

A NEW CROSS-SECTION GENERATION MODEL IN THE FAST CODE SYSTEM AND ITS APPLICATION TO THE GEN-IV GAS-COOLED FAST REACTOR

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ABSTRACT

The cross-section generation scheme employed in the 3D spatial kinetics, PARCS subroutines of the FAST code system being used and developed at the Paul Scherrer Institute (PSI) is currently based on the use of pre-processed region-wise macroscopic cross-sections for reference conditions, and their first order derivatives with respect to the state variables. In this study, this approach is compared for both steady-state and transient conditions to a more rigorous background cross-section, or sigma-zero (σ_0 -) model accounting for interrelations between the various feedback effects. Thereby, use is made of the simulation of hypothetical unprotected overcooling and loss of flow transients for the Gen IV Gas-cooled Fast Reactor (GFR). As expected, for this kind of transients without strong interrelations of the feedback effects, reactivity and power evolutions indicate overall good agreement of the two methods, which systematically use ERANOS cross-sections and consistent delayed neutron data. In addition, the relative differences of steady-state values between the σ_0 -model and corresponding ERANOS calculations are rather small. These findings give a certain confidence in the correct implementation and suitability of the new methodology. After completion of these verifications, it is foreseen to make additional comparisons for control assembly fast movements or accidental ejections. As opposite to the cases investigated in this study, larger differences may then be expected.

Key Words: Cross-section generation, Gen IV Gas cooled Fast Reactor (GFR), transient analysis, spatial kinetics, ERANOS.

1. INTRODUCTION

We briefly recall that the FAST code system being currently used and developed at the Paul Scherrer Institute (PSI) is characterized by a unique capability for the core and safety analysis of advanced fast-spectrum systems for a wide range of different systems [1]. Both static and transient core physics, as well as the transient behavior of the power plant as a whole, can be analyzed. The neutron kinetics part of the code system performs a calculation for each time step of (1) in the case of point kinetics: reactor fission and decay heat power, concentration of the precursors of the delayed neutrons, using the thermal-hydraulics (TRACE) and eventually the fuel behavior (FRED) codes, and (2) in the case of spatial neutron kinetics: 3D fields of neutron fluxes, power, concentrations of precursors of delayed neutrons, etc., using the nodal diffusion-theory code PARCS [2] coupled to the TRACE and FRED codes. Since the 3D spatial kinetics scheme implemented in PARCS was primarily developed for light water reactor applications in

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its original form, the associated cross-section parameterization has been revised and modified for fast-spectrum system analysis [1]. In addition to Doppler-effect and coolant density changes, other effects might be equally important for safety-related issues, depending on the specific core design. Clearly, these include fuel and core structure thermal expansions, which are generally benign for fast spectrum systems, since they lower the reactivity when the fuel temperature is increased. Having impact on both core dimensions and fuel density, thermal expansion influences the core behavior mainly through reactivity changes resulting from leakage and self-shielding effects.

Despite this improvement, in general terms, the feedback effects cannot be precisely approximated in their interrelation through polynomial expansions in the state variables with respect to pre-computed macroscopic cross-sections for reference conditions. Therefore, the functional form of the cross-section parameterization used in PARCS [2], which assumes a linear dependence on the state variables, was recently complemented by a more advanced cross-section representation scheme.

First, we estimated the possibility of integrating parts of the ECCO cell code of ERANOS [3] in the FAST system, to perform explicit criticality or slowing down calculations for the actual state parameters. Such a development would aim at obtaining a kind of reference macroscopic cross-sections for each physical region, the thermal-hydraulic (TRACE) and neutronic (PARCS) models being coupled through their original external mapping scheme. However, there was clear evidence that this approach would be too time-consuming for practical applications, especially if the advanced capabilities of the cell code, including collision probabilities in conjunction with fine group calculations based on the subgroup method, were fully exploited in the framework of a detailed core description.

Therefore, we decided, instead, to implement in PARCS a faster methodology which though ensures accurate modeling of the interactions between the different feedback mechanisms. From previous experience, we have opted for a background cross-section, or sigma-zero (σ_0) methodology [4] which is based on the use of microscopic instead of macroscopic cross-sections.

Section 2 describes and indicates features of the envisaged σ_0 -model, including the general ideas of the current developments (Section 2.1), the generation of temperature- and σ_0 -dependent sets of microscopic cross-sections using ECCO (Section 2.2), and the interpolation procedure to generate the macroscopic cross-sections used in the transient analysis (Section 2.3). Section 3 is devoted to results of comparative verification studies, in which the σ_0 -model is compared to the old PARCS cross-section generation scheme. Finally, Section 4 gives some conclusions and recommendations for further work.

2. THE BACKGROUND CROSS-SECTION METHODOLOGY

2.1. General approach

The main idea behind the proposed approach is that of preparing sets of microscopic multi-group cross sections for a studied design. The full library consisting of such isotopic tables in ASCII format is generated based on using the ECCO cell code of ERANOS [3] for a suitable range of temperatures and background cross sections on a common grid (see Section 2.2.).

The temperature-dependent self-shielded data include total, transport, fission, absorption (equal to capture, i.e. the sum of (n,γ) , (n,α) , (n,d) , etc, plus fission), and total scattering matrix cross-sections including elastic, inelastic and (n,xn) reactions. The temperature-dependent, unshielded data include v , which is used for calculating the neutron production cross-section, and thermal scattering matrix cross-sections. Thermal cross-sections are not relevant for the present investigations, but were also considered in view of a generalization for envisaged water ingress studies. The fission spectrum data available for the individual fissionable nuclides was neither shielded nor made temperature-dependent.

The core is subdivided into physical regions. To limit computational time and storage requirements, a physical region of the system to investigate is assumed to consist of groups of selected neutronic nodes characterized by the same reference material composition and similar transient behavior, whereas nodal feedbacks were so far considered individually in case of the old scheme with cross-section derivatives. For these lumped physical regions, at each time of the transient simulation, a newly developed set of PARCS subroutines and input specifications enable to explicitly calculate average macroscopic cross sections to be used in the respective core simulation. These macroscopic cross-sections are generated by interpolating microscopic cross sections from the pre-generated tables, by using, for each time step, region-averaged values for the individual isotopic densities, pre-computed temperatures from TRACE, and associated background cross-sections (see Section 2.3). Changes of the state variables, e.g. coolant density, fuel temperature, core dimensions etc, leading to perturbations of the neutron spectrum, are caught in their interrelations through corresponding σ_0 variations.

A similar methodology is used in LOOP2 [5], and also in the Los Alamos code TRANSX [6] serving as a basis for the cross-section generation scheme available in the transient code SIMMER [7]. However, the sets of multi-group microscopic cross-sections are prepared with the NJOY modular system [8] instead of with a cell code. The proposed scheme with ECCO in conjunction with dedicated NJOY based data additionally guarantees the excellent treatment of resonance overlapping effects for the different situations.

The broad use of the TRANSX code worldwide, and the adequacy of LOOP2 for the neutronics analysis of fast-spectrum systems, which has been successfully demonstrated on the basis of the MUSE-4 benchmark [9] by comparison with MASURCA experimental data and also with analytical predictions of other codes including stochastic values, clearly support the current choice of implementing a background cross-section methodology in PARCS.

2.2. The microscopic cross-section library

Depending on fuel and coolant types, the microscopic cross-sections, which are typically described with 33 neutron groups or more, are generated for basic lattice data (heterogeneous or homogeneous) through precise ECCO calculations in 1968 groups using the subgroup method [3]. These cell calculations are called for by a dedicated UNIX script outside the FAST code system, to determine the data associated to a given nuclide and the different temperature and σ_0 values aimed for. For the σ_0 dependence, these calculations are carried out in an iterative process by means of variations of a parameter p , $0 \leq p \leq 100$, in order to reach, in turn, a targeted σ_0 value. E.g. in the case of a homogeneous cell, p might equal 100 minus the ratio of the changed number density to the original nuclear density of the nuclide under investigation. Obviously, $p=100$ corresponds to infinite dilution ($\sigma_0 = \infty$), the nuclide being not present. Moreover, with decreasing p , the current nuclide density increases and correspondingly σ_0 decreases (see Eq. (1) below), the minimum possible σ_0 value being thus obtained for $p=0$.

For each energy group, by omitting the group index for simplicity, the background cross-section $\sigma_{0,i}$ for nuclide i is expressed as [4]:

$$\sigma_{0,i} = 1/N_i \sum_{j \neq i} N_j \sigma_{tot,j}, \quad (1)$$

where N_i is the cell-averaged, homogeneous atom number density for nuclide i , and $\sigma_{tot,j}$ the total microscopic cross-section for background nuclide j .

For a given p , the corresponding ECCO spectrum is used to carry out the σ_0 condensation, from e.g. 33 to one group, in which only the epithermal groups with energies above 4 eV are considered [3]. For a nuclide not explicitly appearing in the basic lattice description, before iterating, an arbitrary mass is added to the original composition, in order to be able also in this special case to reproduce the targeted σ_0 values.

More specifically, since the density of the nuclide under investigation is proportional to $1/\sigma_0$ (see Eq. (1)), the iterative process uses a suitable two point interpolation scheme based on the function

$$p = a/\sigma_0 + b \quad (2)$$

For each pair of targeted temperature- σ_0 values, starting from the third iteration, which is the third ECCO calculation, the iteration dependent parameters a and b are determined from the solution of a system of two equations (2), using the p and associated one-group σ_0 value corresponding to the current and to the previous ECCO calculation as was explained earlier in this session. Once a and b have been determined, Eq. (2) is used once more, this time in conjunction with the targeted σ_0 value, to derive the next value for p . The first two iterations use $p=0.001$ and $p=99.99999$ to cover the almost entire σ_0 range.

Convergence, which is obtained when the relative difference between current and targeted σ_0 does not exceed 10^{-5} in absolute terms, is usually achieved within a few dozen iterations. Once it has been reached, the ECCO microscopic cross-sections associated to the converged p are saved. After having processed all envisaged pairs of temperature and σ_0 values, the individual microscopic cross-sections are finally combined into a single library data set, terminating the execution of the UNIX script. Iterations on temperature are not needed, since the temperature is input to ECCO. Within the script, as many ECCO inputs are thus needed as the envisaged number of temperatures.

In general terms, since σ_0 is proportional to $1/N$, p can be correlated to parameters on which N depends, i.e. in addition to the cell-averaged or region-wise atom number density of the specific nuclide i to investigate, to the fuel radius in the case of a cylindrical pin cell, or to the subassembly pitch in the case of a more detailed 2D lattice description, etc.

For fast-spectrum systems, except for the special case of strong absorbers like ^{10}B requiring different sets to account for specific heterogeneities of the control rods, the self-shielded tables generated with the proposed approach were found almost independent of the cell specifications, e.g. heterogeneous or homogeneous, the calculation options used in ECCO, e.g. fundamental mode, zero-buckling or slowing-down scheme with an external fix source. They were also found almost independent of the specific choice of the iteration parameter p . These findings clearly support the adequacy and also indicate a certain robustness of the selected approach for fast-spectrum system analysis.

The temperatures being considered in the current transient analyses of the Gen IV Gas-cooled Fast Reactor (GFR) range from 300 to 3000 K in steps of 300 K. The systematic 20-point σ_0 -grid assuming piecewise equal logarithmic spacing comprises the values of 10^{10} , 10^5 , 10^4 , 5620, 3160, 1780, 1000, 562, 316, 178, 100, 56.2, 31.6, 17.8, 10, 5.62, 3.16, 1.78, 1, and 0.1 barns. The value of 10^{10} barns nearly represents infinite dilution. This grid is the result of a series of preliminary optimization calculations not reported here. In particular, the use of more refined values was found so far not to significantly alter the computational results. However, the associated computational time and especially the overall storage requirements of the FAST code system would remarkably increase.

A complete data library of 33 neutron group cross-sections has been generated for the GFR, including 6 pseudo fission products for ^{235}U , ^{238}U , ^{239}Pu , ^{240}Pu , ^{241}Pu , and ^{242}Pu , allowing transient analyses also for irradiated fuel compositions. This data is based upon the adjusted JEF-2.2 cross-sections available in Edition 2.1 of the ERANOS package [3]. It is worthwhile noticing that the entire library preparation did not take more than a few days work, without requiring particular skills.

2.3. The macroscopic cross-section generation

Nuclide-wise atom number densities corresponding to reference conditions are supplied for each physical region (see Section 2.1) by means of a newly developed PARCS input deck option.

For a given vector or scattering matrix microscopic cross-section, σ , the macroscopic cross-section of the physical region is then obtained by computing

$$\Sigma = \sum_i N_i \sigma_i. \quad (3)$$

Thereby, the original input concentrations are modified according to the actual core dimensions, control rod positions, fuel temperature and coolant density distributions, to derive the N_i , using average TRACE values.

To evaluate the σ_i values, the following steps are carried out in chronological order, by sometimes omitting, for simplicity, the energy group dependence:

- (1) For the actual temperature, interpolation of the data sets available in the microscopic cross-section library is performed on the basis of the same, consistent $\log(T)$ polynomial interpolation as it occurs in ECCO [3]: More precisely, a cubic polynomial passing through the values of 4 points, two on each side of T , is used. In the special case of the outermost tabulation interval at either end of the temperature range, the polynomial is quadratic through the 3 outermost tabulation points.
- (2) The nuclide-wise background cross-sections $\sigma_{0,i}$ for each energy group (see Eq. 1 above) are determined using the previously estimated N_i values for current conditions, in conjunction with total microscopic cross-sections for the given temperature after completion of step (1). This occurs in an iterative process, since σ_{tot} depends on σ_0 (refer to step (3) below for the σ_0 interpolation). Fortunately, tight convergence, i.e. within maximum relative $\sigma_{0,i}$ variations of 10^{-5} , in absolute terms, between two successive iterations, is achieved quite rapidly, the number of iterations being found < 5 , in most cases.

Normally, the $\sigma_{0,i}$ resulting from step (2) for each energy group are directly used in the case of physical regions with fuel material, to compute the σ_i values required in Eq. 3 (see step (3) below). However, in two special cases, averaged σ_0 values over a certain energy range are used instead. More specifically, these two cases are

- a. Regions of fuel cooled with sodium for energies covering the 2.8 keV elastic scattering sodium resonance, i.e. between 0.75 and 15 keV. The rather empirical choice of these two values, corresponding to group boundaries of the 33 neutron group structure, is the result of comparing sodium void predictions, not reported here, with corresponding ERANOS values.
- b. Structural material and absorber regions without fuel, i.e. reflector, control rod materials, etc, in the entire epithermal range. In this case, the intermediate resonance approximation is additionally accounted for [10], which results in increased $\sigma_{0,i}$ by $\lambda_i \sigma_{pot,i}$, where λ_i is the Goldstein Cohen intermediate resonance factor for nuclide i ($0 \leq \lambda_i \leq 1$, $\lambda_i \sim 0.5$ for structural materials), and $\sigma_{pot,i}$ is its almost energy-independent elastic scattering cross-section in the lower epithermal range.

In steps (2) a and (2) b group-averaging is performed on the basis of $1/E$ or a user-supplied, pre-determined adjoint function which is provided in a new card of the PARCS input deck called “*group_bdry*”.

- (3) σ_i is then determined based upon a hyperbolic-tangent σ_0 interpolation using the data for the given temperature after completion of step (1). The interpolation is similar to the scheme used in TRANSX [6], except that only those two library points encompassing $\sigma_{0,i}$ are considered.

More precisely, by omitting the σ_0 nuclide index for simplicity,

For large σ_0 values, i.e. for $\sigma_0 \geq 10^4$, $1/\sigma_i$ is assumed to have linear dependence on $1/\sigma_0$.

For low σ_0 values, i.e. for $\sigma_0 < .10^3$, $\log(\sigma_i)$ is assumed to have linear dependence on $\log(\sigma_0)$.

Whereas for intermediate σ_0 values, i.e. for $10^3 \leq \sigma_0 < 10^4$, the arithmetic average of the values obtained with the previous two laws is used.

The time-dependent, global fission spectrum of a physical region with fuel material is obtained by weighting the individual nuclide fission spectra available on the library with the fractional fission production rates of these nuclides being obtained with the current flux distribution from PARCS. The kinetic parameters are supplied, in PARCS, using the original input specifications.

3. VERIFICATION STUDIES

3.1. Steady-state results

In Table I, steady-state values are compared between the new σ_0 -model within the FAST code system and corresponding ERANOS nodal diffusion-theory predictions for a model of the large 2400 MWth Gas-cooled Fast Reactor (GFR) [11]. These include multiplication factor k_{eff} , all control rod assemblies being located at their parking position, Doppler constant, full depressurization reactivity, and control rod worth for the Control System Devices (CSDs) and for the Diverse System Device (DSD).

Results for the Experimental Technology Demonstration Reactor (ETDR), a low power (~50 MWth), helium-cooled fast reactor currently seen as the first necessary step towards the electricity generating prototype GFR [12], are summarized in Table II as an additional illustration.

Table I. GFR neutronic parameters (pcm, 1pcm = 10⁻⁵)

Code	FAST (σ_0 -model)	ERANOS
k_{eff}	1.062	1.057
Doppler constant ($\Delta\rho/\Delta\log(T)$)	-1483	-1521
Full depressurization reactivity	175	187
CSD worth (internal ring)	2574	2502
CSD worth (total)	17383	16167
DSD worth	5278	5035
Control rod worth (total)	21355	20304

Table II. ETDR neutronic parameters (pcm, 1pcm = 10⁻⁵)

Code	FAST (σ_0 -model)	ERANOS
k_{eff}	1.077	1.076
Doppler constant ($\Delta\rho/\Delta\log(T)$)	253	250
Full depressurization reactivity	-149	-127
CSD worth (1/4 of the length inserted)	811	813
CSD worth (3/4 of the length inserted)	10890	10876

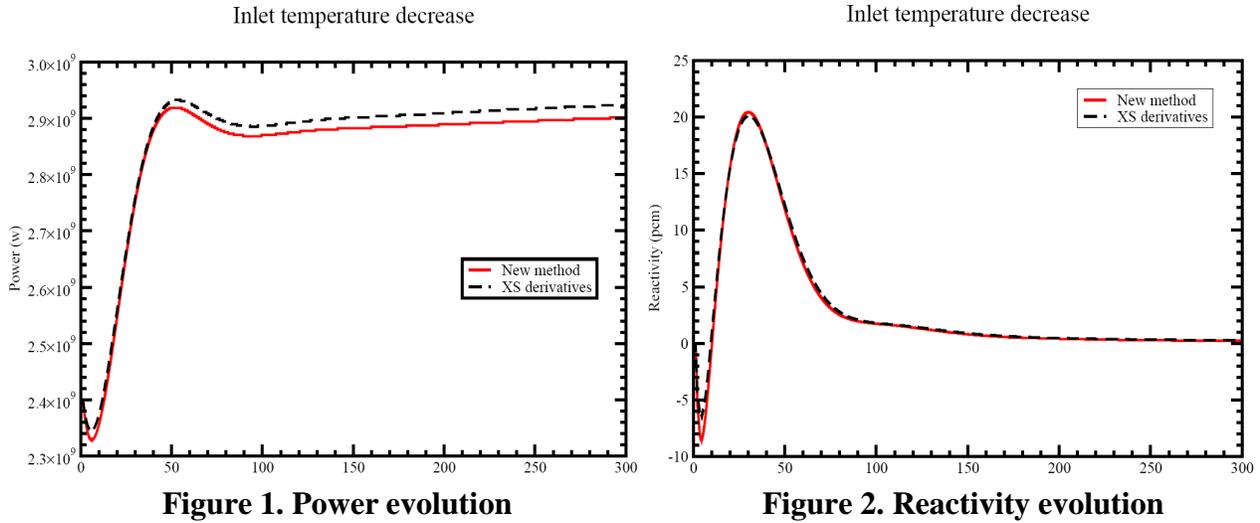
As expected, by inter-comparing the two systems, a better overall agreement of the two methods is shown in the case of the ETDR, which is characterized by harder neutron spectrum and therefore lower resonance importance for the fuel nuclides. A consistent trend of better agreement with less moderation between the σ_0 -model and ERANOS was found by additional analyses of systems with different coolant types including sodium and lead, not reported here.

3.2. Transient results

The first GFR transient comparing the σ_0 -model (“New method”) to the old PARCS method (“XS derivatives”) originates from the 5 minute simulation for a hypothetical linear decrease of the inlet temperature by 100 C, i.e. from 480 to 380 C, taking place during 1s. Core overcooling starts after the simulation of steady-state conditions.

For the initial “zero-transient” calculation, the computed dynamic reactivity is exactly zero, and the power stays at its nominal value of 2400 MWth, indicating correct FAST code predictions using both methods. Excellent agreement within 1pcm between forward and adjoint steady-state static reactivity was obtained for very tight convergence criteria in PARCS.

Figs 1-2 display the time-dependent power and reactivity evolutions during the transient.



Decreasing the inlet temperature primarily decreases the overall coolant temperature first, thus increasing the coolant density. As a result, in the first 5 seconds of the simulation, small reactivity and power decreases are noticeable. These are due to the negative coolant density feedback, consistent with Table I. As a consequence of these coolant temperature and power decreases, the fuel also starts becoming colder, whereas the diagrid temperature decreases with certain inertia as a result of the inlet coolant temperature decrease. This further temperature reduction leads to a more significant increase of the reactivity followed by a corresponding power increase. This effect can be explained, in order of importance, with the positive contribution of Doppler and thermal-mechanical core compaction feedbacks to the reactivity. After that, reactivity and power decrease again, tending, in turn, to reach asymptotic values, primarily due to negative contributions of Doppler and thermal-mechanical core expansion feedbacks in this latter phase of the transient.

The agreement of the two methods is quite satisfactory, bearing in mind that the transient conditions considered deviate significantly from the steady-state values.

An additional transient used for the current verification purposes was a loss of flow without scram. The flow rate is supposed to rapidly decrease to ~5% of its nominal value (natural circulation). The transient simulates, with the use of boundary conditions in TRACE, a primary system pump trip which activates the Decay Heat Removal System (DHR). Figs 3-4 display the time-dependent power and reactivity evolutions for a 10 minute simulation.

In this study we did not consider possible severe consequences of the accident. The transient behavior is dominated by enhanced Doppler and core expansion effects arising from a significant increase of the fuel temperature. These favorable feedbacks result from the loss of forced gas circulation, nearly leading to decay heat conditions 5 minutes after pump trip. Especially the very strong Doppler effect brings the power down to about 15% of its nominal value.

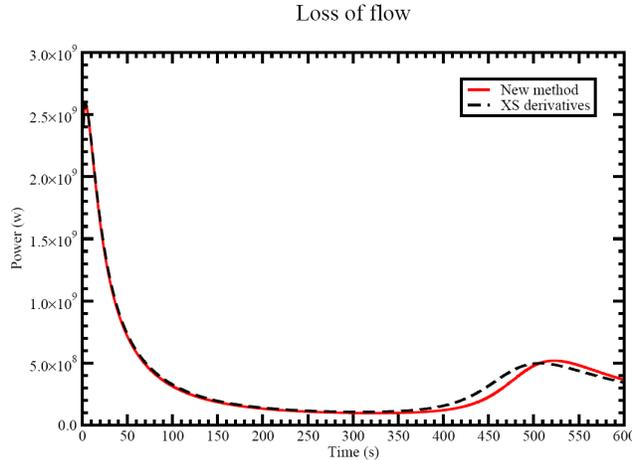


Figure 3. Power evolution

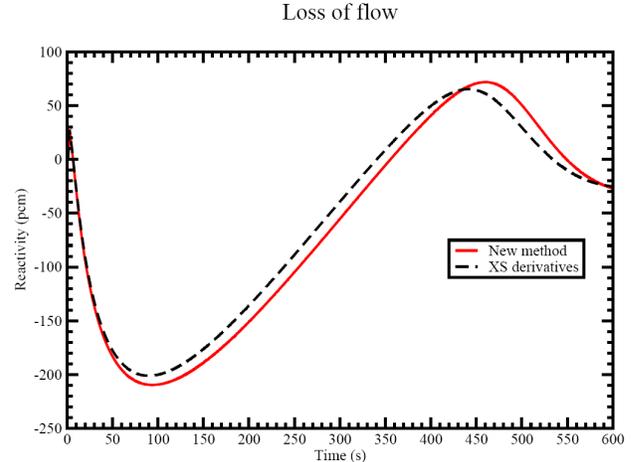


Figure 4. Reactivity evolution

The agreement of the two methods in analyzing this transient is also overall satisfactory. Small differences being observed especially for longer term values can mostly be attributed to the fuel temperature distribution, which has been averaged in space over large core regions in both the radial and axial directions, to reduce the computational time in case of the σ_0 -model (see Section 2.1 above).

As opposite to these two transients, overpower due to progressive or rapid control rod withdrawal as well as loss of coolant accidents, particularly in conjunction with sodium systems, are expected to cause simultaneous changes of the feedback parameters in their interrelation and time evolution [13]. Clearly, these effects are indicative for the necessity of the new σ_0 -model within the FAST code system, and will be studied in detail in a next step of the study.

4. CONCLUSIONS

The cross-section generation scheme employed in the 3D spatial kinetics, PARCS subroutines of the FAST code system is currently based on the use of pre-processed region-wise macroscopic cross-sections for reference conditions, and their first order derivatives with respect to the state variables. In previous studies [13-15], detailed comparisons between spatial and point kinetics have been made on the basis of this cross-section generation scheme, indicating good agreement between the two methods. However, feedback effects cannot, in general terms, be precisely approximated in their interrelation through polynomial expansions in the state variables with respect to pre-computed macroscopic cross-sections for reference conditions. Therefore, it was decided to improve the cross-section representation in the PARCS code of the FAST system. The paper dealt with a detailed description of these enhancements. We implemented a fast-running method based on the use of background cross-sections [4] (σ_0 -model), by maintaining the original coupling between thermal-hydraulics and neutronics. At each time of the transient simulation, a newly developed model enables to explicitly calculate macroscopic cross-sections to be used in the respective core simulation. Using TRACE values for the actual state parameters, i.e. coolant density, fuel temperature, core dimensions, etc, the macroscopic cross-sections are generated for the current isotopic nuclear densities, by interpolating pre-generated

microscopic cross-sections tabulated for different temperature and σ_0 values. Variations of the state variables e.g. leading to spectral perturbations are then caught in their interrelations through corresponding σ_0 variations. The dedicated use of ECCO with the associated data for preparing system-dependent libraries of such microscopic cross-sections in a multi-group structure, additionally guarantees the excellent treatment of resonance overlapping effects for the different situations.

In this study which was dedicated to necessary verification calculations, the new σ_0 -model was compared to the old PARCS method. Thereby, use was made of the simulation of overcooling and loss of flow transients for the Gen IV Gas-cooled Fast Reactor (GFR), without scram. As expected, for this kind of transients without strong interrelations of the feedback effects, reactivity and power evolutions were overall indicating good agreement of the two methods, which systematically use ERANOS cross-sections and consistent delayed neutron data. In addition, the small relative differences of steady-state values between the σ_0 -model and corresponding ERANOS calculations obtained for a larger spectrum of systems with different coolant types give indeed a certain confidence in the correct implementation and suitability of the new cross-section generation scheme.

As opposite to the so far studied transients, overpower due to progressive or rapid control rod withdrawal might induce significant interrelations between the feedback parameters in their time evolution [13]. Therefore, it is recommended, as a next step of the study, to make additional comparisons for control assembly fast movements or accidental ejections due to, for instance, the failure of a control assembly drive. It is foreseen to use the detailed, assembly-wise core behavior model developed in a preparatory study for the most recent GFR design [16]. Since the interrelation of the various feedback mechanisms will definitely play a major role, larger differences between the two methods are expected, in this case.

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