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Transient analysis in the 3D nodal kinetics and thermal-hydraulics *ANDES/COBRA* coupled system

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Abstract

Neutron kinetics has been implemented in the 3D nodal solver *ANDES*, which has been coupled to the core thermal-hydraulics (TH) code *COBRA-III* for core transient analysis. The purpose of this work is, first, to discuss and test the ability of the kinetics solver *ANDES* to model transients; and second, by means of a systematic analysis, including alternate kinetics schemes, time step size, nodal size, neutron energy groups and spectrum, to serve as a basis for the development of more accurate and efficient neutronics/thermal-hydraulics tools for general transient simulations.

The PWR MOX/UO₂ transient benchmark provided by the OECD/NEA and US NRC was selected for these goals. The obtained *ANDES/COBRA-III* results were consistent with other solutions to the benchmark; the differences in the TH feedback led to slight differences in the core power evolution, whereas very good agreements were found in the other requested parameters. The performed systematic analysis highlighted the optimum kinetics iterative scheme, and showed that neutronics spatial discretization effects have stronger influence than time discretization effects, in the semi-implicit scheme adopted, on the numerical solution. On the other hand, the number of energy groups has an important influence on the transient evolution, whereas the assumption of using the prompt neutron spectrum for delayed neutrons is acceptable as it leads to small relative errors.

1. Introduction

A best-estimate neutronics/thermal-hydraulics coupled code system is required to predict the transient response of LWR. With this purpose, neutron kinetics has been implemented in the 3D nodal solver *ANDES*, and then, it has been coupled to the core thermal-hydraulics (TH) code *COBRA-III*.

In order to verify the capability and convergence of the coupled code, the PWR MOX/UO₂ transient benchmark provided by the OECD/NEA and US NRC has been performed. Some of the reasons of this choice are:

- Rod ejection benchmark with a final asymmetric configuration.
- Core partially loaded with MOX fuel, having lower values of β (fraction of

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delayed neutrons) and thus more abrupt transients.

- Transient leads to a core power level high enough to have a strong thermal-hydraulic feedback which allows testing the coupling with the TH code *COBRA-III*.
- Benchmark specifications include a library with a complete set of cross sections and ADF's in 2, 4 and 8 energy groups. This last number of energy groups allows to assess the effect of the delayed neutron spectrum.
- The high agreement between solutions of benchmark participants provides reliability of the results.

This benchmark is also used in this paper to provide a better understanding of the sensitivity of the transient solution to different factors involved in the kinetics equations. The effects of the time step, nodal discretization, number of energy groups and neutron spectrum, as well as the effects of the iterative scheme chosen to solve the kinetics equations, are analyzed.

2. Methodology: neutron kinetics equations and coupling of neutronics and TH

ANDES is a 3D multi-group nodal diffusion solver based on the Analytic Coarse-Mesh Finite-Difference (ACMFD) method. The theory involved in steady-state problems has been developed and extensively tested recently (Aragonés et al., 2007) (Lozano et al., 2007). Under transient conditions, both the time-dependent multi-group diffusion (Eq. 1) and the balance equations of the six neutron precursors (Eq. 2) have to be solved together. The idea is to treat the temporal dependence in such a way that it yields a fixed source problem (FSP), which can be solved utilizing the methodology already developed for the steady-state FSP.

The neutron kinetics equations can be written in a matricial way as follows:

$$\left\langle \frac{1}{D_g \mathbf{v}_g} \frac{\partial \phi_g}{\partial t} \right\rangle = \nabla^2 \langle \phi_g \rangle - \mathbf{A} \langle \phi_g \rangle - \mathbf{F}_d \langle \phi_g \rangle + \sum_{k=1}^6 \lambda_k C_k \left\langle \frac{\chi_{dk}^g}{D_g} \right\rangle \quad (1)$$

$$\frac{\partial C_k}{\partial t} = f_k \beta \sum_{g=1}^G \frac{\nu \Sigma_f^g}{k_{eff}} \phi_g - \lambda_k C_k \quad \text{for } k=1,6 \quad (2)$$

where \mathbf{A} is the steady-state multigroup diffusion matrix, χ and χ_d refer to the prompt and delayed neutron spectrum respectively, and the ig - kg element of the \mathbf{F}_d matrix is defined as:

$$F_d(ig, kg) = \frac{\beta \chi^{ig}}{D_{ig}} \frac{\nu \Sigma_f^{kg}}{k_{eff}}$$

To treat the time dependence, the first step is to discretize the time domain into discrete time steps. Focusing on the neutron precursor balance equation and using a finite difference implicit scheme for the time derivative (neutron precursor concentrations are assumed to have smooth variations with time steps employed in core transient analysis), we can obtain a relation between every precursor concentration and the prompt neutron flux per energy group:

$$C_k(t, \vec{r}) = \frac{C_k(t - \Delta t, \vec{r}) + \Delta t \cdot f_k \beta \sum_{g=1}^G \nu \Sigma_f^g \phi_g(t, \vec{r})}{1 + \lambda_k \Delta t} \quad (3)$$

On the other hand, to approximate the time derivative of the neutron kinetics equation, we use the method of exponential extrapolation, $\phi_g(r, t) = \tilde{\phi}_g(r, t) \cdot e^{\omega_g t}$, and then the time derivative of the form function $\tilde{\phi}_g$ is approximated by an implicit linear forward difference scheme, which results appropriate for most of the nodes (those that are far from moving control rods). Thus the neutron flux time derivative can be written as follows:

$$\frac{1}{D_g \mathbf{v}_g} \frac{\partial \phi_g(t, \vec{r})}{\partial t} = \left(\frac{\omega_g}{D_g \mathbf{v}_g} + \frac{1}{D_g \mathbf{v}_g \Delta t} \right) \cdot \phi_g(t, \vec{r}) - \frac{1}{D_g \mathbf{v}_g \Delta t} \cdot \phi_g(t - \Delta t, \vec{r}) \cdot e^{\omega_g \Delta t} \quad (4)$$

The frequency ω_g is recursively computed for each node and energy group using the nodal average flux:

$$\omega_g = \frac{1}{\Delta t} \ln \left(\frac{\bar{\phi}_g(t)}{\bar{\phi}_g(t - \Delta t)} \right) \quad (5)$$

The iterative process over the frequency ω_g is performed until the required convergence in the fission source distribution is achieved.

Regarding to the spectrum of delayed neutrons, it is known that it is softer than the prompt fission

spectrum. Thus the delayed neutrons have a greater importance in thermal reactors than do the prompt neutrons. For instance, in the point kinetics approximation, we can see that the effective β can be greater than the physical β by 20% or so. However, henceforward it will be assumed the same neutron spectrum for prompt (χ) and delayed neutrons (χ_d), as specified in the benchmark presented in this paper. In section 4.3, the influence of this assumption will be analyzed, comparing the results with those obtained using an appropriate spectrum for the delayed neutrons.

Introducing those approximations into the balance equations of neutron precursors and into Eq. 1:

$$\nabla^2 \langle \phi_g \rangle - \mathbf{A} \langle \phi_g \rangle - \mathbf{A}_{kin} \langle \phi_g \rangle = - \left[\frac{e^{\omega_g \Delta t}}{D_g \mathbf{v}_g \Delta t} \phi_g^0 \right] - \left(\sum_{k=1}^6 \frac{\lambda_k C_k^0}{1 + \lambda_k \Delta t} \right) \left[\frac{\chi^g}{D_g} \right] \quad (6)$$

$$A_{kin}(ig, jg) = \frac{1}{D_{ig}} \left[\left(\sum_{k=1}^6 \frac{\Delta t f_k}{1 + \lambda_k \Delta t} \right) \chi^{jg} \beta \nu \Sigma_f^{jg} + \delta_{ig, jg} \left(\frac{\omega_{ig}}{\mathbf{v}_{ig}} + \frac{1}{\mathbf{v}_{ig} \Delta t} \right) \right] \quad (7)$$

We can see that Eq. 6 is a FSP with additional terms respect to the steady-state FSP: the multigroup matrix is now $\mathbf{A} + \mathbf{A}_{kin}$, and the external source has an additional term determined by both the flux spatial distribution and the precursor concentrations in the previous time step (ϕ_g^0 , C_k^0). As a first approach, it was considered a flat distribution of C_k^0 inside every node, but it induced unexpected insertions of negative reactivity (~ 10 pcm) at the beginning of the transient. To reduce this effect, a polynomial fit has been chosen for this term of the external source, leading to values of spurious reactivity smaller than 2 pcm. The cause of the error is that the precursor concentration distribution inside a node at the beginning of the transient come from the equilibrium of Eq. 2:

$$C_k(0, \vec{r}) = \frac{\beta \cdot f_k \sum_{g=1}^G \nu \Sigma_{fg} \phi_g(0, \vec{r})}{\lambda_k} \quad (8)$$

If we apply a flat distribution to C_k ($t=0$), we will be neglecting the neutron flux distribution of

the eigenvalue calculation previous to the transient, resulting the error previously pointed out.

In order to obtain an accurate ACMFD relation for transient problems, the most important is to decide which terms are included in the multigroup diffusion matrix ($\mathbf{A} + \mathbf{A}_{kin}$) and the spatial distribution assigned to the terms included in the external source. Attending to this criterion, three different schemes are proposed in this paper:

- *Explicit scheme*

This approach consists on considering all the kinetics terms of Eq. 6 known from the previous iteration and thus included in the RHS as an external source. All the neutron fluxes included in this source are supposed to have a flat spatial distribution and the precursor concentrations, a polynomial fit:

$$|S_g^{kin}(\vec{r})\rangle = \mathbf{A}_{kin} \langle \bar{\phi}_g \rangle - \left[\frac{e^{\omega_g \Delta t}}{D_g \mathbf{v}_g \Delta t} \bar{\phi}_g^0 \right] - \left(\sum_{k=1}^6 \frac{\lambda_k C_k^0(\vec{r})}{1 + \lambda_k \Delta t} \right) \left[\frac{\chi^g}{D_g} \right] \quad (9)$$

- *Pure exponential time derivative scheme*

In this second scheme, it has been supposed that the time-dependence of the neutron flux within a node is purely exponential. It is also considered that the flux distribution in the node does not change during the time step:

$$\phi_g(\vec{r}) - e^{\omega_g \Delta t} \phi_g^0(\vec{r}) = 0 \quad (10)$$

With this hypothesis, which is true when the reactor is evolving with the fundamental mode (no changes in physical properties), Eq. 6 and 7 are simplified:

$$A_{kin}(ig, jg) = \frac{1}{D_{ig}} \left[\left(\sum_{k=1}^6 \frac{\Delta t f_k}{1 + \lambda_k \Delta t} \right) \chi^{jg} \beta \nu \Sigma_f^{jg} + \delta_{ig, jg} \left(\frac{\omega_{ig}}{\mathbf{v}_{ig}} \right) \right] \quad (11)$$

$$|S_g^{kin}(\vec{r})\rangle = - \left(\sum_{k=1}^6 \frac{\lambda_k C_k^0(\vec{r})}{1 + \lambda_k \Delta t} \right) \left[\frac{\chi^g}{D_g} \right] \quad (12)$$

In this case the multigroup diffusion matrix will be modified by the addition of matrix \mathbf{A}_{kin} , inducing a change in the eigenvalues.

- *Non-pure exponential time derivative scheme*

This scheme is an improvement of the previous one and it consists on a better approximation of the time derivative. In this case, relation (10) transforms as follows:

$$\begin{aligned} \phi_g(\vec{r}) - e^{-\omega_g \Delta t} \phi_g^0(\vec{r}) &= \delta_g(\vec{r}) \\ \delta_g(\vec{r}) &= a + u_1 x + u_2 x^2 + v_1 y + v_2 y^2 + w_1 z + w_2 z^2 \end{aligned} \quad (13)$$

where the 7 coefficients of the function δ_g can be computed from the values of the nodal average flux and the 6 interface average fluxes at the current and previous time steps. This way, a change in the flux distribution during the time step is allowed, which is the case of nodes placed near moving control rods.

As a consequence of this approach, the external source (Eq. 12) will have an additional term, resulting:

$$|S_g^{kin}(\vec{r})| = - \left(\sum_{k=1}^6 \frac{\lambda_k C_k^0(\vec{r})}{1 + \lambda_k \Delta t} \right) \cdot \left| \frac{\chi_g}{D_g} \right| + \left| \frac{\delta_g(\vec{r})}{D_g v_g \Delta t} \right| \quad (14)$$

A comparison of the three above methods will be performed in section 4.1. A common strategy of the three methods is to put together the terms derived of Eq. 4 that are divided by Δt , independently whether they are included in the multigroup diffusion matrix or in the external source. The reason is that problems arise when we include the current time step flux term in the multigroup diffusion matrix and the previous time step flux term in the external source. The differences between the analytic and the interpolated profiles increase as the time step is shorter because it appears in the denominator. Thus the transient results differ more and more from the real solution as the time step is shorter.

The NK-TH (*ANDES/COBRA-III*) coupling is done internally by a semi-implicit scheme, using a staggered alternate time mesh, as shown in (Merino et al., 1993). The TH solution is advanced over one-half of the NK time step. Then, the implicitly calculated TH variables are extrapolated over another half of the time step for the NK solution. The neutronics constants are thus nearly implicitly calculated in the next time step as a function of the extrapolated TH variables, where the limited half-

step extrapolation prevents significant oscillations, allowing for larger time steps.

3. Application problem definition

The objective of the benchmark problem is to model a rod ejection transient in a core partially loaded with mixed-oxide (MOX) fuel from HZP conditions. The reactor core chosen for the simulation is based on four-loop Westinghouse PWR power plant. The benchmark specifications are given in (Kozłowski et al., 2003). Four different benchmark parts were defined: three corresponding to different steady-state calculations and one corresponding to the transient response to control rod ejection. Results of this last part, and reported in this work, have been used to analyze the different scheme approximations. The steady-state results of *ANDES* have been reported elsewhere (Lozano et al., 2007), to show the adequacy of the nodal method and cross section library implementation.

4. Results

The simulations performed with *ANDES+COBRA-III* were based on the benchmark-specified 2G nodal library, using a reference nodalization scheme of 4 nodes and 4 channels per assembly, a time step $dt = 0,005$ sec and an exponential time derivative kinetics scheme. A comparison with the solutions to the benchmark obtained with the codes *PARCS* and *CORETRAN* (Kozłowski et al., 2007) were performed. Solutions of both codes correspond to the same spatial discretization of the 2G diffusion equations.

The main requested result concerned the temporal evolution of the total core power during the transient. As shown in Fig. 1, the results provided by the three code systems are consistent. It can be observed that the power increase in *CORETRAN* solution is quicker than in the others due to the higher level of reactivity obtained with this code after the rod ejection. On the other hand, the figure shows differences in the TH feedback of *ANDES* and *PARCS*, stronger in the last one. Transient reactivity, transient assembly peaking and Doppler temperature are in a good agreement as it can be seen at Table 1.

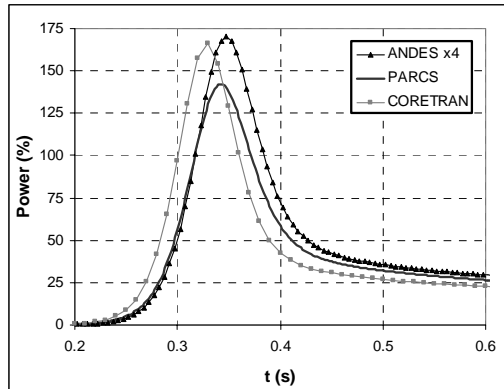


Fig. 1. Transient core power

Table 1
Comparison with other code solutions

	<i>ANDES</i>	<i>PARCS</i>	<i>CORETRAN</i>
Peak time (sec)	0.3475	0.342	0.330
Peak power (%)	170.0	142.2	166.2
Maximum reactivity (\$)	1.1125	1.1226	1.1374
Power integral (%)	30.7	28.9	26.2
$T_{Dop}(t = 1 \text{ s})$ ($^{\circ}\text{C}$)	309.6	308.8	312.7

Table 2
Solution sensitivity to different factors

	Sensitivity to the time step		Sensitivity to the NK and TH nodalization			Sensitivity to the kinetics scheme		
	$\Delta t=0.005$	$\Delta t=0.0025$	NK=4 TH=4	NK=4 TH=1	NK=1 TH=1	Scheme 1	Scheme 2	Scheme 3
Peak time (sec)	0.3475	0.3437	0.3475	0.3475	0.3425	0.3325	0.3475	0.3475
Peak power (%)	170.0	171.9	170.0	173.9	178.9	184.89	170.0	170.01
Maximum reactivity (\$)	1.1125	1.1125	1.1125	1.1125	1.1144	1.1198	1.1125	1.1125
Power integral (%)	30.70	30.78	30.70	31.42	31.72	31.74	30.70	30.71
$T_{Dop}(t = 1 \text{ s})$ ($^{\circ}\text{C}$)	309.6	309.6	309.6	310.1	310.3	310.2	309.6	309.6

4.1. Analysis of convergence for different scheme approximations

In order to test the accuracy of ACMFD method for kinetics equations, a comprehensive analysis to study the influence of the time step, the nodal discretization and the kinetics scheme was performed. Comparisons of peak time, peak power, peak reactivity, power integral and Doppler temperature for the different cases are shown in Table 2.

The columns 2-3 refer to the time discretization effects. A mean of verifying the reliability of the NK-TH numerical scheme is to change the time step during the transient simulation. Calculations taking $dt = 0.005$ sec. and $dt = 0.0025$ sec. were performed. Peak power is the most sensitive parameter to the time step, showing a slight tendency to reduce the peak power as the time step increases. Other magnitudes remain almost unaffected.

Columns 4-6 show the sensitivity of the transient solution to the radial spatial discretization in the NK and TH codes. A moderate difference is found in the transient peak power, because of the neutronics and thermal-hydraulics meshes, specially the first one.

The effect of the scheme chosen to solve the ACMFD kinetics equations is shown in columns 7-9. Calculations were performed using the three iterative schemes described in section 2. Significant differences are found when using the first scheme, while the other two are almost equivalent. As explained in section 2, in scheme 1 all the kinetics terms are assumed to be a flat external source. Results show that this approach is not good enough, especially due to the term of fissions of delayed neutrons, which requires a more accurate spatial definition. Results obtained with scheme 3 do not differ from those of scheme 2, proving that the last one is a suitable approach.

4.2. Influence of the number of energy groups

It has also been studied the influence of the number of energy groups over the main transient results obtained with *ANDES*. They have been compared with the available solutions of *PARCS* in 2, 4 and 8 groups. Fig. 2 shows the power evolution during the transients for all cases.

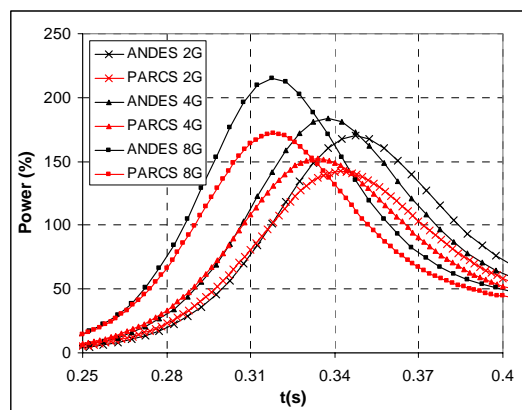


Fig. 2. Transient core power for 2, 4 and 8 energy group solutions

Both *ANDES* and *PARCS* solutions show a tendency to increase the peak power and reactivity as the number of groups is higher. The three solutions (2, 4 and 8 groups) in the figure above confirm the lower thermal-hydraulic feedback observed in *ANDES* solutions.

4.3. Delayed neutron spectrum

Until now all results presented have been obtained using the fission spectrum of prompt

neutrons also for delayed neutrons, as it was specified in the benchmark. It is quite straightforward to see that this approach results appropriate for 2 group diffusion equation. However, in 8 groups it is necessary to assess the error introduced by this assumption. An analytic approximation for the energy spectrum of delayed neutrons from thermal neutron induced fission of U235 has been taken from (Doroshenko et al., 2002), which gives a distribution for every neutron precursor group.

Two *ANDES* calculations of the previous rod ejection transient have been performed using 8 energy groups and the same spatial and time discretization. The first one uses the same spectrum for both delayed and prompt neutrons. The second one uses for delayed neutrons an 8G spectrum obtained from integration of the analytic approximation in the group structure. Prompt and delayed neutron spectrums in 8 groups are compared in Fig. 3. For the sake of clarity, spectrums of delayed neutrons from precursor groups 2 to 5 are not plotted, being very similar to those of groups 1 and 6. We can see that the energies of emerging delayed neutrons are lower than those of prompt neutrons, as expected.

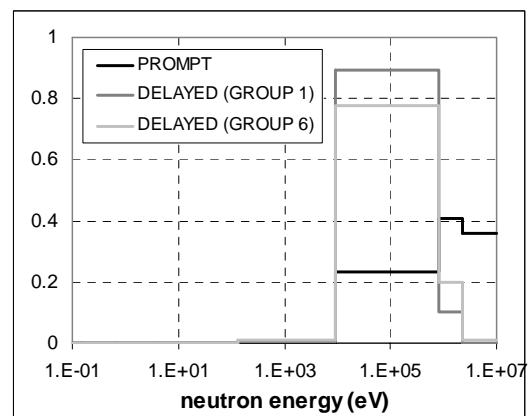


Fig. 3. Prompt and delayed neutron spectrums in 8 energy group structure

In Fig. 4 we can see the relative error in core power when the prompt neutron spectrum is applied to delayed neutrons. This approach leads to underestimate the value of the power during most of the transient, except the moment of the peak power. Anyway, results obtained in the two calculations are similar, so we can conclude that the assumption

adopted in the benchmark definition is suitable as it does not introduce relevant errors.

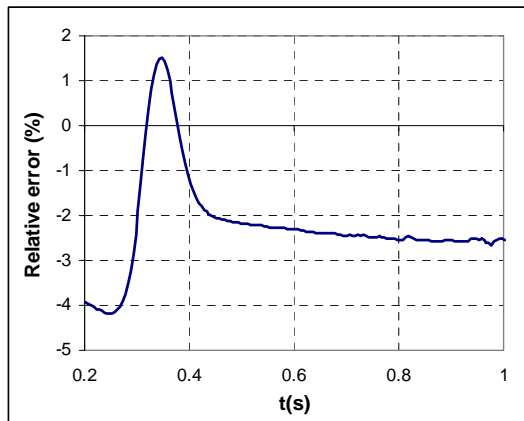


Fig. 4. Relative error in transient core power

5. Conclusions

ANDES was found to give consistent results for the transient solution of the MOX core. The largest differences are in the transient peak power and Doppler temperature evolution and minor differences are found in other requested parameters.

The analysis showed that:

- the numerical solution is not very sensitive to the time discretization effects, proving that the kinetics equations are well implemented and that approaches for time derivatives are suitable for fast transients as the one presented in this paper.
- the neutronics spatial discretization effects are significant for this problem and slightly more relevant than those derived of the thermal-hydraulic mesh. It has been stated that using 1 node/FA the relative error introduced in peak power is kept below 5.5% while the error of using 1 channel/FA is only 2.3%. Calculations with more than 2 energy groups have shown that the spatial discretization error is independent of the number of groups.
- the second iterative scheme used to solve the kinetics problem is the optimum one, since it is found that neglecting the non-exponential dependence of the flux does not affect the solution, while maintaining more

simplicity. First iterative scheme has resulted quite inaccurate due to the poor spatial approach of kinetics terms in the external source.

- the number of energy groups of the cross section library has an important influence in reactivity and peak power. Comparison with PARCS solutions shows similar power evolutions until TH feedback.
- the assumption of using the prompt neutron spectrum for delayed neutrons is acceptable as it leads to relative error in transient power lower than 4%.

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