuclear cross section sets is strongly problem-dependent; in our model we determine them from a large number of pre-calculated libraries, which have been generated in advance for certain discrete triplets of the relevant thermal hydraulic quantities T_{Fuel}, $T_{Coolant}$ and $\rho_{Coolant}$. Multigroup cross sections are then evaluated for each zone by three-dimensional interpolation from the pre-calculated values. The zonewise cross sections are then passed in DORT-compatible format to the transport code, which determines the nodal power densities. After projection of the power distribution onto the ATHLET nodalisation, the thermal hydraulics computation can start over again and so on. In our code system, we build new cross sections for each single time step, regardless how much the system conditions have actually changed.

5. THE RESEARCH REACTOR FRM-II

To test the capabilities of the coupled neutron transport code, we decided to analyse the research reactor FRM-II in Garching (Germany) [4]. The system is characterised by a small, compact reactor core in a large heavy water tank. The FRM-II is cooled by forced light water flow (mass flow rate ~300 kg/s) at a nominal power of ~20 MW. The cylindrical fuel assembly contains 113 evolvent shaped fuel plates of 1.36 mm thickness, separated by water gaps of 2.2 mm width. The moderator tank containing the reactor core is situated in a large light water pool.

The reactor has a few features, which make it interesting both from the thermal hydraulics and the neutron kinetics point of view. The reactor core is quite inhomogeneous and contains, apart from the

fuel, several water channels and a central control rod, which can be moved up- and downwards inside the core for reactor start-up, power control and burn-up compensation. In our model, all components can adequately be described in two-dimensional cylindrical coordinates. Due to the complicated geometry it is advisable to perform coupled analyses using transport theory instead of the usual point kinetics or diffusion approach.

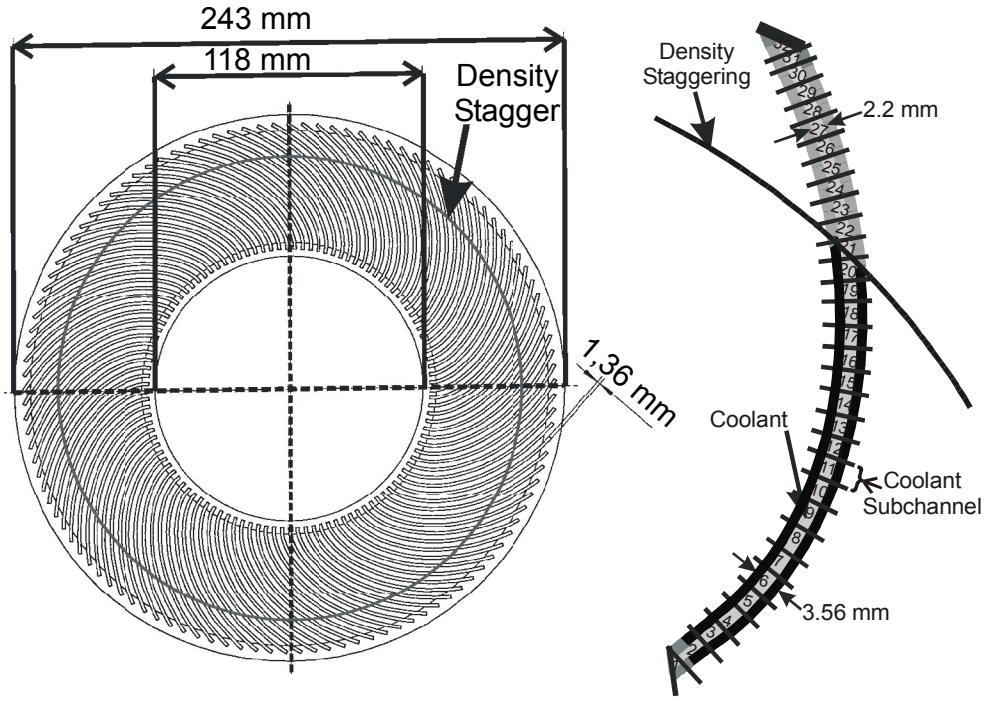

Figure 5: The left picture shows the reactor core of the FRM-II with its evolvent shaped fuel plates; observe the density staggering line, which separates the inner region with high fuel density from the outer region with low fuel density. The right picture shows the corresponding ATHLET model.

The thermal hydraulics of the FRM-II is only considered for the reactor core. In Fig. 5 we show a radial cut through the fuel assembly. Due to the rotational symmetry of the neutron kinetics model it is sufficient to model only one of the 113 coolant channels, as shown on the right hand side of Fig. 5. Along the fuel plates, the coolant channel is divided into 32 parallel ATHLET subchannels. Each of these subchannels is further divided into 28 axial nodes in flow direction. Changes in mass flow, inlet temperature or inlet pressures are simulated by appropriate boundary conditions at the core inlet. While the description of single-phase flow conditions is well established, the modelling of two-phase flow for research reactor conditions is not yet sufficiently validated in ATHLET, which has been primarily applied to nuclear power plants in the past.

One typical transient often considered in research reactor studies is the unintended withdrawl of the control rod. The maximum reactivity insertion of the FRM-II central control rod drive is $4*10^{-4}$ s^{-1}, i.e. an accidental rod movement of 15-18 seconds duration corresponds to roughly 1β (=1$) of reactivity. It is instructive to compare the predictions of transport theory, diffusion and point kinetics. Starting from a reactor power of 10% nominal power (corresponding to ~2 MW), we did several calculations with and without feedback, ignoring all scram signals including the last one at 114% nominal power. At an estimated power of 48 MW, so called flow instabilities are likely to occur, which could damage

the reactor core. It is interesting to ask, whether the duration from scram signal actuation to the onset of flow instabilities is actually long enough to scram the reactor (the duration from scram signal to scram rods being fully inserted amounting to ~1.1 seconds). The results are shown in Fig. 6.

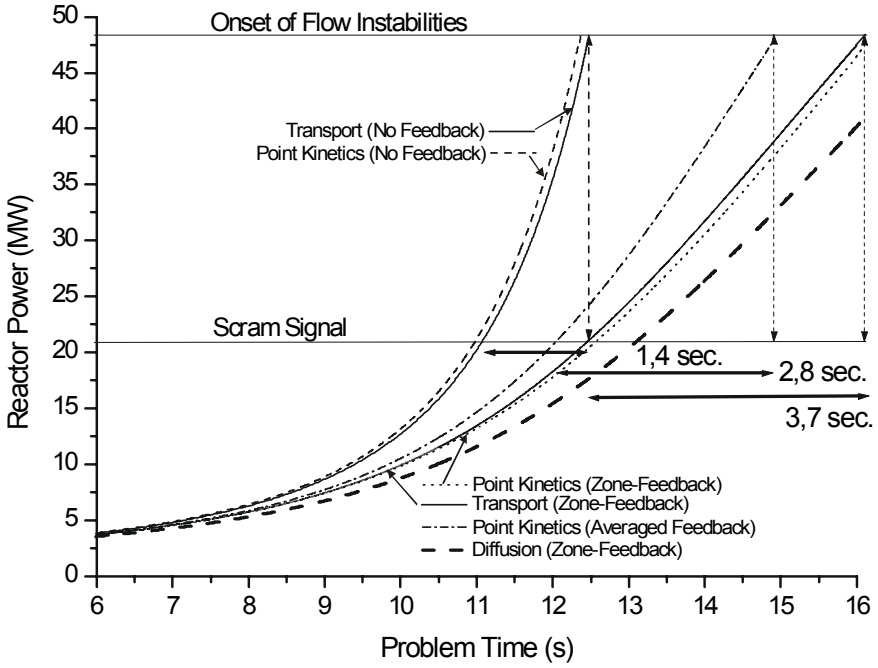

Figure 6: The power excursion of the FRM-II during the unintended withdrawl of the central control rod; we have depicted comparisons of point kinetics, diffusion and transport theory with and without thermal hydraulic feedback.

The first pair of solid/dashed curves shows the power excursion without feedback for point kinetics and transport theory, revealing small deviations only. The good agreement between both approaches is not too surprising, since the main assumption of point kinetics, a constant flux shape function in time, is a good approximation for this rather slow transient. One should, however, keep in mind, that the evaluation of the point kinetics parameters already required a couple of steady-state transport calculations. This also holds for the calculations with feedback, drawn in Fig. 6 as the second pair of solid/dotted lines. Fuel and coolant temperature/density coefficients for the point kinetics solution were derived from fully coupled steady-state calculations. Due to the careful, zonewise evaluation of reactivity coefficients the agreement between both approaches is again very good. In contrast, if one uses global, core averaged temperatures and densities for the determination of reactivity coefficients instead, one obtains misleading results for point kinetics (cf. the dashed-dotted line in Fig. 6). It is obviously necessary to represent feedback effects by spatially resolved cross section sets.

In Fig. 6, we also have indicated the safety margin for scramming the reactor (cf. the thick arrows). Even in the case without feedback, the duration of ~1.4 seconds would be sufficient to protect the reactor from dangerous core conditions; for the core-averaged feedback model we obtain 2.8 seconds, for the model with feedback fully accounted for even 3.7 seconds.

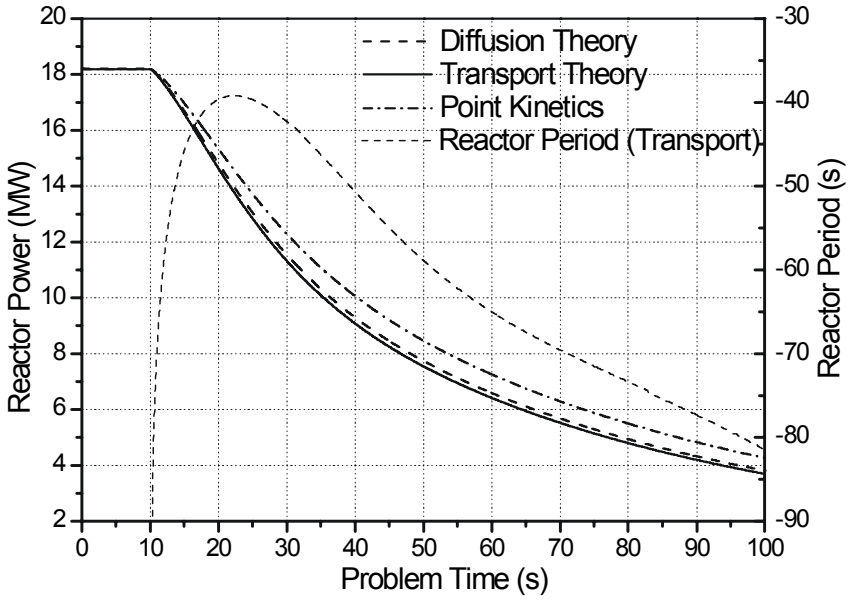

Figure 7: Overall reactor power for diffusion and transport theory as well as point kinetics for the loss of offsite power incident

It is also interesting to compare the diffusion prediction (thick dashed line) with transport theory. On first sight, the significant deviations are surprising. However, these stem exclusively from the fact, that diffusion theory cannot determine the control rod worth correctly, but gives a slightly lower rod worth than transport theory. If the control rod velocity in the diffusion calculation is adjusted such that the net reactivity insertion is identical to the transport case, the prediction of both approaches is in excellent agreement and thus not additionally shown in Fig. 6.

The second accident to be discussed is the loss of offsite power. This causes the primary coolant pumps to run down. Due to the big fly wheels on the main pumps the mass flow reduces to 10% of nominal flow within approximately 100 seconds. Of primary interest in this transient is to ensure, that the heat flux in the core remains at all times below some critical value. This may be characterised by the DNB ratio or the safety margin against the onset of flow instabilities.

Fig. 7 shows reactor power and reactor period during this transient. We again postulated a failure of all scram signals. Obviously, the mass flow reduction gives rise to a higher heat-up of the coolant and hence to a decrease of the coolant density in the core. This in turn causes a strong negative feedback effect and a corresponding decrease in power, with diffusion and transport in quite good agreement. Point kinetics with the simplified estimation of global reactivity coefficients, however, causes significant deviations of several percent.

To judge the thermal hydraulic behaviour of the core, we furthermore depict the maximum fuel and coolant outlet temperatures (Fig. 8) and the two most relevant safety parameters, i.e. the minimum DNB ratio and the minimal safety margin against flow instabilities S_{OFI}, as they occur in different ATHLET subchannels (Fig. 9).

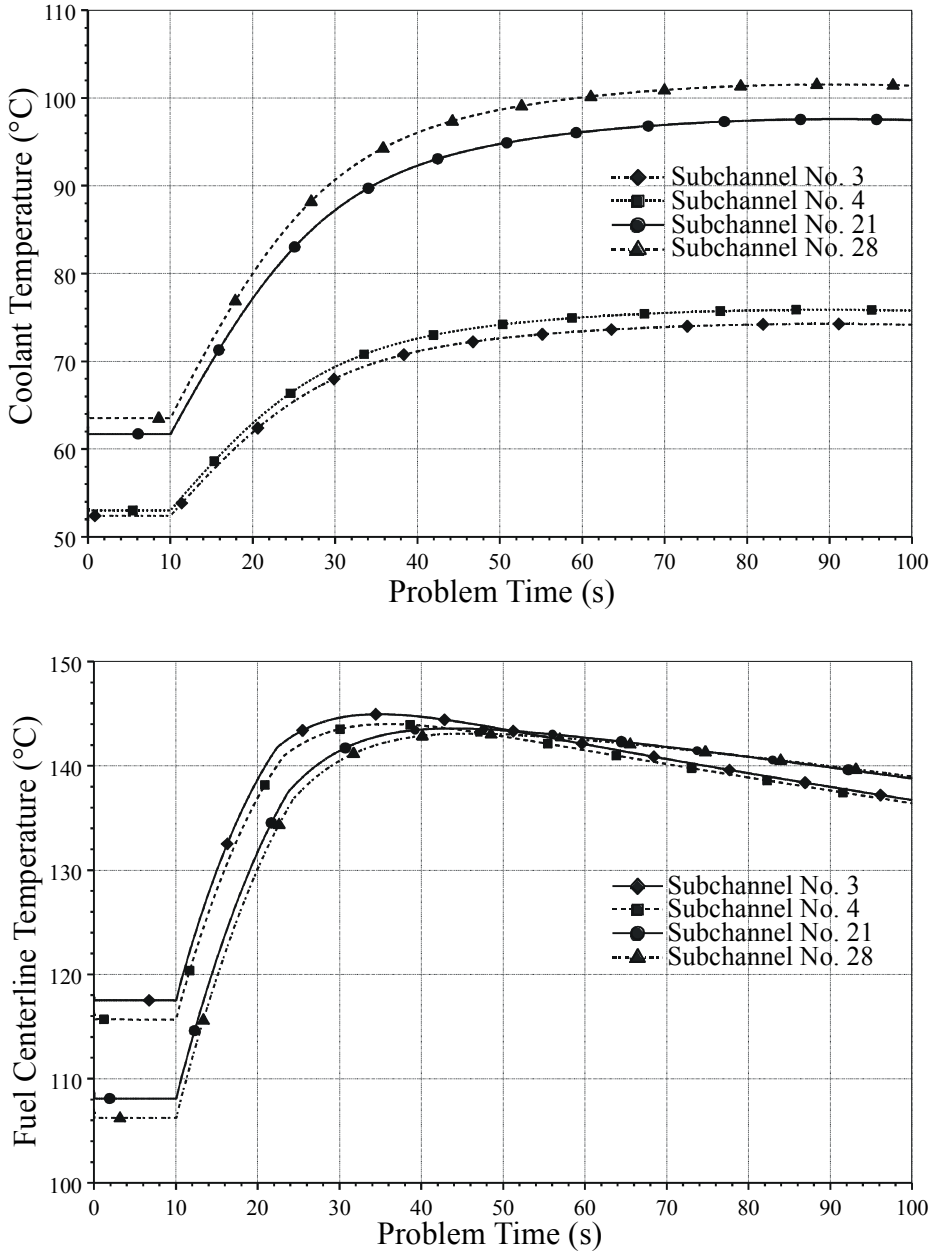

Figure 8: Channelwise coolant temperatures at core outlet and maximum fuel temperatures during the loss of offsite power, shown for the most critical ATHLET channels in the FRM-II core model.

The fuel temperature rises by about 30 K during the transient and assumes a flat maximum roughly 20 seconds after the failure of coolant pumps, while the coolant temperature increases monotonously and assumes a maximum value of ~100 °C, i.e. well below the outlet saturation temperature of ~127 °C. The DNB ratio attains a minimum value of ~1.7, which is still quite far away from the critical value of unity. Finally, even the parameter S_{OFI} remains at all times above one and thus clearly indicates, that the reactor can withstand a loss of offsite power even without reactor scram.

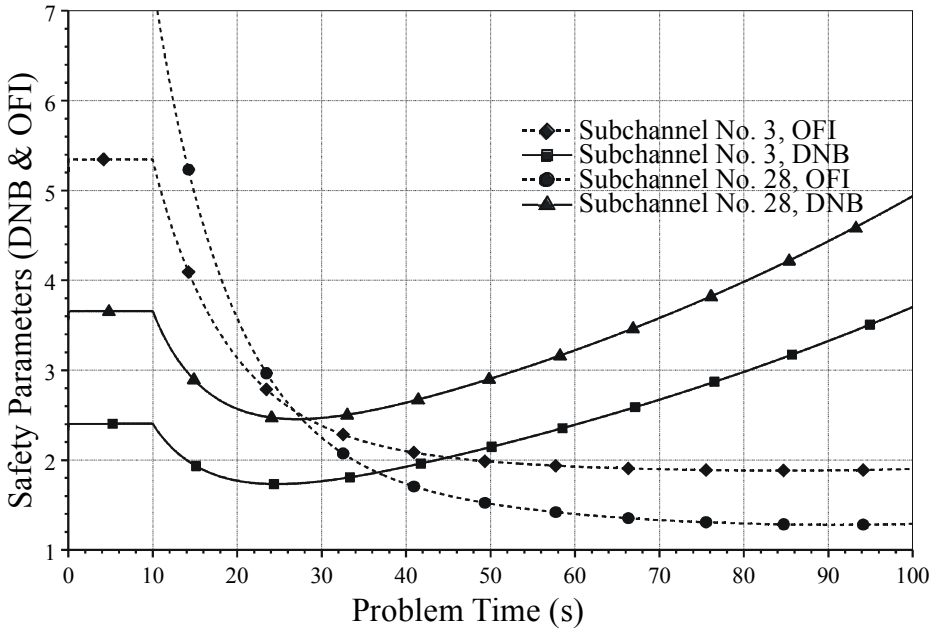

Figure 9: Safety margins against flow instabilities SOFI and DNB ratio for the most critical core positions inside the FRM-II core for the loss of offsite power

CONCLUSIONS

In this paper a new coupled code system was presented and applied to a realistic nuclear system, the research reactor FRM-II. The capabilities of the neutron transport code DORT were extended to transient analyses via the implementation of a fully implicit, unconditionally stable time discretisation, which guarantees a very high accuracy in time-dependent calculations. Furthermore, DORT was coupled to the thermal hydraulics system code ATHLET.
Besides from the application to research reactors with compact core, the code system might as well be used to treat other kinds of nuclear systems, such as ADS (provided a proper source term can be constructed) or innovative reactor designs (like HTR or fast systems). An extension to three dimensions, using DORT's 3D counterpart TORT is intended.

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