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Introduction of a Hybrid Deterministic / Stochastic Calculation Model for Transient Analysis

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Abstract -*This study introduces a concept that includes time-dependent simulations via the coupling of a neutron-kinetic code with a thermal-hydraulic system code in combination with an updating procedure of the lattice-physics parameters during the transient. The idea is to update these parameters during the transient via a Monte Carlo neutron transport calculation of a three-dimensional full-scale model. In this way, lattice-physics parameters can be determined for subregions of the full-scale model taking into account the current spatial distribution of thermal-hydraulic parameters and the actual neutron flux distribution of the full-scale model. Since simulation of transients may involve hundreds of time steps, Monte Carlo full-scale calculations will be performed only after a certain number of time steps. In between, the lattice-physics parameters will be updated by an extrapolation scheme. The method development and testing has been started with the three-dimensional core configuration of the OECD/NEA C5G7-TD benchmark.*

I. INTRODUCTION

Safety evaluations of nuclear power plants involve analyses of normal and abnormal operation states. In particular, transient safety analysis of a nuclear power plant may include the following accidental scenarios: reactivity initiated accidents (RIA), loss of coolant accidents (LOCA), and failure of a single or all the main cooling pumps. Typical RIA events are the ejection of control rods, boron dilution transients, and cool-down transients (under the assumption of a strong negative moderator temperature coefficient). These events can take place in the whole reactor core or only in a localized area (for example due to a partial failure of control rods), which results in different spatial effects. [1]

In order to predict the behaviour of the nuclear power plant during a postulated transient event, coupled neutron kinetic (NK) / thermal-hydraulic (TH) code systems are currently applied. The reason for the necessity of coupled simulations is that the thermal-hydraulics and neutron kinetics build a coupled system through intrinsic feedback effects. For example, Doppler broadening of the U-238 neutron capture cross section is caused by changes of the fuel temperature. Thus, an adequate prediction of the reactor core behaviour is only possible by calculating these reactor dynamics phenomena with coupled code systems.

For the simulation of reactor dynamic problems, the coupling of a three-dimensional nodal diffusion code with a TH system code has been state-of-the-art for many years. The nodal diffusion code solves the diffusion equation in few energy groups on a coarse spatial mesh. The thermal-hydraulics is often modelled by a system code which treats fuel assemblies as thermal-hydraulic channels. In a preceding step to the coupled simulation, lattice-physics calculations are performed for each fuel assembly type in order to provide the neutron kinetic code with homogenized few-group cross sections and kinetic parameters branched with thermal-hydraulic parameters. In other studies, the nodal diffusion code is replaced by a Discrete-Ordinate code. Beside a finer spatial grid and an explicit treatment of the angular dependence, these methods allow a finer discretisation of the energy-dependent variables. The utilisation of a neutron transport code is advantageous over a conventional diffusion code if the nuclear system exhibits inhomogeneities and strong flux gradients on a small distance. [2]

Over the last years, codes such as nTRACER have been developed. These codes use the subgroup method for the self-shielding of cross sections, which are in turn used for the transport solution by means of the method of characteristics and a lower order axial solver. In this way, a homogenization of the fuel assemblies or the fuel pins is not required. [3]

Beside the deterministic neutron transport methods, the time-dependent Monte Carlo (MC) method has been further developed in the last years. The method is similar to a fixed source calculation, and in addition to the neutron position, direction and energy, the time is tracked. The capability of the time-dependent MC method has been demonstrated on various transient cases, although a description of transients for power reactors in full-scale representation is still very challenging. [4, 5]

On the other hand, for steady-state problems, full-scale MC solutions are possible with a reasonable amount of CPU time. For instance, a coupling of the MC code MCNP [6] and the TH system code ATHLET [7] has already been realized and applied to large reactor cores [8].

In this work, a method is developed that utilises a MC neutron transport code in order to update the lattice-physics parameters by means of a three-dimensional MC full-scale

model during the transient. In this way, the advantages of the MC method can be implemented into transient analysis. They are the application of continuous-energy cross section libraries, and geometrically complex models for generating few-group cross sections and kinetic parameters for the nodal code, as well as the calculation of results with a detailed spatial resolution without the necessity of additional methods such as pin power reconstruction. The first goal is to apply this method on simpler systems, such as the OECD/NEA C5G7-TD benchmark [9]. Later these studies will be extended to larger systems including more complex transients.

II. CALCULATION METHOD

This section briefly describes the intended concept of the hybrid deterministic / stochastic calculation model including thermal-hydraulic feedback.

1. Codes and Coupling Scheme

The intended concept includes time-dependent simulations via the coupling of the neutron-kinetic code QUABOX/CUBBOX [1] with the thermal-hydraulic system code ATHLET in combination with an updating procedure of the lattice-physics parameters during the transient. The idea is to update these parameters at time steps during the transient on the basis of a three-dimensional full-scale model using the MC neutron transport code Serpent 2 [10]. This code has the functionality to determine lattice-physics parameters for single fuel assemblies in an infinite lattice or for several subregions in a three-dimensional full-scale model. In the latter case, the lattice-physics parameters are generated with the current spatial distribution of thermal-hydraulic parameters and with the actual neutron flux distribution of the full-scale model.

The integration of full-scale MC calculations into the NK/TH code system will be based on the established staggered time synchronisation scheme, which solves the time-integration explicitly, as shown in Fig. 1.

The TH system code and the NK code perform the time-integration separately; however, the time step size in both codes is synchronised during the transient. Before the NK code proceeds in time, it receives the thermal-hydraulic conditions from the next time step. The NK code interpolates the lattice-physics parameters according to these conditions and proceeds in time. As a first step, this scheme will be changed in a way that the thermal-hydraulic conditions will be passed to the full-scale MC model in order to determine new lattice-physics parameters. Afterwards, the new parameters will be used by the NK code to advance over time as well.

Since simulation of transients may involve hundreds of time steps, the generation of lattice-physics parameters at every time step using a full-scale MC calculation is not practical in terms of computing time. Therefore, full-scale MC calculations will be performed only after a certain number of time steps. In between, the lattice-physics parameters will be updated by an extrapolation scheme (cf. Section II.2).

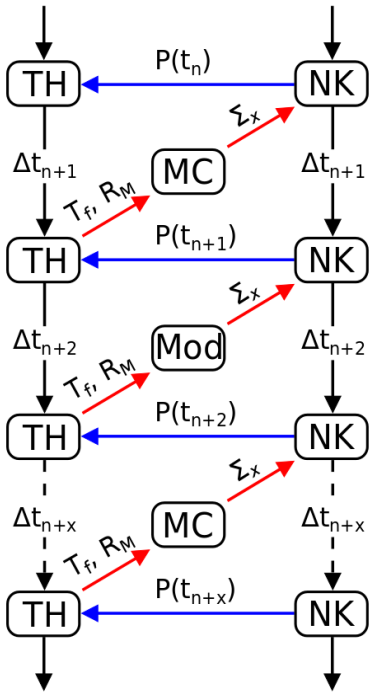

Fig. 1: Simulation scheme for transients with updating of lattice-physics parameters using Monte Carlo calculations or extrapolation; NK: neutron-kinetics, TH: thermal-hydraulics, MC: Monte-Carlo, Mod: Extrapolation method for updating lattice-physics parameters.

Because the concept involves lattice-physics analysis, coupled core calculations, and data transfer and storage between the codes, it is appropriate to make use of the KMacs infrastructure, the core simulator developed by GRS [11]. Within the KMacs project, codes developed at GRS as well as other established codes are coupled by a modular interface.

2. Extrapolation Scheme of Lattice-Physics Parameters

The extrapolation scheme uses lattice-physics parameters that are determined in preceding branch calculations as a basis, i.e. data that is parametrised on thermal-hydraulic conditions, e.g. fuel temperature, moderator density and boron concentration. During the transient, at a time step in which a full-scale MC calculation is performed, lattice-physics parameters are determined for selected subregions with the current thermal-hydraulic conditions in these subregions. At a time step, in which a full-scale MC calculation is avoided, new lattice-physics parameters are calculated through multidimensional linear extrapolation. As a starting point, the conventional lattice-

physics parameters σ and the underlying distribution of branched thermal-hydraulic parameters, fuel temperature T_f, moderator density ρ_M, boron concentration C_B, are used to calculate the gradients $\frac{\partial\sigma}{\partial T_f}, \frac{\partial\sigma}{\partial\rho_M}, \frac{\partial\sigma}{\partial C_B}$ on the grid of the branched thermal-hydraulic parameters. By means of the MC full-scale calculation, lattice-physics parameters σ_{Fs} are obtained taking into account the current thermal-hydraulic condition $T_{f\,Fs}, \rho_{M\,Fs}, C_{B\,Fs}$ present in a subregion of the MC full-scale model. With $T_{f\,Fs}, \rho_{M\,Fs}, C_{B\,Fs}$ lying in the grid of the branched thermal-hydraulic parameters, the corresponding gradients are picked. Finally, by means of the extrapolation ranges $\Delta T_f = T_f' - T_{f\,Fs}$, $\Delta\rho_M = \rho'_M - \rho_{M\,Fs}$, $\Delta C_B = C'_B - C_{B\,Fs}$, the values σ' can be extrapolated:

$$\sigma'\left(T_{f\,Fs} + \Delta T_f, \rho_{M\,Fs} + \Delta\rho_M, C_{B\,Fs} + \Delta C_B\right) = \sigma_{Fs}\left(T_{f\,Fs}, \rho_{M\,Fs}, C_{B\,Fs}\right) + \frac{\partial\sigma}{\partial T_f}\Delta T_f + \frac{\partial\sigma}{\partial\rho_M}\Delta\rho_M + \frac{\partial\sigma}{\partial C_B}\Delta C_B.$$

For one dimension, for example the fuel temperature T_f, the intended extrapolation scheme is presented in Fig. 2. The gradient $\frac{\partial\sigma}{\partial T_f}$ is picked according to the temperature interval that contains $T_{f\,Fs}$. With σ_{Fs} from the MC full-scale calculation used as a grid point and the extrapolation range $\Delta T_f = T_f' - T_{f\,Fs}$, a new value σ' can be calculated.

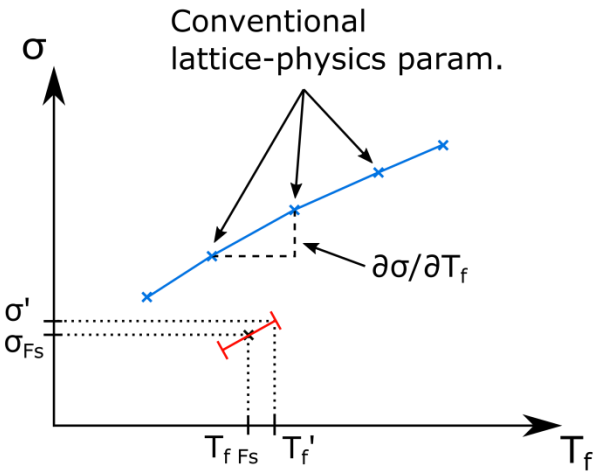

Fig. 2: Scheme for extrapolation of full-scale cross sections with conventional lattice-physics parameters; for simplification, presented for one dimension only.

In further studies, the maximum possible value of the extrapolation ranges needs to be investigated. Moreover, it is planned to implement a control mechanism that limits the maximum number of time steps where extrapolation can be performed.

3. Implementation

Since Serpent 2 has not been integrated into the KMacs infrastructure yet, a new Python module was implemented to perform pre- and post-processing steps for lattice-physics analysis for fuel assemblies in an infinite lattice or full-scale models with Serpent 2. The pre-processing involves the setup of fuel assembly models with branched thermal-hydraulic conditions from the generic KMacs input or, in case of the full-scale model, the assignment of the thermal-hydraulic conditions to the material cards of the full-scale model. The post-processing includes parsing the lattice-physics parameters from the Serpent outputs.

III. APPLICATION

This section outlines results of first calculations based on the OECD/NEA C5G7-TD benchmark.

1. The C5G7-TD Benchmark

Since method development and testing are facilitated with simple models, it is decided to start with the three-dimensional core configuration of the OECD/NEA C5G7-TD benchmark [9].

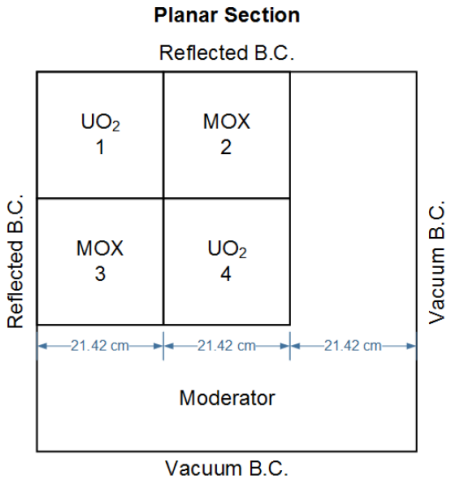

Fig. 3: Planar section of the C5G7-TD core [9].

The C5G7-TD core is a 2x2 lattice with two UO_2 and two MOX fuel assemblies arranged in a checkerboard scheme (cf. Fig. 3). In the x-y plane, reflective boundary conditions are specified for the rear and left of the geometry and vacuum boundary conditions to the front and right of the geometry. The overall length of the core is 128.52 cm, including a top and bottom water reflector of 21.42 cm thickness.

By applying Serpent 2, branched lattice-physics parameters are generated for both fuel assembly types through the conventional manner, namely, fuel assemblies

in an infinite lattice. The thermal-hydraulic conditions are branched as follows: i) fuel temperature [K]: 560.0, 900.0, 1000.0; ii) moderator density [g/cm^3]: 0.66114, 0.71186, 0.75206, iii) boron concentration [ppm]: 0.0, 1000.0, 2000.0. Based on the specification, models of the core are developed for the NK/TH code system. The active length of the core is subdivided into four nodes, each with a height of 21.42 cm. The lattice-physics parameters are then used in the coupled NK/TH calculation in order to yield the boron concentration according to a multiplication factor of 1.00. The total power is set to 50.0 MW. After that, the resulting thermal-hydraulic parameters (fuel temperature, moderator density, boron concentration) of each node are processed and inserted into the full-scale model. Finally, a MC neutron transport calculation is performed with this model.

IV. RESULTS

The MC neutron transport calculation of the full-scale model yields a reactivity difference of -141 pcm to the coupled NK/TH calculation. Keeping in mind that the neutron transport codes are based on different methods, the obtained reactivity difference is considered as a satisfactory result. Table I provides the radial power distribution compared between the Serpent full-scale model and the coupled NK/TH calculation for the C5G7-TD core. Overall, there is a reasonable agreement between the codes.

Table I. Rel. power of the UO_2 and MOX fuel assemblies and the rel. deviation between the codes.

	Serpent	Athlet / QC	rel. dev. [%]
UO2 (1)	1.641(1)	1.678	2.30
MOX (2)	0.890(1)	0.878	-1.30
MOX (3)	0.891(1)	0.878	-1.43
UO2 (4)	0.579(1)	0.565	-2.32

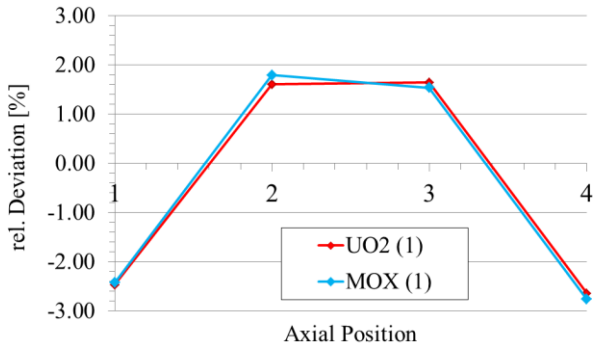

Fig. 4: Rel. deviation between the axial power distribution obtained by Serpent (stat. error < 0.1 %) and Athlet-Q/C for the UO_2 and MOX fuel assembly.

Fig. 4 shows the relative deviation between the axial power distribution calculated by the Serpent full-scale model and the coupled NK/TH calculation of a UO_2 fuel assembly (1) and the MOX fuel assembly (2).

Deviations of up to approximately +/- 2.5 % between the nodal and the MC solutions are observed.

For the four fuel assemblies given in the core layout of the C5G7-TD core (cf. Fig. 3), Fig. 5 shows the fuel temperature as a function of the axial node position. Due to the symmetric core configuration in axial direction, all fuel assemblies reach the maximum fuel temperature at the axial node positions 2 and 3. The UO2 (1) fuel assembly next to the reflective boundaries has the highest fuel temperature and the UO2 (2) fuel assembly next to the water reflector shows the lowest fuel temperature. Both MOX fuel assemblies have the same fuel temperature distribution due to the radial symmetric core configuration.

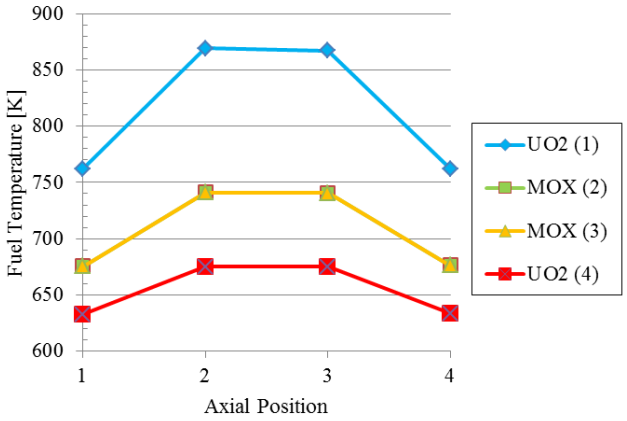

Fig. 5: Fuel temperature as a function of the axial node position.

The axial distributions of the moderator density of the four fuel assemblies are given in Fig. 6. The higher the fuel temperature, the stronger is the decrease of the moderator density as a function of the axial node position.

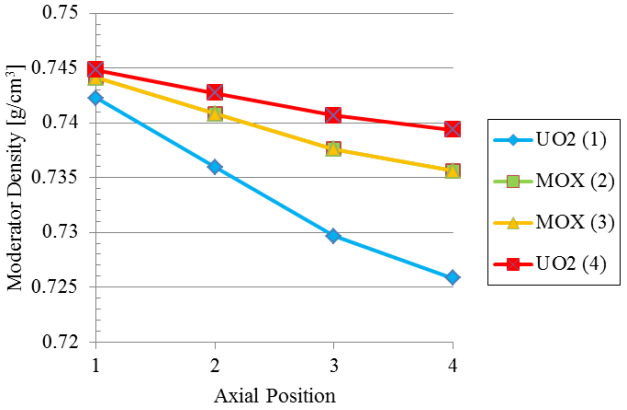

Fig. 6: Moderator density as a function of the axial node position.

It is emphasized here that the coupled NK/TH calculation is only used for describing the time evolution of

the system and updating the TH parameters. The power distributions on node and pin level are evaluated by the MC code, cf. Fig. 7 and Fig. 8; in this way, the need of additional methods such as pin power reconstruction is eliminated.

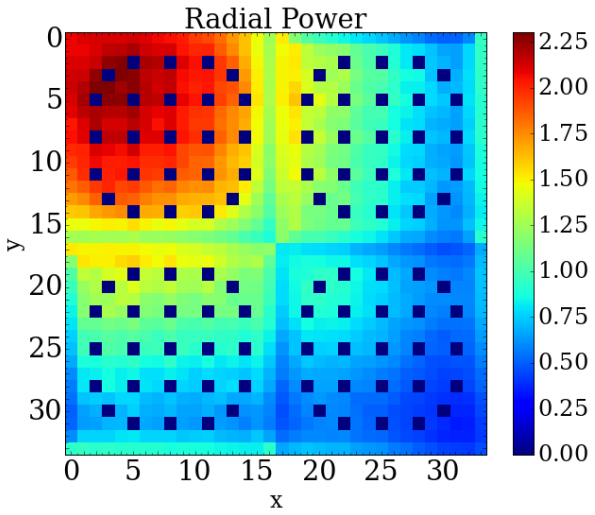

Fig. 7: Radial pin power distribution of the C5G7-TD core obtained from the Serpent Monte Carlo calculation.

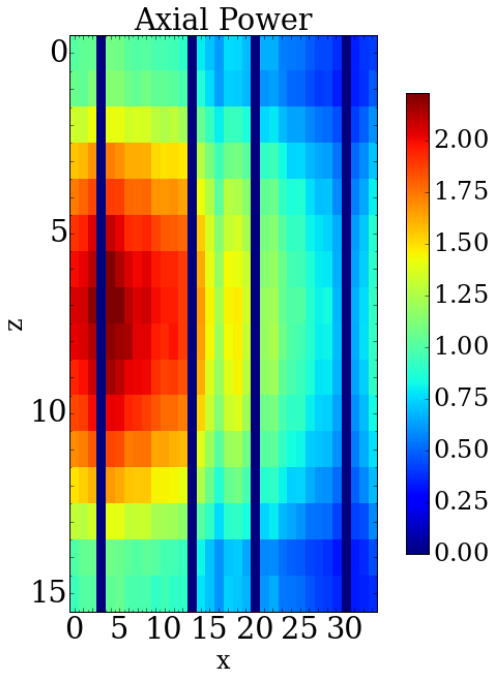

Fig. 8: Axial pin power distribution along the pin row y=4 of the C5G7-TD core obtained from the Serpent Monte Carlo calculation.

V. SUMMARY AND OUTLOOK

The concept of incorporating MC neutron transport calculations into the transient calculation scheme consisting of the NK/TH code system was outlined. The goal of this concept is to update the lattice-physics parameters through a MC neutron transport calculation of a full-scale model at time steps during the transient. The MC code Serpent 2 allows the generation of lattice-physics parameters on the basis of a three-dimensional full-scale model while considering the current spatial distribution of thermal-hydraulic parameters. Furthermore, the full-scale MC calculation offers the possibility to monitor local values during the transient since MC codes are able to perform the neutron transport in complex models with a detailed spatial resolution.

The next steps include the full implementation of the calculation model for transients, and finally, the application of this model on large reactor cores with more complex transients.

ACKNOWLEDGMENTS

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