# DEVELOPMENT OF AN ADVANCED CODE SYSTEM FOR FAST REACTOR TRANSIENT ANALYSIS

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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 behaviour and safety of the power plant as a whole are to be studied. The paper discusses the structure of the code system, the organization of the interfaces and data exchange. Examples of validation and application of the individual programs, as well as of the complete code system, are provided.

# 1. INTRODUCTION

The FAST (<u>Fast-spectrum Advanced Systems for power production and resource managemenT</u>) project is a recently (2003) launched 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 analysing core statics and the dynamic behaviour 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 analyse in a systematic manner a wide variety of transients including those which may lead to a reactivity increase, e.g. water/steam in a gas cooled core. In addition, through the modelling 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 behaviour.

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 for Generation-IV fast reactors 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.

The paper discusses the structure of the code system and the organization of the interfaces and data transfer, providing examples of validation and application of the individual programs as well as of the code system as a whole. The current status of the code system and the validation efforts and the future plans, are discussed in each of the relevant sections.

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# 2. STRUCTURE OF THE FAST CODE SYSTEM

As indicated above, one of the principal goals of the FAST project is to develop a general tool for analysis of core statics and the dynamic behaviour of advanced fast spectrum reactor concepts and to apply it to a selected range of Generation IV reactors. An appropriate detailed 3D fast reactor dynamics code system is assembled. This is based upon the coupled reactor static/kinetics codes ERANOS and PARCS, the thermal-hydraulics code TRAC/AAA and the fuel rod thermal mechanics code FRED. The methods development will be as generic as possible and hence aimed at the different Generation IV fast reactor concepts. In the initial phase, however, separate emphasis will be given to the gas cooled fast reactor (GCFR). The structure of the FAST transient code system is shown in Fig. 1, including major components and exchange of information between them.



Figure 1: FAST code system structure.

Two main options are available in the context of this code structure: one based on point reactor kinetics and another on spatial neutron kinetics.

# 2.1. Core Neutronics Data Preparation

This part of the code system performs for any targeted reactor state as a function of the core burnup a pre-calculation of 1) in case of point reactor kinetics: the core power distribution, kinetics parameters and reactivity coefficients; and 2) in the case of spatial neutron kinetics: basic macroscopic cross-sections and their derivatives, using in both cases the CEA's ERANOS code system.

ERANOS (Doriath et al., 1993) (Version 2.0) is a deterministic code system consisting of the newer generation of neutron and gamma modules developed within the European Fast Reactor collaboration. Among many other capabilities, it performs core, shielding, as well as fuel cycle calculations in conjunction with non-adjusted as well as adjusted JEF-2.2 data (Nuclear Energy Agency, 2000) and includes the most recent developments in calculational methods, such as the collision probability method in many groups and a 3D nodal transport theory variational method with perturbation theory and kinetics options. External neutron sources from MCNPX calculations can be input for accelerator-driven system (ADS) applications.

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#### **2.2.** Neutron Kinetics

The neutron kinetics part of the code system performs a calculation at each time step of 1) in the case of point reactor kinetics: reactor fission and decay heat power, concentration of the precursors of the delayed neutrons, using the TRAC/AAAcode; and 2) in the case of spatial neutron kinetics: 3D fields of neutron fluxes, power, concentrations of precursors of delayed neutrons, etc., using the PARCS code.

PARCS (Joo et al., 1998) 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 using the PVM system.

The cross-section parameterisation currently being used in PARCS was developed for light water reactor applications, and this has been reviewed for fast spectrum system analysis. In particular, in LWRs the dominant transient reactivity feedback effects are the Doppler effect and the change in the coolant density or void, while in fast spectra systems, because of the relatively smaller magnitude of these, other feedback effects are of equal importance, e.g. the fuel and core structure thermal expansion, which changes both the core dimensions and the effective fuel density, influencing the neutron leakage and core reactivity. As a consequence, two important steps need to be investigated:

- First: all the important transient reactivity feedback effects have to be identified;
- Second: the required functional form of the parameterisation has to be determined and implemented, and the adequacy of a new well established formulation based on cross-section derivatives can only be judged by extensive comparisons with other codes using explicitly tabulated cross-sections as a function of suitable, independent state variables.

This work is closely linked to the coupling of the PARCS code to the thermal-hydraulics code TRAC/AAA and the fuel behaviour code, since the derivatives of the cross-sections should be multiplied by the local state variables coming from these codes, e.g. local fuel and coolant temperatures, fuel expansions, etc.

The original (LWR) PARCS model uses the following procedure for re-calculating macroscopic crosssections:

$$\Sigma(T_F, \rho_M, T_M, B) = \Sigma_0 + \frac{\partial \Sigma}{\partial \sqrt{T_F}} (\sqrt{T_F} - \sqrt{T_{F0}}) + \frac{\partial \Sigma}{\partial \rho_M} (\rho_M - \rho_{M0}) + \frac{\partial \Sigma}{\partial T_M} (T_M - T_{M0}) + \frac{\partial \Sigma}{\partial B} (B - B_0),$$
(1)

where  $\Sigma$  is the macroscopic cross-section,  $T_F$  the fuel temperature,  $\rho_M$  the moderator density,  $T_M$  the moderator temperature and *B* the boron concentration. The subscript "0" means related to reference conditions.

One of the simplest ways to functionalize the cross-sections for fast spectrum systems is as follows:

$$\Sigma(T_F, \rho_C, R, H) = \Sigma_0 + \frac{\partial \Sigma}{\partial \ln T_F} (\ln T_F - \ln T_{F0}) + \frac{\partial \Sigma}{\partial \rho_C} (\rho_C - \rho_{C0}) + \frac{\partial \Sigma}{\partial R} (R - R_0) + \frac{\partial \Sigma}{\partial H} (H - H_0)$$
(2)

where  $\rho_C$  –is the coolant density, R the average core radius and H the average core height.

The modifications of the PARCS cross-section parameterization model, based in the first phase on Eq. 2, are currently under way. The fuel temperature and coolant density components are already implemented and tested.

### 2.3. Core and System Thermal Hydraulics

The system thermal-hydraulics part of the code system calculates, using the TRAC/AAA code (Spore et al., 2001), the coolant temperatures, velocities, pressure, etc., in the core and reactor plant, at each time step. The TRAC/AAA code is based on the USNRC LWR transient (safety) analysis code TRAC-M and includes a 3D (hydraulic) vessel component, a generalised heat structure component to model fuel rods, heat exchangers, environmental heat losses, etc., as well as models for all the "normal" reactor components, e.g. pumps, valves, separators, turbines, etc.

In addition to containing these standard elements, the AAA version was updated at the US Los Alamos National Laboratory to simulate; (1) additional working fluids (including liquid metals and helium), (2) the deposition of power in the working fluid, (3) the tracking of trace material that flows with the fluid, and (4) the heat conduction within the working fluid which is particularly important for liquid metal coolants.

Additional updates have been made to the TRAC/AAA code at PSI, including those necessary; (1) to improve the simulation of gas/heavy-metal two-phase flow, (2) to restructure the code output, (3) for the control of the external source power and (4) to improve the wall heat transfer for gas cooled systems. One of the most important modifications of the TRAC/AAA code was the introduction of the FRED fuel rod model in order to improve the simulation of the fuel rod performance under transient conditions (see next Section).

Since for the majority of the fast reactor concepts envisaged within Generation IV (and in particular GCFR) the coolant remains single phase, no significant work is expected to validate or modify the interfacial relations. The one known exception to this is for the gas lift pump driven coolant flow in the Ansaldo eXperimental Accelerator-Driven System (XADS) and other designs, and for this phenomenon assessment against experimental data and code improvements have been performed and are described in Section 3.2 below.

### 2.4. Fuels and Structures Thermal Mechanics

The fuel and structure thermal mechanics part of the code system performs, at each time step a calculation of temperature, and the stresses and strains in the fuel and structures (i.e. fuel pin, core diagrid, heat exchanger tubing, reactor vessel, etc.), using either the FRED thermal-mechanical code (Mikityuk and Fomitchenko, 2000) or the TRAC/AAA heat structure model. The choice of the model used depends upon the nature of the structure and the level of detail required.

The 'on-line' modelling of thermal-mechanical fuel behaviour during transients is an important feature of the FAST code system to account both for reactivity effects (due to core thermal expansion) and to estimate the fuel failure probability. Because of the tight coupling between the fuel rod and core structure behaviour, and the reactivity feedback in fast systems, it is more important to establish an implicit coupling (see Fig. 1) between the reactor kinetics (PARCS), thermal-hydraulics (TRAC/AAA) and the fuel thermal mechanics code (FRED) than is usual for LWR applications. Thus, for example, because of the possible smaller Doppler and coolant density reactivity effects (compared to LWRs), the reactivity feedback due to fuel and core structural material thermal expansion can be of equal magnitude. Therefore, in order to capture these effects, an integral code including fuel behaviour effects is needed.

In the initial phase of the work, emphasis is given to the improvement of the transient modelling of the current fast reactor fuel types, i.e. pelleted  $(U,Pu)O_2$  fuels, and will include improvements to the modelling of the pellet restructuring, transient fission gas release, fuel/clad interaction, etc. At some point during this phase, a link to an established fuel performance code will be developed in order to provide steady-state characterisation of burnt fuel. In parallel, a study on the development of a transient thermal-mechanical model of the advanced fuel concepts for gas-cooled fast reactors, in particular for carbide and oxide composite fuel in the form of coated particles in a ceramic silicon-carbide matrix as well as dispersed fuels is being initiated.

#### 2.5. Code Module Interface and Data Transfer

A special interface code, ERANOSTOPARCS, has been developed at PSI to convert, for any reactor state, ERANOS cross-sections produced with the cell code ECCO, as well as dedicated delayed neutron data, into a form suitable for use in PARCS, including the aforementioned cross-section derivatives. The ERANOSTOPARCS code was developed for this purpose and is currently being validated on the basis of extensive criticality calculations performed in conjunction with the VARIANT module of ERANOS. Thereby, analogous analyses conducted with PARCS by using these ERANOSTOPARCS cross-sections are based upon equivalent options. On the other hand, kinetics (dynamics) calculations carried out with TRAC/PARCS are compared with KIN3D, the kinetics module of ERANOS which was originally developed at CEA and FZK. In the latter dynamics calculations, feedback effects, such as fuel Doppler, coolant density and thermal expansions, are accounted for within the scope of this preliminary comparison study, in an approximate manner, i.e. by means of channel-averaged TRAC-values being introduced in KIN3D as suitable material changes at selected time points. Some results of this study are given below in Section 3.1.

As stated above, one advantage of using the PARCS and TRAC/AAA codes is that the interface software is supplied as part of the code package and this has been implemented and tested at PSI. The coupled code system PARCS and TRAC has been extensively used for LWR applications by the code developers. In addition, a first phase linking of the TRAC/AAA code to the FRED fuel rod code has been completed (Mikityuk, 2003). The main task in this area, therefore, is the extension of the interface to include all the additional feedback variables that are important for the change in the transient reactivity for fast spectrum systems. This work will therefore be performed in parallel with the cross-section parameterisation described above. For application to fast systems with many energy groups, further work may be required to optimize the overall convergence procedure.

The FRED fuel rod code has been included in the TRAC/AAA code as a subroutine. The FRED code includes its own internal time integration scheme and has the option to divide the TRAC/AAA time-step into sub time-steps if convergence is not obtained. Representative fuel rods are specified in both the TRAC/AAA and FRED input decks. At each time step, TRAC/AAA performs thermal-hydraulic and power calculations using the temperature distribution in the fuel rods obtained from FRED at the previous time step and transfers to FRED the axial distribution of the clad-to-coolant heat flux and power distribution (obtained from PARCS) in the fuel; then, with this data FRED calculates fuel pin properties and temperatures for the same time step and returns to TRAC/AAA the temperature distribution in fuel rods. Temperatures in the heat structures calculated by TRAC/AAA are overwritten by these FRED data. In the considered applications this does not significantly increase the CPU time.

#### **3. VALIDATION OF THE FAST CODE SYSTEM**

In addition to the development of the code system, it is important to benchmark and/or validate the individual elements, as well as the code system as a whole. In this respect, advantage is taken of the fact that "well developed" individual elements are available in many cases. However, it needs to be borne in mind that their envisaged use will often be at the limits of their original development window. Thus, for example, the application of the planned code system to the highly (neutronically) heterogeneous gas cooled fast reactor or to heavy-metal coolant thermal hydraulics will require significant further development and validation.

In the initial phase, emphasis has been placed on the validation of the separate parts of the code system for fast reactor designs and related phenomena. The examples of such validation presented here include: TRAC/PARCS benchmarking against ERANOS and KIN3D; TRAC/AAA validation against two-phase liquid-metal/nitrogen flow data.

### 3.1. Benchmarking of TRAC/PARCS against ERANOS and KIN3D

The PARCS code is currently being benchmarked against ERANOS for fast spectrum steady-state cores. This benchmarking is being performed for both lead-bismuth eutectic (LBE) and gas cooled XADS systems. It has been shown that transport effects are relatively unimportant for LBE systems (Pelloni, 2003), while for gas cooled systems, because of the voided core, neutron transport effects can contribute up to 2000 pcm in the calculation of  $k_{eff}$ . These effects need to be further evaluated by comparison against ERANOS for steady-state configurations and KIN3D for kinetics. Only after these investigations will it be possible to determine if the transport effects are of sufficient importance to require changes to the PARCS code.

As one of the first applications of the coupled PARCS and TRAC/AAA codes to a fast-spectrum system, a modified model of the CAPRA-CADRA gas-cooled core (Murgatroyd et al., 2002) has been used for test calculations of the steady-state and transient behaviour and for comparison with the ERANOS and KIN3D codes. One of the main aims of this study was to check the preparation of the basic cross-sections and their derivatives with respect to fuel temperature and coolant density. For this reason, the diffusion option in both ERANOS and KIN3D was used to correlate with the PARCS predictions. The nodalization diagrams used for PARCS and TRAC/AAA are presented in Fig. 2a and 2b, respectively. Comparison of ERANOS and TRAC/PARCS predictions for the Doppler constant and coolant density reactivity coefficient is presented in Table 1. Comparison of the relative power evolution in a test calculation of a control rod ejection transient using KIN3D and TRAC/PARCS is shown in Fig. 3. The results of the comparison demonstrate the reliability of the procedure developed to prepare the basic cross-sections and their derivatives with respect to fuel temperature and coolant density. A similar study will be performed for the derivatives with respect to core dimensions changes (Eq. 2).



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

Reactivity coefficients	ERANOS	T/P
Coolant density, pcm/°C	0.85	0.80
Doppler constant, pcm	-389	-448



fill

b)

 Table 1: Comparison of ERANOS and

 TRAC/PARCS predictions for reactivity coefficients

**Figure 3**: Comparison of relative power evolution in test calculation of control rod ejection transient using KIN3D and TRAC/PARCS.

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#### 3.2 TRAC/AAA Validation against Two-Phase Liquid-Metal/Nitrogen Flow Data

A gas lift pump concept based on the bubbling of inert gas in liquid metal to enhance the natural circulation of the primary coolant is currently being considered in a number of LBE cooled reactor projects. Thus, verification of the two-phase heavy metal/gas flow model in the FAST code system becomes an important issue. An analysis has therefore been performed, using the TRAC/AAA code, to simulate three sets of experiments with two-phase heavy metal/nitrogen flow, corresponding to different geometries, coolants, flowrates and void fraction ranges (Mikityuk et al., 2004). The predictions of the TRAC/AAA code versus the test data for void fraction are presented in Fig. 4a for the standard TRAC/AAA bubble drag model and in Fig. 4b for a modified model with a reduction of the bubble drag coefficient by a factor of 2. The predictions of the modified model show an improvement in the agreement with test data.



**Figure 4**: Comparison of tests data for void fraction with predictions obtained using (a) original and (b) modified TRAC/AAA.

### 4. APPLICATIONS OF THE FAST CODE SYSTEM

Within the 5th Framework Program of the E.U., the Preliminary Design Study of eXperimental Accelerator-Driven Systems (PDS-XADS) Project was focused on the study of three design options: 1) with a lead bismuth eutectic (LBE) cooled 80 MWt core (Cinotti and Gherardi, 2002), 2) with a gas (helium) cooled 80 MWt core (Giraud, 2003) and 3) with a lead bismuth eutectic (LBE) cooled 50 MWt core (i.e. the MYRRHA design), all designs being driven by a neutron spallation source corresponding to a proton accelerator beam impacting an LBE windowless target. One of the work packages of the PDS-XADS project was concerned with the assessment of the safety of the two 80 MWt designs (Coddington et al., 2004). A wide range of transients was analysed using the TRAC/AAA code, including, for example, protected and unprotected transient overpower, spurious beam trip, loss of flow, loss of heat sink, loss of coolant accidents, overcooling, etc. This section presents selected results of the application of TRAC/AAA, which is a part of the FAST code system to the safety analysis of LBE- and gas-cooled eXperimental Accelerator-Driven Systems.

#### 4.1 Example from LBE and Gas-Cooled XADS Transient Analysis: PLOF and ULOF

As an illustration of the PSI analysis (Coddington, et al., 2004.), the calculational results for the core temperatures in a protected loss of flow accident (PLOF) are shown in Figs. 5a and 5b for LBE- and gas-cooled systems, respectively. The beam trip in the He-cooled XADS (Fig. 5b) occurs, at the beginning of the transient, using the "main blower status" as signal. For this reason, all temperatures decrease in the gas system, while in the LBE case, there is some temperature increase (70°C for fuel and 150°C for cladding) until the coolant outlet temperature reaches 420°C, generating the beam trip signal (Fig. 5a).



Figure 5: Results of protected loss of flow accident.

In the unprotected case (Figs. 6a and 6b for LBE- and gas-cooled systems, respectively), the temperature increase in the gas system is much higher than in the LBE case. The natural circulation level of LBE coolant is very high (more than 40% of the nominal value) and the peak temperatures stabilize at 1120°C in fuel and at 640°C in cladding. For the gas system, two units of the safety cooling system provide a flow rate of about 20% of the nominal value and the peak temperatures stabilize at 2000°C in fuel and at 1220°C in cladding.



Figure 6: Results of unprotected loss of flow accident.

In summary, the results obtained show that the LBE-cooled XADS exhibits a very wide safety margin (for both protected and unprotected transients) as a consequence of very favourable safety characteristics, including excellent heat transfer properties and high boiling point of the coolant, favourable in-vessel and secondary system coolant natural circulation flow characteristics, and the large thermal inertia within the primary system as a result of the large coolant mass (pool design). For the gas-cooled XADS, the results demonstrate the importance of the core heat transfer, the adequacy of the decay heat removal system for protected depressurization and loss of flow transients, and appropriate definition of the time window for backup proton beam shutdown systems in the event of an unprotected transient.

#### 4.2 Example from LBE Transient Analysis: Beam Overpower

The transient chosen to test the integration of the different code modules into the FAST code system is a linear increase of the external source power (for an ADS) up to six times the nominal value over a 10 second period. The external source power was kept constant and after 80 seconds of the transient the external source was switched off. The scenario is not realistic, but demonstrates the coupling of thermal, hydraulic and mechanical modules, and in particular shows the closed gap regime and cladding plastic deformation.

The exercise was performed in three phases:

- first, the TRAC/AAA original fuel rod model was used;
- second, the reactivity feedback due to fuel axial expansion was also taken into account; and,

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• third, both the FRED fuel rod model and reactivity feedback due to fuel axial expansion were used.

The calculational results are presented in Figure 7. The time history of the relative power calculated using the TRAC/AAA point kinetics model is shown in Fig. 7a. The lower power levels in the second and third calculations are a consequence of the negative reactivity effect due to the fuel axial expansion. (Note without any reactivity feedback the relative power would increase to a value of 6.) The time history of the peak fuel temperature is shown in Fig. 7b. The fuel temperature in the third calculation is significantly (about 200°C) lower because the FRED model accounts for a "contact" component in the fuel-to-clad heat conductance, following the closure of the fuel-clad gap. For this reason, the Doppler effect is smaller and the power level is slightly higher (Fig. 7a) in the third case as compared to the second calculation.



Figure 7: Relative power (a) and peak fuel temperature (b) in 3 stages of the exercise:

1 – TRAC/AAA original fuel rod model;

2 – TRAC/AAA original fuel rod model and reactivity feedback due to fuel axial expansion;

3 – FRED fuel rod model and reactivity feedback due to fuel axial expansion.

Although the transient chosen, i.e. a six times increase in the external source power for an accelerator driven system, is somewhat arbitrary, the exercise demonstrated the operability of the modified TRAC/AAA code, including the integration of the FRED fuel rod model. It also showed that, under closed gap conditions, changes in the fuel rod model can lead to noticeable changes in the fuel temperatures and in the power.

### **5. CONCLUSIONS**

The FAST project is a recently (2003) launched 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 code capability for the core and safety analysis of critical (and sub-critical) fast spectrum systems. The paper discusses the structure of the code system, the organization of the interfaces between the individual modules and data exchange, provides examples of the validation and application of the individual codes and the system as a whole, and indicates the status of the current research and future plans.

In the initial phase of this activity, emphasis has been placed on the validation of the separate parts of the code system for advanced fast reactor designs and related phenomena. The examples of such validation presented in the paper include: TRAC/PARCS benchmarking against the ERANOS and KIN3D codes; TRAC/AAA validation against two-phase liquid-metal/nitrogen flow data.

TRAC/AAA which is an important part of the FAST code system was successfully applied to the analysis of LBE and gas-cooled XADS as part of the EU PDS-XADS project, in the frame of which intercode comparison from the different partners was used to benchmark the analytical models of the TRAC/AAA code.

The main conclusions from the above mentioned FAST code system validation activities are as follows: i) the validation results demonstrate the reliability of the developed procedure for preparing the basic cross-sections and their derivatives with respect to fuel temperature and coolant density, ii) the predictions of the FAST code system are in a good agreement with test data (and corresponding predictions with other code systems) for natural and gas-lift enhanced natural circulation flows, iii) the FAST code system could be successfully used for the LBE and gas cooled XADS transient analysis.

The following developments and applications of the FAST code system are currently in progress:

- validation of the FAST code system against MUSE4, TALL and other available experimental data;
- extension of the cross-section parametrisation formalism to model moderator ingress in gascooled fast-spectrum systems and gas entrainment in liquid metal systems;
- inclusion of a procedure for modelling of fuel behaviour with the steady-state fuel code necessary to provide for any burnup state initial conditions for transient fuel calculations.

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