

## VERIFICATION OF REACTOR DYNAMICS CALCULATIONS USING THE COUPLED CODE SYSTEM FAST

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### ABSTRACT

The FAST project is a PSI activity in the area of fast-spectrum core and safety analysis with emphasis on generic developments and Generation IV systems. One of the main goals of the project is to develop a unique analytical code capability for the core and safety analysis of critical (and sub-critical) fast spectrum systems, with an initial emphasis on gas-cooled fast reactors. Both static and transient core physics, as well as the behavior and safety of the power plant as a whole are to be studied. In the framework of the overall development of the FAST code system, it is important to verify its individual parts, including the links between them. The paper is focused on this detailed verification procedure. Steady-state conditions as well as a series of hypothetical control rod ejection accidents are investigated based on a CAPRA-CADRA reactor core loaded with Superphénix-like MOX fuel. In particular, the TRAC-AAA/PARCS elements of the FAST code system are compared with the stand-alone ERANOS/KIN-3D code, using as far as possible equivalent options for a series of hypothetical control rod ejection accidents.

**KEYWORDS:** CAPRA-CADRA, dynamics, ERANOS, PARCS, TRAC-AAA.

### 1. INTRODUCTION

The FAST (Fast-spectrum Advanced Systems for power production and resource management) project is an activity in the area of fast spectrum core and safety analysis with emphasis on generic developments and Generation IV systems. One of the objectives is to develop a general tool for analyzing core statics and the dynamic behavior of the whole reactor system, which is devoted to advanced fast spectrum concepts in multi-domains including different coolants. A code system of this complexity is particularly attractive in the context of safety-related studies aimed at establishing the basic feasibility of the advanced fast reactors being proposed by the Generation IV International Forum. Using this code system, it will be possible to analyze in a systematic manner a wide variety of transients including those, which may lead to asymmetric core conditions. An example is the insertion of moderating material, which may lead to a reactivity increase, e.g. water/steam in a gas-cooled core. In addition, through the modeling of the whole reactor system, it will be possible to assess those phenomena, which depend on the direct interaction between the primary and secondary systems and the core behavior.

The driving force to achieve this ambitious goal lies in the fact that: (a) a unified system for the analysis of a broad range of hypothetical scenarios is not available currently, and (b) the stand-alone codes being foreseen as part of the package are state-of-the-art as regards a certain domain of applications, but are currently either not coupled together or adequately qualified and tested for advanced fast spectrum system analysis.

In addition to a brief general discussion of the structure of the new FAST code system and the organization of the interfaces and data transfer, special emphasis is given, in this paper, to examples of verification of the reactor dynamics parts, i.e. TRAC-AAA/PARCS being used in conjunction with ERANOS-based cross sections.

## 2. STRUCTURE OF THE FAST CODE SYSTEM

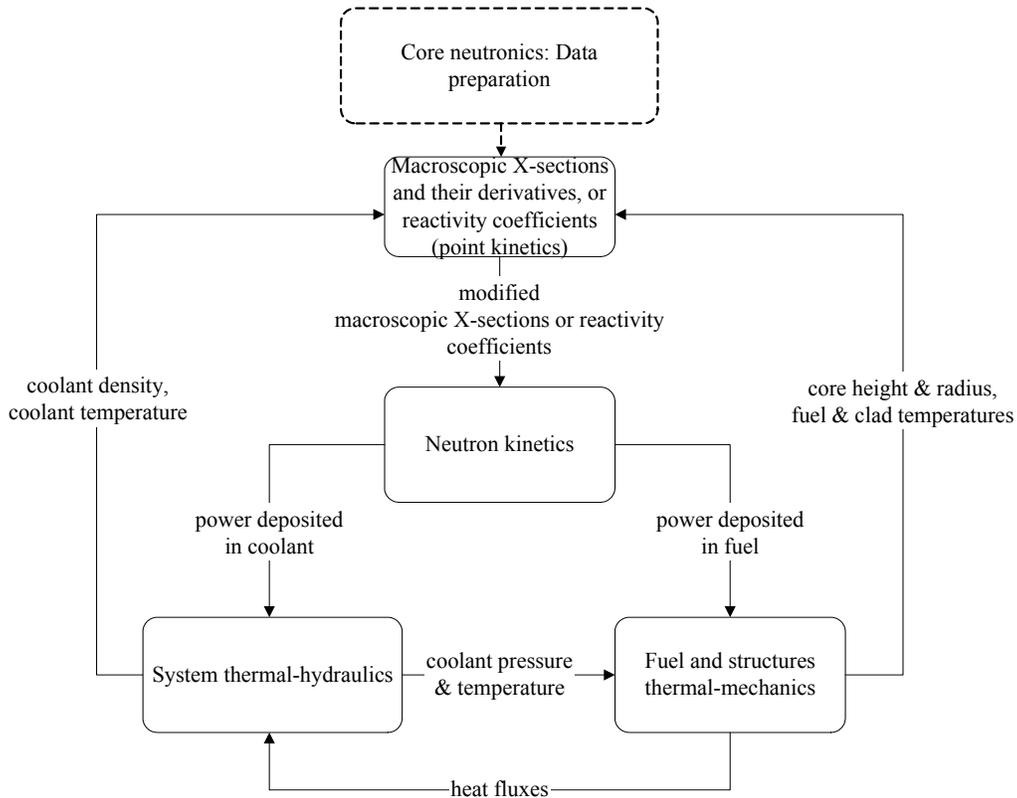
The FAST code system being assembled [1] is based on the coupled reactor static/kinetic codes ERANOS [2], [3], [4] and PARCS [5], the thermal-hydraulics code TRAC-AAA [6] and the fuel rod thermal mechanics code FRED [7]. The structure of the overall system, viz. the FAST transient code system, is shown in Fig. 1, which indicates its major parts as well as the key-information being exchanged between the individual units. Inputs to FAST are, besides the basic geometric and thermal-hydraulics specifications, the kinetic parameters, including the delayed neutron fractions ( $\beta_i$ ) and decay constants of the precursors ( $\lambda_i$ ). In the point reactor kinetics approach the neutron generation time ( $\Lambda$ ), as well as the “average” reactivity coefficients such as fuel Doppler, coolant density and material expansion, which are all important in the analysis of fast spectrum systems, are needed to estimate the reactivity ( $\rho$ ). In the case of spatial kinetics, explicit zone-wise macroscopic cross-sections are required, in conjunction with suitable cross section derivatives. The simple formulation being used to functionalize the cross sections is:

$$\begin{aligned} \Sigma(T_F, \rho_C, R, H) = \Sigma_0 + & \left[ \frac{\partial \Sigma}{\partial \ln T_F} \right]_{T_{F0}} (\ln T_F - \ln T_{F0}) + \\ & + \left[ \frac{\partial \Sigma}{\partial \rho_C} \right]_{\rho_{C0}} (\rho_C - \rho_{C0}) + \left[ \frac{\partial \Sigma}{\partial R} \right]_{R_0} (R - R_0) + \left[ \frac{\partial \Sigma}{\partial H} \right]_{H_0} (H - H_0), \end{aligned} \quad (1)$$

where  $T_F$  is the fuel temperature,  $\rho_C$  the coolant density,  $R$  the average core radius and  $H$  the average core height; the subscript “0” indicates reference conditions for which the basic cross sections ( $\Sigma_0 = \Sigma(T_{F0}, \rho_{C0}, R_0, H_0)$  in Eq. (1)) have been generated.

For any targeted reactor state as a function of the core burnup, all the required nuclear data is generated using the French code ERANOS (Version 2.0), which consists of the newer generation of neutron and gamma modules developed within the European Fast Reactor collaboration. Among many other capabilities, ERANOS performs core, shielding and fuel cycle calculations in conjunction with adjusted as well as non-adjusted JEF-2.2 data. It includes the most recent developments in calculation methods, such as the collision probability method in many neutron groups and a 3D nodal transport-theory variational method with perturbation-theory as well as kinetic options. The latter method is currently used in the module TGV-VARIANT, i.e. the VARIANT code with its extension KIN-3D, where KIN-3D is a time-dependent 3D nodal

transport code, which takes its cross-sections directly from ECCO. A dedicated procedure has been developed to convert ERANOS cross sections produced with the cell code ECCO, as well as delayed neutron data, into a form suitable for use in PARCS, including the aforementioned cross section derivatives.



**Figure 1. Structure of the FAST code system**

In point kinetic calculations, fission, decay heat power, as well as precursor concentrations, are determined within TRAC-AAA.

PARCS is in its current version a 3D nodal-method, transient multi-group, neutron diffusion code for hexagonal and square geometries, having an interface with TRAC-AAA based on the PVM system. Where spatial kinetics is important, these effects are treated by means of explicit 3D flux and power distribution fields, which are determined using a suitable modification of the 3D reactor kinetics solver of PARCS, in which the original cross section parametrization devoted to Light Water Reactor (LWR) applications has been modified to account for the specific fast reactor thermal-hydraulic feedbacks outlined above (see Eq. (1)).

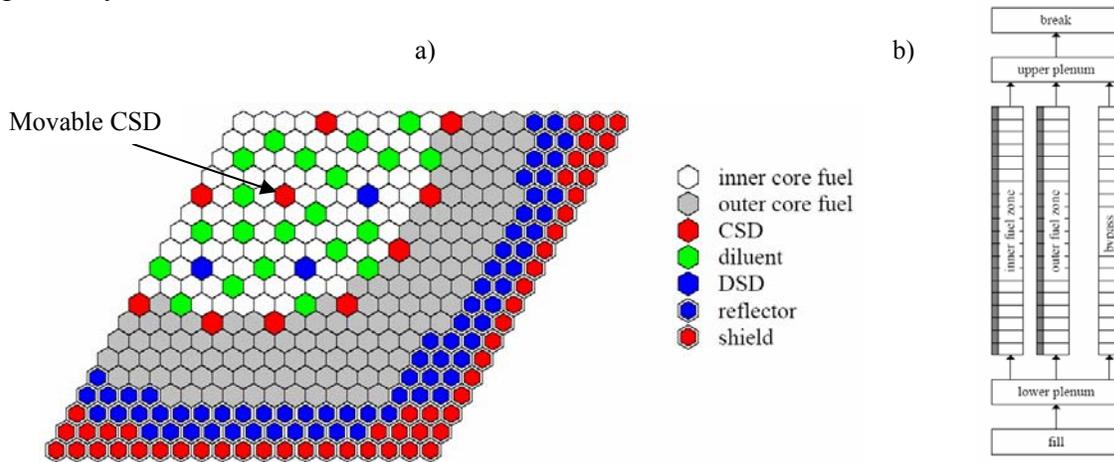
Thermal-hydraulic calculations of the full reactor plant, resulting in time-dependent fuel and coolant temperatures, coolant velocities pressures, etc., are carried out using TRAC-AAA, which is a modification of the USNRC code TRAC-M, coupled to FRED. The integration of the FRED code is needed for the accurate refined modeling of fuel rods under transient conditions. In

addition to the original TRAC models for standard reactor components, e.g. pumps, valves, separators, turbines, 3D vessel and the generalized heat structure component, TRAC-AAA includes a methodology for analyzing additional fluids, e.g. liquid metals, helium, etc., which is clearly important in the application to fast spectrum systems. On-line modeling of thermal-mechanical phenomena, implying an implicit coupling of PARCS, TRAC-AAA and FRED, is especially important for fast-spectrum systems, to evaluate the thermal expansion reactivity effects in an appropriate manner and to estimate the fuel failure probability.

### 3. COMPARISONS BETWEEN TRAC-AAA/PARCS AND ERANOS/KIN-3D

#### 3.1. Introduction

As one of the first applications of the coupled TRAC-AAA and PARCS codes to a fast-spectrum system, a modified model of the CAPRA-CADRA gas-cooled MOX core (20% Pu) [8] (with a 120 degree rotational symmetry) has been used for test calculations of the steady-state and transient behavior, and for comparison with the ERANOS and KIN-3D codes (see Fig. 2). The nodalization diagrams used for PARCS and TRAC-AAA are presented in Figs 2a and 2b, respectively.



**Figure 2. CAPRA-CADRA core test model for a) PARCS (120-degree rotational symmetry) and b) TRAC-AAA**

Such investigations are primarily aimed at checking the preparation of the basic cross-sections and their derivatives with respect to the most important reactivity feedback effects envisaged so far, e.g. fuel temperature (Doppler), coolant density and thermal-mechanical expansions in both the radial and axial directions. It is in this framework that a special interface code, ERANOSTOPARCS, was developed to convert ERANOS multigroup cross-sections originally produced with the cell code ECCO, as well as delayed neutron data, into a form suitable for use in PARCS, including the aforementioned cross-section derivatives (see Eq. (1)). The additional use of a dedicated ALOS procedure of ERANOS (UPDEDLMILIEU) [9], also developed at PSI in the framework of the FAST project, makes it possible to generate this data for any reactor state such as for equilibrium cycle concentrations.

### 3.2 Steady-State Calculations

UPDEDLMILIEU/ERANOSTOPARCS is being verified on the basis of several comparative criticality, reactivity coefficient and control rod worth calculations of arrangements of fresh/burnt fuel. The calculations, performed with PARCS and the TGV-VARIANT module of ERANOS, are based upon equivalent options and consistent ERANOS cross-sections. Such an analysis for the CAPRA-CADRA core with its fresh fuel compositions (Superphénix-like MOX fuel, (hex,z) geometric model), which has been performed by using 4 neutron broad group cross-sections with energy boundaries at 19.6, 1.35, 0.111 MeV, 4 eV and 0.11 meV (diffusion theory, default options for the discretization of the source in TGV-VARIANT), shows good agreement between PARCS and TGV-VARIANT (see Table 1). The  $k_{\text{eff}}$ -difference of 232 pcm between the two calculations (see Table 1) results from the different numerical solution schemes of the diffusion equation. It has to be borne in mind that similar detailed 3D-calculations of LWRs are carried out mostly using only 2 group cross sections, the choice of accurately prepared 4 group cross sections with 3 epithermal groups being thus a reasonable initial approach which also provides significant savings in computing time.

**Table 1: Criticality and reactivity coefficients for the CAPRA-CADRA core model**

$k_{\text{eff}}$		Control rod worth (pcm) <sup>a</sup>		Doppler constant (pcm) <sup>a</sup>		Coolant Density (pcm/°C) <sup>a</sup>		Radial Expansion (pcm/°C) <sup>a</sup>		Axial Expansion (pcm/°C) <sup>a</sup>	
PARCS	TGV	PARCS	TGV	PARCS	TGV	PARCS	TGV	PARCS	TGV	PARCS	TGV
1.00293	1.00525	242	243	-466	-467	1.025	1.027	-1.376	-1.375	-0.519	-0.490

a) 1pcm = 10<sup>-5</sup>.

The control rod worth reported in Table 1 was computed for a representative case, in which three control rods are simultaneously withdrawn by 60 cm (see Fig. 2a). In view of the subsequent transient calculations, a small number of movable control rods was deliberately chosen to enhance spatial effects and the value of 60 cm was chosen such that the total control rod worth is close to, but smaller than, the effective delayed neutron fraction ( $\beta_{\text{eff}} = 380$  pcm). The generation time  $\Lambda$  amounts to 0.7 $\mu$ s in this case.

The transport-theory effect and the effect coming from the use of a finer 33-group library, which is what is broadly used in design calculations of sodium-cooled fast cores, have also been studied (see Table 2).

**Table 2: Criticality and reactivity coefficients for the CAPRA-CADRA core model computed using TGV-VARIANT in conjunction with more refined methods**

$k_{\text{eff}}$		Control rod worth (pcm)		Doppler constant (pcm)		Coolant Density (pcm/°C)		Radial Expansion (pcm/°C)		Axial Expansion (pcm/°C)	
$P_1^a$	33 gs <sup>b</sup>	$P_1^a$	33 gs <sup>b</sup>	$P_1^a$	33 gs <sup>b</sup>	$P_1^a$	33 gs <sup>b</sup>	$P_1^a$	33 gs <sup>b</sup>	$P_1^a$	33 gs <sup>b</sup>
1.01000	0.99911	227	220	-462	-627	1.031	0.959	-1.378	-1.300	-0.481	-0.467

a) 4-group,  $P_1$  transport-theory calculation. b) 33-group, diffusion-theory calculation.

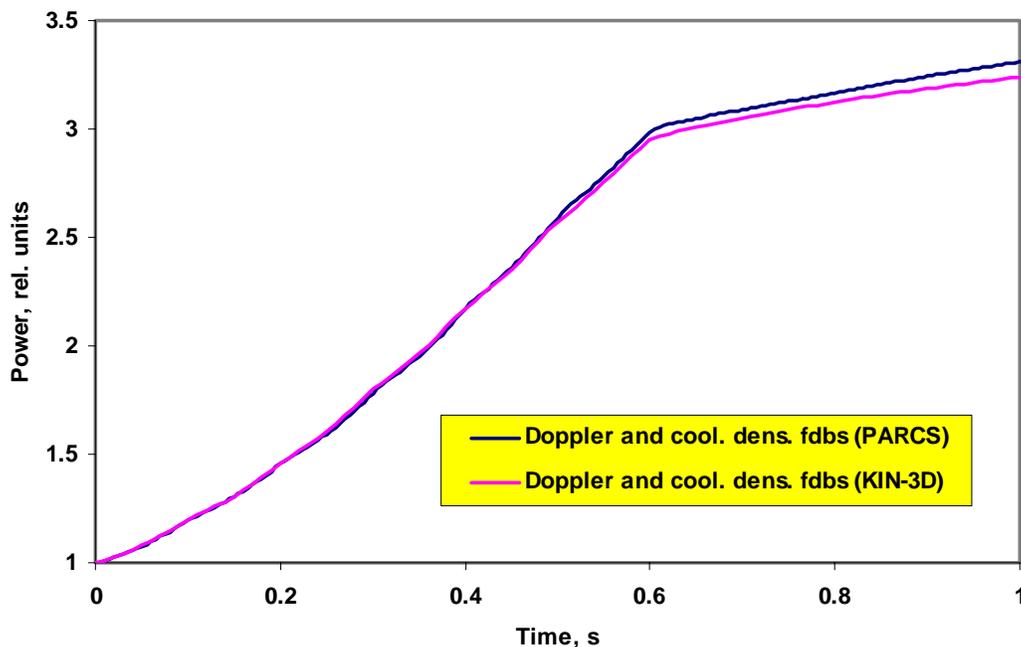
The effects are significant especially with respect to the criticality of the system (the reactivity change being much larger than 1\$), the control rod worth (which decreases by ~10%), and to the

magnitude of the Doppler constant (where the 33-group calculation leads to an increase of ~40%). This indicates that an accurate description of the steady-state behavior of a CAPRA-CADRA core based on the use of few-group cross sections in conjunction with diffusion theory is quite difficult, the main reason being the complex core/reflector interaction in systems with high contents of iron-based structural materials.

### 3.3 Transient Calculations

Within the scope of a preliminary study, transient calculations carried out with TRAC-AAA/PARCS are compared with KIN-3D, the kinetics module of ERANOS, which was originally developed at CEA and FZK. The dynamic calculations involve a steady-state analysis to check with the static parameters, followed by studies of various control rod movements, in which the feedback effects envisaged so far, i.e. fuel Doppler, coolant density and thermal expansions, are accounted for in KIN-3D in an approximate manner, i.e. channel-averaged TRAC-AAA-values are introduced in KIN-3D as material changes at selected time points. In the reference analysis, the 3D spatial kinetics approach based on the direct method is used, while the alternative use of the adiabatic or quasi-static method leads to more or less equivalent results.

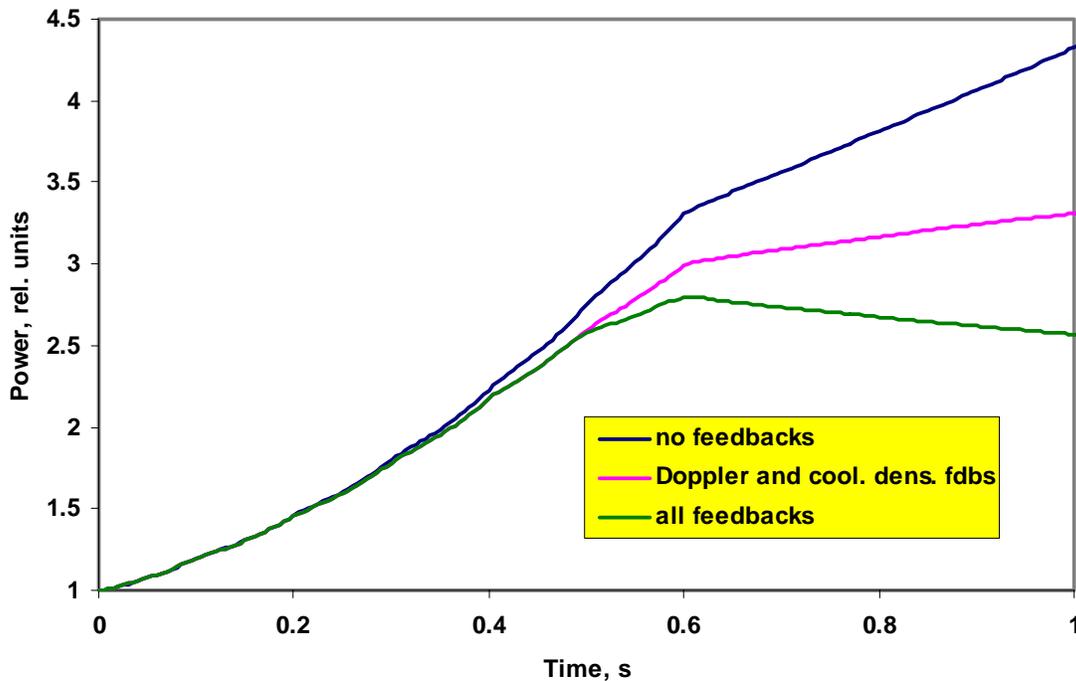
As an example, Fig. 3 displays the power evolution for a representative case, the dynamics calculation having been performed with the 4 group cross-sections, in which the 60 cm withdrawal of the three control rods studied before from a static viewpoint occurs in a time frame



**Figure 3. Comparison of the relative power evolution in the calculation of the control rod ejection transient using TRAC-AAA/PARCS and KIN-3D**

of 0.6 s, after which the overall control rod positions are unchanged during the remaining 0.4 s. The total time being considered for this “delayed critical” transient, the reactivity change of which is smaller than the delayed neutron fraction, is thus 1 s. The results of the comparison, showing good agreement between the two curves, demonstrate the reliability of the procedure developed so far to prepare the basic cross-sections and their derivatives with respect to fuel temperature and coolant density; material expansions implying changes in the original core geometry cannot be simulated with the current version of KIN-3D and were thus not taken into account.

Fig. 4 displays the TRAC-AAA/PARCS power evolution in three cases where (a) no feedback effects are accounted for, (b) only fuel temperature and coolant density effects are accounted for, which obviously is identical to one of the curves displayed previously in Fig. 3, and (c) all effects envisaged so far, i.e. including axial expansions, are considered, radial expansions playing no part in this transient.

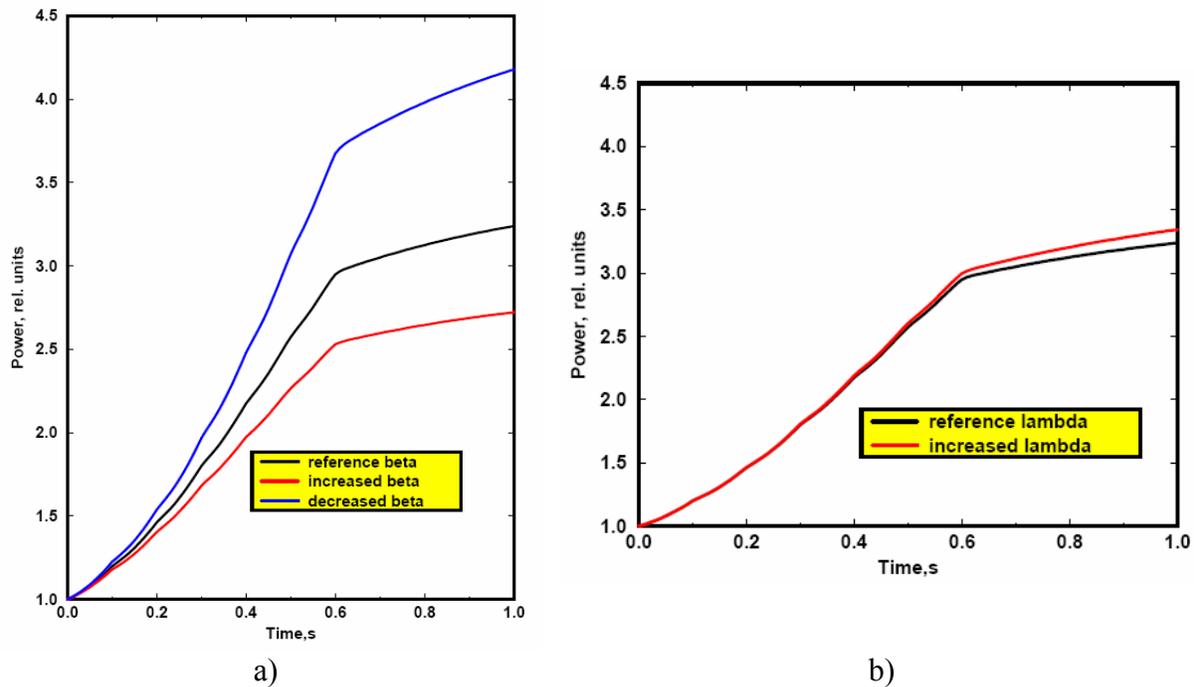


**Figure 4. Comparison of the relative power evolution in the calculation of the control rod ejection transient by considering different feedback effects.**

For CAPRA-CADRA cores with MOX type fuels, core expansion effects are of similar importance to the Doppler feedback in mitigating the power excursion. For a control rod ejection transient, the dominant thermal-mechanical effect, neglecting of which would clearly lead to conservative results, comes from the axial expansion, since the inlet temperature driving the radial expansion remains unchanged during the entire transient.

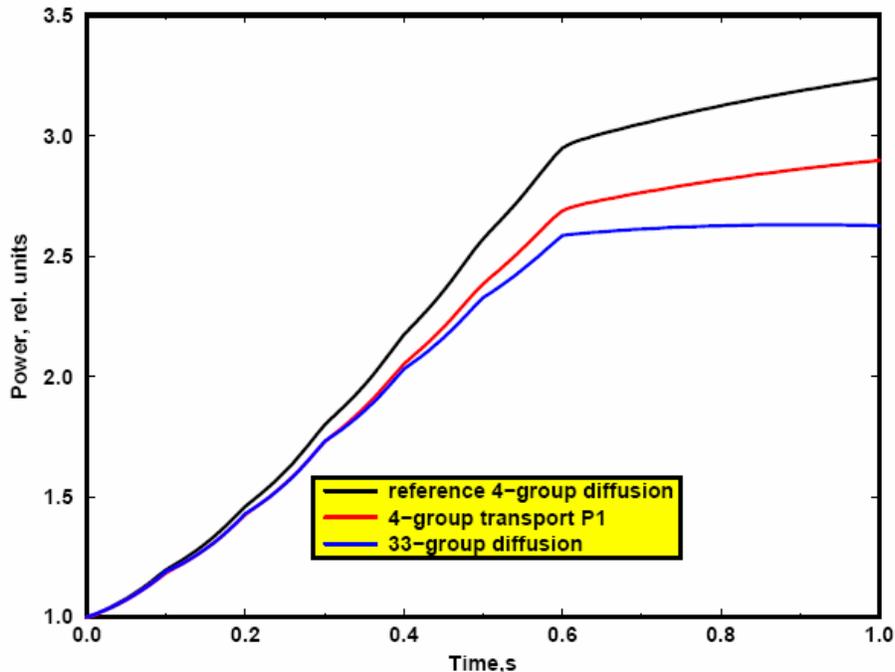
### 3.4 Sensitivity Calculations

“Delayed critical” control rod ejection transients in gas-cooled fast-spectrum systems are found to be weakly sensitive to the neutron velocities. Low sensitivity of the results, including the evolution of both the total power and power distribution, is also observed with respect to the energy distribution of the prompt and delayed fission spectra, as well as the time step being used in the temporal discretization. A value as low as 0.01 s is sufficient to obtain asymptotic results for the particular transient scenario, which has been considered in Fig. 3. Obviously, these transients are somewhat more sensitive to the decay constants of the precursors and much more to the delayed neutron fractions. In Fig. 5, a 10% uncertainty of these values is assumed, which corresponds more or less to the uncertainty of these parameters in current-day data libraries.



**Figure 5. Sensitivity of the relative power evolution in the calculation of the control rod ejection transient with respect to a) the delayed neutron fractions ( $\beta_i$ ) and b) the decay constants of the precursors ( $\lambda_i$ ).**

The transport-theory effect and the effect coming from the use of more groups have also been studied (see Fig. 6). In the transport-theory calculation, the power excursion is less pronounced as a result of the reduced control rod worth. A 33-group diffusion calculation results in an even milder transient in which the power excursion is reduced by  $\sim 20\%$  as compared to the original 4-group diffusion results, due to the significantly larger magnitude of the Doppler constant and the somewhat further reduced control rod worth; the opposite effect coming from the decrease of the expansion coefficients is less important in this context, because the relative decrease of these coefficients is smaller when compared to the relative increase of the magnitude of the Doppler constant (compare Table 2 with Table 1). Increasing the number of groups from 4 to 33 thus results in a significantly different power evolution.



**Figure 6. Comparison of the relative power evolution in the calculation of the control rod ejection transient by using different methods.**

### 3.5 Envisaged Methods Improvements

For such “delayed critical” transients dealing with control rod movements, it is found that the spatial kinetics solution is mainly determined by the cross-section dependence on the control rod position, fuel temperature, core expansion, coolant density, etc. Tuning the cross-section parametrization might reduce the dependence of the spatial kinetics solution on the methodology, e.g. transport or diffusion theory, larger or smaller number of energy groups, etc. For example, it is likely possible to modify the cross-section derivatives to improve the PARCS diffusion-theory solution. The envisaged modification is based upon the comparison of a limited number of integral parameters, i.e. the reactivity worth of the control rods, average fuel temperature, average core expansions, average coolant density, etc.

As an illustrative example, the transient shown in Fig. 3 has been reanalyzed. A complex spatial kinetics transport-theory calculation in 4 groups was compared with a new diffusion-theory calculation in 4 groups, in which the cross section derivative with respect to the control rod position is suitably scaled to match the transport-theory value of the control rod worth. This is equivalent to a reduction of the control rod withdrawal length by ~5% in this specific case. While the computing time required by the diffusion-theory calculation was about 10 times smaller compared to the transport-theory calculation, the agreement in the power evolution was nevertheless quite satisfactory. Obviously, a similar approach could also be used for scaling the cross-section derivatives with respect to the fuel temperature, core expansions, coolant density, etc.

## 4. CONCLUSIONS

The FAST project launched at PSI is an activity in the area of fast spectrum core and safety analysis with emphasis on generic developments and Generation IV systems. One of the main aims of the project is to develop a unique code capability for the core and safety analysis of critical (and sub-critical) fast-spectrum systems. In addition to the overall development of the FAST code system, it is important to verify its individual parts, including the different links between them. In one of the initial phases of this detailed verification procedure on which this paper is focused, the TRAC-AAA/PARCS elements of the FAST code have been compared with the stand-alone code ERANOS/KIN-3D, using as far as possible equivalent options, e.g. diffusion theory and ERANOS-based cross sections, which are supplied to PARCS, for any reactor state, via the new interface code UPDEDLMLIEU/ERANOSTOPARCS.

One of the main objectives of this analysis is a thorough check of the cross sections and their derivatives used in PARCS and the identification of key parameters to which dynamic calculations of gas-cooled fast-spectrum systems are particularly sensitive. Steady-state conditions as well as a series of hypothetical control ejection accidents have been investigated based on a CAPRA-CADRA reactor core loaded with Superphénix like MOX fuel. In the calculations based on KIN-3D, feedback effects have been accounted for in an approximate manner, e.g. by means of channel-averaged TRAC-AAA-values introduced as material changes for selected time points. The satisfactory agreement systematically achieved between TRAC-AAA/PARCS and ERANOS/KIN-3D for this analysis (see Fig. 3) provides confidence in the methodology used to obtain the basic cross-sections and derivatives for the analysis of fast-spectrum reactor transients. (It needs to be borne in mind that, for CAPRA-CADRA cores with MOX type fuels, core expansion effects are of similar importance to the Doppler feedback in mitigating the power excursion.)

The sensitivity of the reactivity and reactivity coefficients, as well as the transient behavior resulting from various control rod movements, has been examined with ERANOS/KIN-3D, by varying the number of neutron groups being used in the flux calculation and using transport-instead of diffusion-theory. The dynamic calculations have been performed using spatial kinetics (direct, quasi-static and adiabatic methods). The sensitivity of the results with respect to the kinetic parameters has also been investigated. The basis for this study is a 120-degree rotational symmetric, 1 s transient, in which three control rods are simultaneously withdrawn by 60 cm (see Fig. 2 a) in a time frame of 0.6 s, after which the overall control rod positions remain unchanged.

It is found that (a) the reactivity and reactivity coefficients are quite sensitive to the methods, particularly to the number of groups. For example, the magnitude of the Doppler constant of the CAPRA-CADRA core being investigated increases from 467 to 627 pcm and the control rod worth decreases from 243 to 220 pcm, if 33 groups are used instead of 4 groups; (b) for such “delayed critical” transients, in which the control rod worth is smaller than the delayed neutron fraction amounting to 380 pcm in this specific case, the spatial kinetics solution is mainly determined by the cross-section dependence on the control rod position, fuel temperature, core expansions, coolant density, etc.; (c) the resulting power excursion is particularly sensitive to the delayed neutron yield data: A 10% decrease of the reference  $\beta_i$ -values being obtained with ERANOSTOPARCS, bearing in mind that a 10% uncertainty corresponds to current-day nuclear

data uncertainties, leads to a significant increase of the maximum power by almost 50% as compared to the reference solution. A major need for reducing this uncertainty is thus clearly highlighted.

## ACKNOWLEDGMENTS

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## REFERENCES

1. K. Mikityuk, S. Pelloni, P. Coddington, E. Bubelis, "Development of an Advanced Code for System Fast Reactor Transient Analysis", *International Topical Meeting on Nuclear Reactor Thermal-Hydraulics (NURETH-11)*, Popes' Palace Conference Center, Avignon, France, October 2-6, 2005.
2. J. Y. Doriath, et al., "ERANOS 1: The Advanced European System of Codes for Reactor Physics Calculations", *Joint Conference on Mathematical Methods and Supercomputing in Nuclear Applications*, Karlsruhe, Germany, (1993).
3. G. Rimpault, et al., "The ERANOS Data and Code System for Fast Reactor Neutronic Analyses", *Int. Conf. On the New Frontier of Nuclear Technology: Reactor Physics, Safety and High-Performance Computing, PHYSOR*, Seoul, Korea, (2002).
4. G. Palmiotti et al., "VARIANT: Variational Anisotropic Nodal Transport for Multidimensional Cartesian and Hexagonal Geometry Calculation", Technical Report, ANL-95/40, Argonne National Laboratory (1995).
5. H.G. Joo, D. Barber, G. Jiang, T. Downar, "PARCS, A Multi-Dimensional Two-Group Reactor Kinetics Code Based on the Nonlinear Nodal Method", Technical Report, PU/NE-98-26, Purdue University (1998).
6. K. Mikityuk, P. Coddington, R. Chawla, "TRAC-M/AAA Code Assessment for Transient Analysis of Pb-Bi Cooled Fast-Spectrum Reactor Systems", *PHYSOR 2004 - The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments*, Chicago, Illinois, (2004).
7. K. Mikityuk, P. Fomitchenko, "FRED: Computational Model of Fuel Rod Behavior Under Accident Conditions Coupled with RELAP5/MOD3", *8th Int. Conf. On Nuclear Engineering (ICONE-8)*, Baltimore, Madison, (2000).
8. J.T. Murgatroyd et al., "Optimisation of the CO<sub>2</sub> Cooled Fast Reactor for Plutonium and Minor Actinide Management", *ENS 2002*, World Nuclear Expo (2002).
9. S. Pelloni, "UPDEDLMILIEU: A new ERANOS procedure LU", TM-41-04-21, Technical PSI Report, (2004).