Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007)
Monterey, California, April 15-19, 2007, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2007)

ANALYTICAL BENCHMARKS FOR THE KINETICS OF ACCELERATOR-DRIVEN SYSTEMS

S. Dulla, P. Ravetto, P. Picca, D. Tomatis
Politecnico di Torino, Dipartimento di Energetica
Corso Duca degli Abruzzi, 24 - 10129 Torino, Italy
sandra.dulla@polito.it

J.R. Maiorino, T. Carluccio, A. Antunes, A. Santos, F. de Oliveira
Instituto de Pesquisas Energeticas e Nucleares, IPEN
Cidade Universitaria USP
Av. Prof.Lineu Prestes, 2242 05508-000, São Paulo, Brazil

R.S. Santos
Instituto de Engenharia Nuclear
Caixa Postal 68 550, 21945-970, Rio de Janeiro, Brazil

ABSTRACT

The work presented in this paper illustrates the analytical benchmark philosophy with applications to subcritical source-driven system dynamics. Results for different complexity problems are presented in the frame of multigroup diffusion theory. The analysis performed on systems having physical characteristics typical of the Yalina Booster experiment are presented. The comparisons with the results of numerical calculations enlighten the convergence trend of discretized schemes and the limits of applicability to the analysis of experiments.

Key Words: analytical benchmarks, ADS kinetics, numerical code validation

1. INTRODUCTION

A Coordinated Research Project (CRP) under the auspices of IAEA is on-going on *Analytical and Experimental Benchmark Analyses of Accelerator Driver Systems (ADS)* [1]. One of the work tasks concerns the development of ADS kinetics analytic benchmarks suitable for the assessment of models, numerical methods and codes for the time dependent analysis of source-driven multiplying systems. Within this framework, a collaboration is established between Politecnico di Torino (Italy), the University of São Paulo and the IEN (Brazil).

The project involves the study and interpretation of kinetic experiments performed on the subcritical facility Yalina [2]. The work presented here illustrates some analytical benchmarks which are intended for physical situations comparable to the Yalina assembly, as far as nuclear data and geometrical configuration are concerned. The work involves both a fully analytical approach and a numerical investigation. The analytical approach produces paradigmatic results which are used for the study of convergence trends of numerical techniques and for their error control.

2. THE NEED OF BENCHMARKS FOR ADS DYNAMIC SIMULATION TOOLS

The study of time-dependent problems for neutron multiplying structures is usually carried out by high performance computers using numerical codes which can adequately handle the large physical complications associated to realistic full scale system configurations. The computational tools use algorithms which reduce the model equations to algebraic problems that are then numerically solved. When the tools are used for real simulations, the first question that needs to be answered concerns the adequateness of the model which usually includes some simplifications with respect to the exact reference model (e.g., diffusion in place of the full Boltzmann equation) for the physical situation at hand. Furthermore, the numerical procedures show two inherent shortcomings:

- differential and integral operators are treated by discretization schemes;
- iterative procedures are made use of to obtain the full solution.

The following concerns need to be considered with regards to the full simulation tool:

- is the model adequate to describe the physical situation of interest?
- is the algorithm properly coded?
- is the algorithm suitable to obtain numerical results with a defined level of accuracy?
- for what physical systems a code can be retained a suitable computational tool?

To answer in a satisfactory way, various successive steps need to be taken for the evaluation of a numerical high performance code. A verification procedure obviously has to be carried out, to guarantee that the software has been coded in such a way that the required operations are correctly performed (software verification). A validation process will then assure that the model adopted can capture the physical phenomena of interest (validation of model) and that the numerical schemes and techniques can provide the required accuracy of the numerical results (validation of numerical method). This steps may also focus on the determination of the numerical requisites (mesh sizes, convergence criteria, number of iterations and so on) which are needed to obtain certain levels of accuracy in the results. At last, the code will be tested to verify its capability to describe certain specific situations, thus defining its limits of validity (qualification).

The above steps constitute a benchmarking process and can be conducted through different analytical, numerical and experimental approaches. The need of reliable benchmarking procedures is particularly felt by code developers for the dynamics of accelerator-driven systems, because available methods were usually developed for reactors in the vicinity of the critical situation or departing from a critical state. For the analysis of accelerator-driven systems different physical situations have to be dealt with; in fact high energy neutrons play an important role and it has been shown that the source dominance may have important consequences in the dynamic characteristics of the systems. Therefore, it is foreseeable that numerical methods need to be properly adapted.

3. THE PRINCIPLE OF ANALYTICAL BENCHMARKING

An analytical benchmark can be defined as a closed-form solution to some reference problems that are significant for the physical situation of interest [3]. Hence, the solution must be obtained using purely analytical techniques as much as possible, with a full error control at all steps. The precision of the numerical results produced (e.g., number of significant figures) should be fully certain. Of course, being the elective methods mainly analytical, only highly simplified and idealised configurations may be treated. However, for this purpose it is of great importance to construct problems that can be informative with regards to the physical situations of interest. The work by Barry Ganapol has led over the years to important achievements in deriving and organizing analytical benchmarks. Ganapol published a library of analytical benchmarks that includes also time-dependent problems [3].

The analytical benchmark can thus perfectly serve the following scopes:

- to verify that the equations are adequately solved by numerical schemes;
- to separate model and numerically induced effects;
- to fully comprehend and interpret physical phenomena;
- to determine the limitations of approximate models (diffusion vs. transport, anisotropy effects, definition of kinetic parameters).

An important aspect is error control. Analytical formulae must be numerically calculated. This operation unavoidably introduces some sort of error, which must be controlled and upper-limited. For instance, a truncation of a series representation should be accompanied by an evaluation of the truncation error, which must be supplied together with the benchmark results.

In conclusion, they have a role for both the validation of models and of algorithms. A general golden rule may be stated at this point: a numerical technique that gives bad results for a simple system cannot be expected to give reliable results for complicated systems.

In the field of neutron kinetics, the principle of analytical benchmarking was used successfully in the past for the validation of numerical codes [4]. More recently, a first attempt has been made also in the field of source-driven systems [5].

4 PHYSICAL PROBLEMS CONSIDERED IN THE WORK

The work considers problems of different and increasing complexity. The Yalina structure is a multiplying system characterised by an inner fast core surrounded by a thermal zone. Starting from simple homogeneous systems, problems for a multilayer reactor with an inner source are considered. Analyses are performed for one dimensional configurations for a three-energy group structure, which is the minimum needed to simulate the physical features of the assembly. For the generation of the few group macroscopic constants of the facility, the ENDF-B-VI.8 nuclear data library is used by processing the basic data with the NJOY system version 97.115 with AMPX-II.

The system is supposed to be injected by a pulsed source. When analysing a single pulse, delayed neutron contributions may be disregarded, while their effect must be taken into account for multiple pulse analyses. The results of analytical evaluations are compared with results obtained by simplified kinetic models (point, multipoint) which are widely used in practice. Furthermore, a study on the convergence pattern and accuracy of the numerical finite difference scheme is performed. The assessment of the CINESP code [6] is also among the objectives of the present research.

5 A THREE-GROUP DIFFUSION THEORY EXAMPLE AND SELECTED RESULTS

In the following the analytical solution of the three-group diffusion equations for a homogeneous pulsed system is given. The general problem can be solved fully analytically since an explicit formula for the solution of third-order algebraic equations is available. The balance equations are the following:

$$\begin{cases} \dfrac{1}{\mathrm{v}_1}\dfrac{\partial\Phi_1}{\partial t} = D_1\nabla^2\Phi_1 - \Sigma_1\Phi_1 + Q \\ \dfrac{1}{\mathrm{v}_2}\dfrac{\partial\Phi_2}{\partial t} = D_2\nabla^2\Phi_2 - \Sigma_2\Phi_2 + \Sigma_{1\longrightarrow 2}\Phi_1 + \nu\Sigma_{f_3}\Phi_3 \\ \dfrac{1}{\mathrm{v}_3}\dfrac{\partial\Phi_3}{\partial t} = D_3\nabla^2\Phi_3 - \Sigma_3\Phi_3 + \Sigma_{2\longrightarrow 3}\Phi_2 + \Sigma_{1\longrightarrow 3}\Phi_1, \end{cases} \tag{1}$$

complemented with initial and flux vanishing boundary conditions. The first group includes high energy source neutrons, the second one is dominated by fission emissions, while the third one describes thermal neutrons.

The source vector is introduced as:

$$|Q(x,t)\rangle = \left| \begin{array}{c} \mathrm{v}_1 Q(x,t) \\ 0 \\ 0 \end{array} \right\rangle, \tag{2}$$

together with the balance matrix $\hat{\mathbf{M}}_\phi$:

$$\hat{\mathbf{M}}_\phi = \left\{ \begin{array}{ccc} \mathrm{v}_1 D_1\nabla^2(\cdot) - \mathrm{v}_1\Sigma_1 & 0 & 0 \\ \mathrm{v}_2\Sigma_{1\longrightarrow 2} & \mathrm{v}_2 D_2\nabla^2(\cdot) - \mathrm{v}_2\Sigma_2 & \mathrm{v}_2\nu\Sigma_{f_3} \\ \mathrm{v}_3\Sigma_{1\longrightarrow 3} & \mathrm{v}_3\Sigma_{2\longrightarrow 3} & \mathrm{v}_3 D_3\nabla^2(\cdot) - \mathrm{v}_3\Sigma_3 \end{array} \right\}. \tag{3}$$

Expanding in a series of Helmholtz eigenfunctions φ_n, for each mode the following matrix is introduced:

$$\hat{\mathbf{M}}_{\phi,n} = \left\{ \begin{array}{ccc} -\mathrm{v}_1(D_1 B_n^2 + \Sigma_1) & 0 & 0 \\ \mathrm{v}_2\Sigma_{1\to 2} & -\mathrm{v}_2(D_2 B_n^2 + \Sigma_2) & \mathrm{v}_2\nu\Sigma_{f_3} \\ \mathrm{v}_3\Sigma_{1\to 3} & \mathrm{v}_3\Sigma_{2\to 3} & -\mathrm{v}_3(D_3 B_n^2 + \Sigma_3) \end{array} \right\}. \tag{4}$$

Defining:

$$_i\delta_n = -\mathrm{v}_i(D_i B_n^2 + \Sigma_i) \tag{5}$$

one can write the third-order characteristic equation for the matrix in Eq. (4), introducing the eigenvalues ω_n, as:

$$(_1\delta_n - \omega_n)\left[\omega_n^2 - \xi_n\omega_n + \zeta_n\right] = 0, \tag{6}$$

Table I. Cross sections for the homogeneous 1D system treated in three-group diffusion approximation.

		$g=1$	$g=2$	$g=3$
$1/\mathrm{v_g}$	[s cm^{-1}]	$5.35994e-8$	$1.47756e-7$	$1.33310e-6$
$\Sigma_{tot,g}$	[cm^{-1}]	$2.83110e-1$	$3.65360e-1$	$6.65500e-1$
$\Sigma_{a,g}$	[cm^{-1}]	$1.40280e-2$	$1.63760e-2$	$6.98540e-2$
$\nu\Sigma_{f,g}$	[cm^{-1}]	$3.45310e-2$	$3.28690e-2$	$1.20020e-1$
χ_g	$-$	0.7112	0.2886	0.0002
$\Sigma_{g\to g}$	[cm^{-1}]	$2.36040e-1$	$3.48954e-1$	$5.95640e-1$
$\Sigma_{g\to g+1}$	[cm^{-1}]	$3.31803e-2$	$3.45000e-5$	$-$
$\Sigma_{g\to g+2}$	[cm^{-1}]	$1.16620e-5$	$-$	$-$

where:

$$\xi_n = (\ {}_2\delta_n + \ {}_3\delta_n) \tag{7}$$

and:

$$\zeta_n = (\ {}_2\delta_n\ {}_3\delta_n - \mathrm{v}_2\mathrm{v}_3\nu\Sigma_{f_3}\Sigma_{2\to 3}). \tag{8}$$

Eigenvalues as well as direct and adjoint eigenvectors can be found, in order to write the full vector solution whose components are the group fluxes as:

$$|\Xi(x,t)\rangle = \sum_{n=1}^{\infty} \left[{}_1a_n(t)\,|{}_1U_n\rangle + \ {}_2a_n(t)\,|{}_2U_n\rangle + \ {}_3a_n(t)\,|{}_3U_n\rangle\right] \varphi_n(x). \tag{9}$$

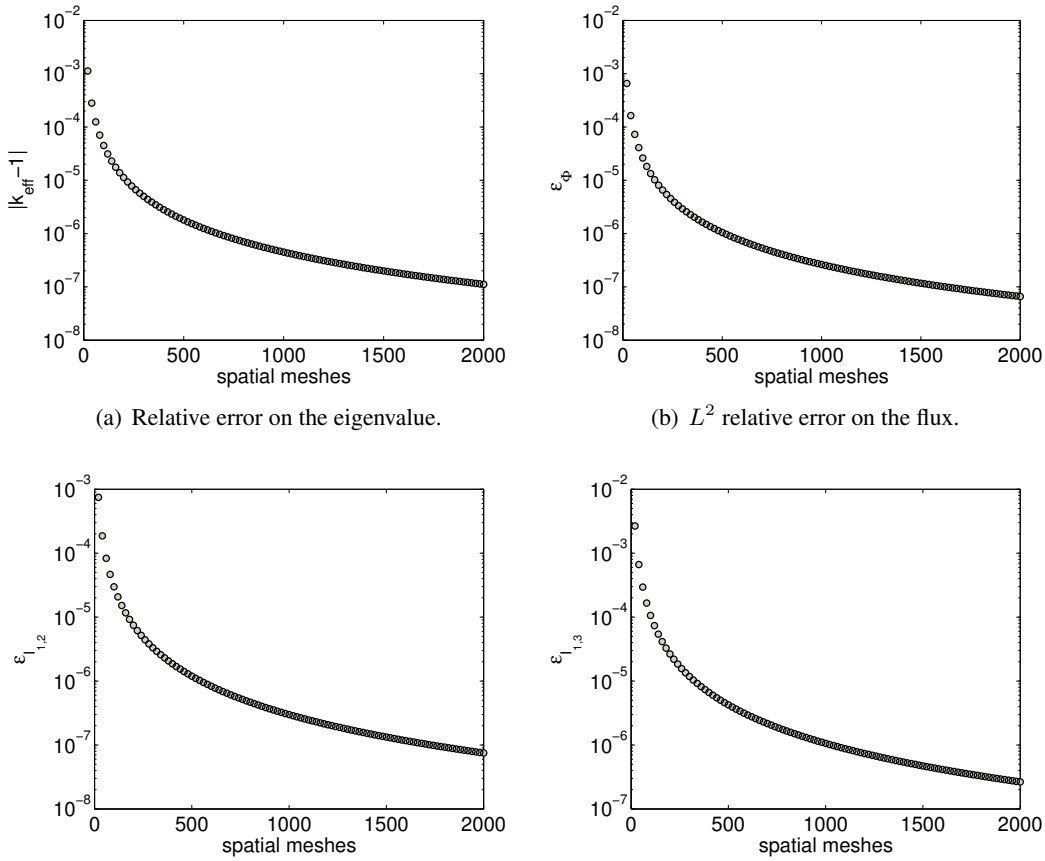
This analytical procedure can be easily extended to the general case with fast and epithermal fissions and emissions by properly modifying the matrix appearing in Eq. (3).

6 Results

The first configuration analyzed is a homogeneous slab, characterized by material parameters as in Table I. Diffusion coefficients are evaluated adopting the standard formulation coming out from P_1 approximation:

$$D_g = \frac{1}{3\Sigma_{t,g}} \tag{10}$$

At first, the critical slab dimension for this system is evaluated analytically, by imposing a spatial shape according to the fundamental boundary vanishing eigenfunction for the three-group fluxes and solving the steady-state eigenvalue problem associated to model (1). The critical dimension obtained is $h_{cr} = 23.53185893$ cm, with an imposed relative error of $1e-8$. The criticality problem is then solved numerically, adopting a centered finite-volume discretization scheme for the spatial variable, with equally-spaced meshes and the same boundary condition as in the analytical case. The power iteration



(a) Relative error on the eigenvalue.

(b) L^2 relative error on the flux.

(c) Maximum relative error on $I_{1,2}$.

(d) Maximum relative error on $I_{1,3}$.

Figure 1. Convergence trend of the numerical scheme in the criticality evaluation.

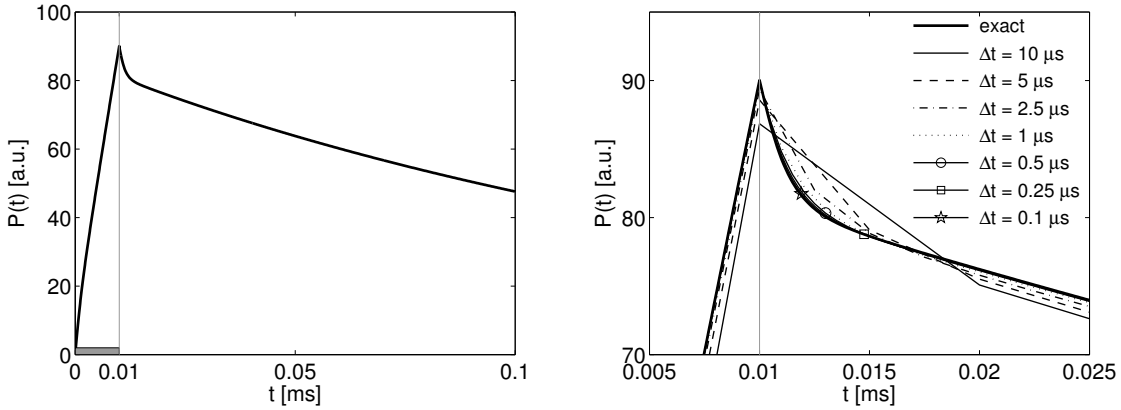
method is adopted to evaluate k_{eff} corresponding to the exact critical arehave been defined as follows:

$$\varepsilon_{\Phi} = \frac{\sqrt{\sum_{g=1}^{3} \int \left(\Phi_{g,num} - \Phi_{g,ex}\right)^2 dx}}{\sqrt{\sum_{g=1}^{3} \int \Phi_{g,ex}^2 dx}},$$
$$\varepsilon_{I_{i,j}} = \frac{\max \left| \left(\frac{\Phi_i}{\Phi_j}\right)_{num} - \left(\frac{\Phi_i}{\Phi_j}\right)_{ex} \right|}{\left(\frac{\Phi_i}{\Phi_j}\right)_{num}}, \tag{11}$$

where the indication num refers to the numerical results and ex to the exact, analytical results.
In Figs. 1(a) and 1(b) the convergence trend of the eigenvalue and of the critical flux is drawn. In such a system the energy spectrum is independent on space; the analytical spectral indeces are compared to the results of the numerical simulation as functions of the spatial mesh in Figs. 1(c) and 1(d).

Table II. Source transients considered.

	Source amplitude	pulse duration	$\Phi_g(t=0)$	description
I	$S_1 = 10, S_2 = S_3 = 0$	$\tau = 10\mu$s	zero-flux	response to a single source pulse
II	$S_1 = 10, S_2 = S_3 = 0$	$\tau = 10\mu$s	equilibrium with $S_1 = 10$	system shut-down
III	$S_1 = 10, S_2 = S_3 = 0$	$\tau = 10\mu$s	equilibrium with $S_1 = 1$	source increase + shut-down



(a) Exact solution. (b) Comparison of numerical simulations.

Figure 2. Power evolution for transient I. The gray lines indicate the duration of the source pulse.

A subcritical configuration is then considered, in order to perform time-dependent simulations of source transients. The dimension of the slab associated to $k_{eff} = 0.98$ is $h = 23.09695823$ cm, evaluated analytically. In order to have a numerical evaluation with a relative error below 1 pcm a minimum of 220 spatial meshes is required. This spatial discretization is adopted for the following time dependent calculations.

Some transients involving a localized source pulse are considered. The source is symmetrically located in the center of the system and its width is $1/10$ of the total slab dimension. In Table II the characteristics of the transients considered are summarized.

The analytical solution for the transients considered is obtained with the above-outlined procedure, by projection of the neutron fluxes on the Helmholtz eigenfunctions. The use of 150 harmonics allows to reduce the error introduced by the series truncation below 10^{-9} on the power at each time instant.

In Fig. 2 the power evolution for transient I is presented, comparing the analytical solution with the numerical evaluations. An implicit Euler scheme is adopted for the time integration with different time steps. The relative error on the power, ϵ_{power}, is reported in Fig. 3.

The three-group flux evolution is reported in Fig. 4 for two spatial points, x_1, located in the center of the system, and x_5, at a distance of $1/10$ of the total dimension of the system from the boundary. The presence of spatial effects and the error introduced by the time discretization is clearly visible.

An analogous analysis is performed for the other two transients, characterized by a source increase

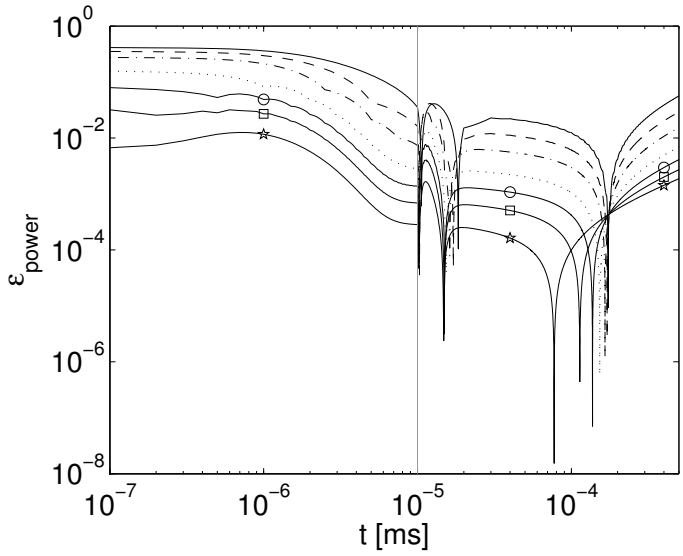


Figure 3. Relative error on power for transient I. Identification of curves as in the previous figure.

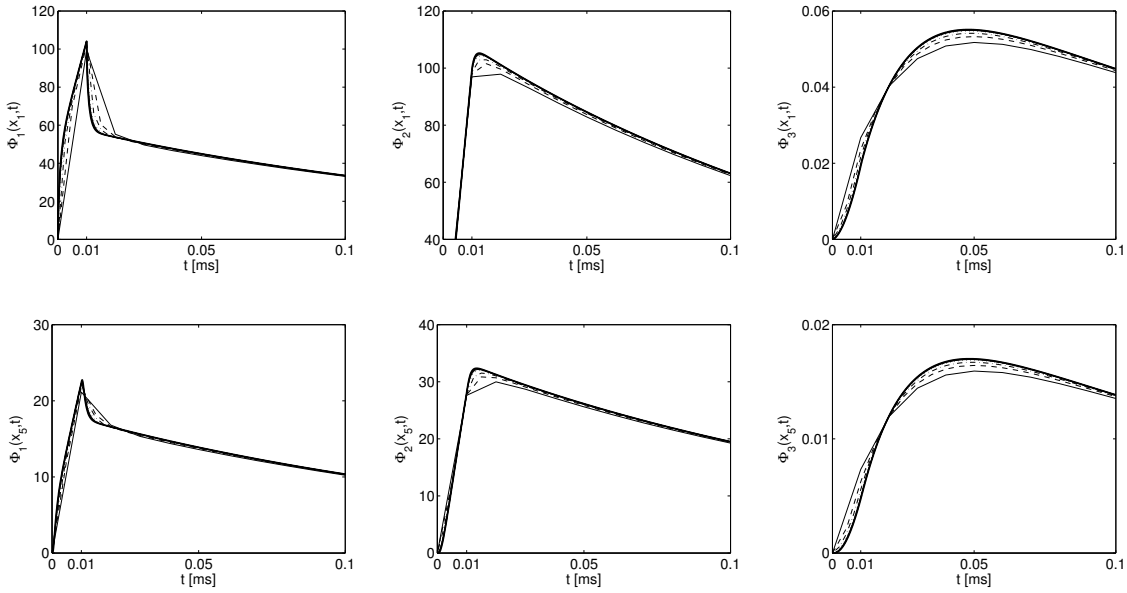
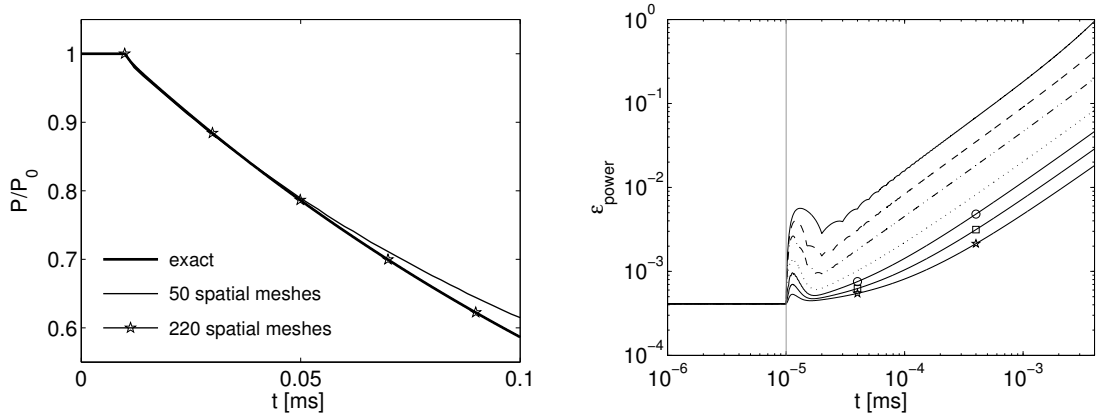


Figure 4. Detector flux evolutions for transient I. Identification of curves as in previous figures.



(a) (b)

Figure 5. Power evolution (left) and relative error (right) for transient II. On the left the effect of spatial discretization is presented, on the right the error introduced by numerical time integration is studied; identification of curves as in previous figures.

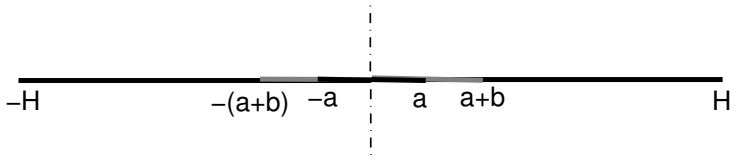


Figure 6. Core composition of the three-group three-region case. Relative dimensions are: $a = 0.20H$, $b = 0.17H$.

(transient III) followed by a system shut-down (both). These two transients are characterized by smaller spatial and spectral effects with respect to the previous one, since the source-driven initial condition for the three-group fluxes is very close to the critical distribution. In Fig. 5 the power evolution for transient II is reported, comparing the analytical result with the values obtained with two different numerical approaches. The time discretization used is the same for both algorithms, with different numbers of spatial meshes, enlightening the effect of the space discretization.

Additional calculations are performed for a one-dimensional heterogeneous system. A source non-multiplying region is surrounded by an highly enriched fissile medium and a lower enriched material is added in the outermost region. The relative dimension of the three regions correspond to the typical geometry of the Yalina Booster core. Three-group cross sections are evaluated on the base of the Yalina fuel composition. In Fig. 6 the structure of the system is sketched.

The critical dimension, critical and source driven flux distributions are evaluated analytically with the standard reactor physics procedure, and the results are compared to a numerical evaluation obtained with the same discretization scheme as in the homogeneous case. The exact critical dimension is $H = 21.229357145$ cm, while a subcritical configuration with $k_{eff} = 0.98$ is obtained with $H = 20.81329856$ cm. The critical flux distributions are reported in Fig. 7.

Figure 8 reports the evolution of the group fluxes and of the power following a localized pulse. The exact

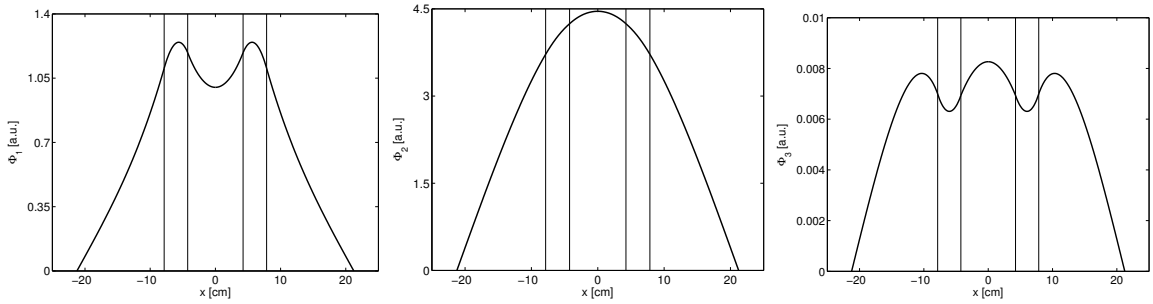


Figure 7. Critical flux distributions for the three-group three-region case.

power is compared to multipoint calculations using one point per energy group [7] and two different projection techniques [8]. As can be seen, the multipoint model is capable to improve the quality of power prediction with respect to point kinetics; however, the choice of the most suitable projection technique plays an important role in producing reliable results.

7. CONCLUSIONS

The work presented in this paper shows that analytical benchmarks can be fruitfully used as reference for code development and for the qualification of numerical algorithms and codes for the kinetic analysis of accelerator-driven system. Some results for different physically significant and increasing complexity problems are presented and discussed to show some specific features in the interpretation of pulsed experiments.

ACKNOWLEDGEMENTS

The work is performed under the auspices of IAEA. One of the Authors (P.R.) is grateful for the nice time spent at the University of São Paulo.

REFERENCES

[1] H. Aït-Abderrahim, A. Stanculescu, “IAEA Coordinated Research Project on Analytical and Experimental Benchmark Analyses of Accelerator Driven Systems,” *Proceedings of ANS Topical Meeting on Reactor Physics, PHYSOR 2006*, Vancouver, 10-14 September, Paper C074 (2006).

[2] V. Bournos, C. Routkovskaia, I. Serafimovich, H. I. Kiyavitskaya, Yu. Fokov, A. Fokov, S. Mazanik, A. Adamovich, T. Korbut, A. Koulikovskaya, A. Khilmanovich, B. Martsinkevich, S. Chigrinov, “Experimental Investigations on ADS at Sub-Critical Facilities of Joint Institute for Power and Nuclear Research-Sosny of the National Academy of Sciences of Belarus,” *Meeting of the CRP Analytical and Experimental Benchmark Analyses of Accelerator Driven Systems*, Minsk, 5-9 December (2005).

[3] B. D. Ganapol, “The Analytical Benchmark Library for Nuclear Engineering: PC Version,” Idaho National Engineering Laboratory, Idaho Falls (1992).

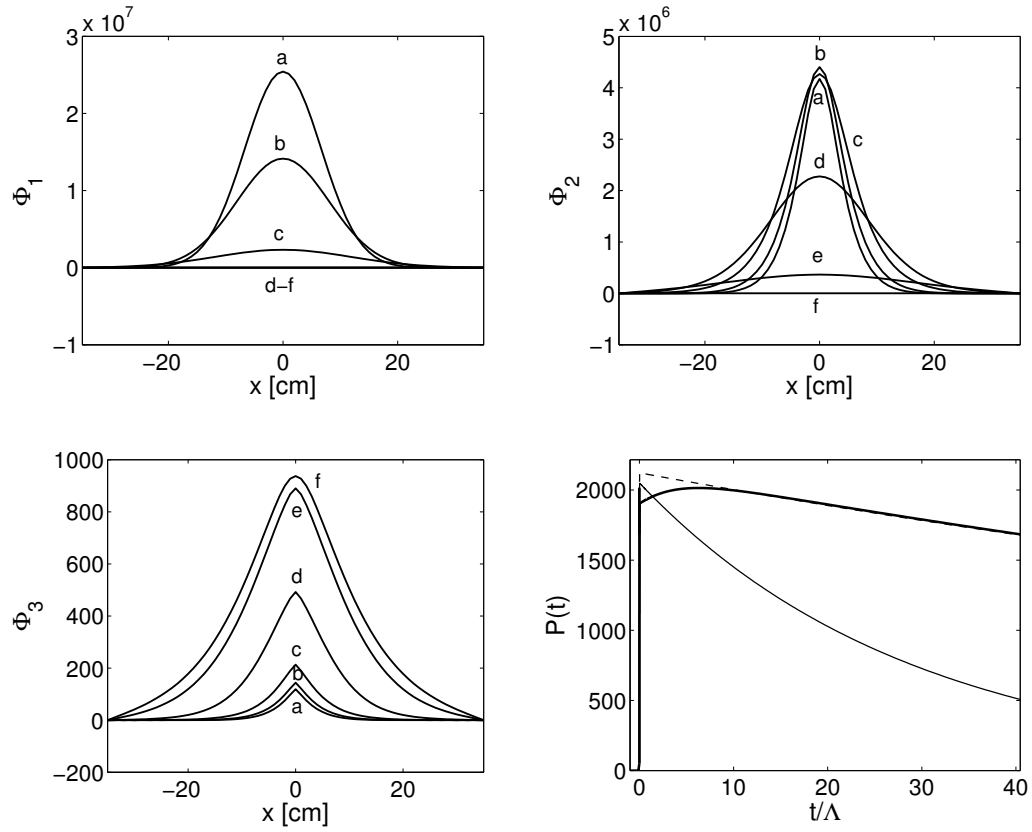


Figure 8. Evolution of the three-group fluxes and of the total power following a localized pulse. The curves are identified as follows: (a) $3.5e-5\ \Lambda$**; (b)** $5e-5\ \Lambda$**; (c)** $1e-4\ \Lambda$**; (d)** $5e-4\ \Lambda$**; (e)** $2.3e-3\ \Lambda$**; (f)** $4.8e-2\ \Lambda$**, where** Λ **is the mean prompt effective generation time. In the graph for the power the bold line is the exact solution while the thin line and the dashed line correspond to three-point calculations with different choices for the projection weight.**

[4] S.E. Corno, G. Manzo, P. Ravetto, R. Ricchena, "Analytical Methods in Local Reactor Dynamics and Validation of the Quasi-Static Approximation," *EUR 6390 EN and European Applied Research Reports*, **1**(4), pp. 831-945 (1979).

[5] E.H. Mund, B.D. Ganapol, P. Ravetto, M.M. Rostagno, "Multigroup Diffusion Kinetics Benchmark of an ADS System in Slab Geometry," *Proceedings of Conference on the New Frontiers of Nuclear Technology: Reactor Physics, Safety and High-Performance Computing, PHYSOR '02*, Seoul, October, Paper 7B-03 (2002).

[6] R.S. Santos, "Dynamics of nuclear cores based on one and two dimensional multigroup diffusion theory," *Proceedings of X ENFIR- Brazilian Meeting on Reactor Physics*, Aguas de Lindoia, Brazil, 7-11 August, pp. 143-148 (1995).

[7] P. Ravetto, M.M. Rostagno, G. Bianchini, M. Carta, A. D'Angelo, "Application of the Multipoint Method to the Kinetics of Accelerator-Driven Systems," *Nuclear Science and Engineering*, **148**(1), pp. 79-88 (2004).

[8] S. Dulla, P. Picca, "Consistent multipoint kinetics for source-driven systems," *Progress in Nuclear Energy*, **48**, pp. 617-628 (2006).