

## Neutron Transport and Diffusion Models for Molten-Salt Reactor Dynamics

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### *Abstract*

The steady state and time dependent equations for a molten-salt reactor are numerically solved adopting the multigroup diffusion and transport models for neutrons. The motion of the multiplying material is properly accounted for in the balance equations for delayed neutron precursors. Non-linear feedback phenomena are also taken into account by coupling the neutron equations with a simplified zero-dimensional thermal model. The analysis of the results presented allows the identification of physical situations for which transport effects can play an important role and thus must be properly described in the study of realistic system configurations.

**KEYWORDS:** *Molten-salt reactors, Non-linear neutron dynamics*

## 1. Introduction

In a previous paper [1] the dynamics of a circulating fuel reactor in the presence of non-linear feedback effects has been analyzed, introducing a one-dimensional multigroup diffusion model for neutrons and a simplified zero-dimensional two-temperatures thermal model for the treatment of the feedback. Some peculiar static and time-dependent effects connected to the motion of the fuel in the reactor and the presence of thermal feedback have been enlightened. As a further step toward the assessment of the safety characteristics of circulating fuel systems, the adoption of more sophisticated models for the analysis of neutronics and thermal-hydraulics is proposed. For some concepts of molten salt reactors neutron transport phenomena may become important. In this paper the results obtained with the diffusion approximation are compared with those obtained by adopting the transport model. The work aims to identify the situations for which the possible appearance of transport phenomena affects the behavior of the system significantly. The transport equation is solved numerically by the discrete-ordinate technique and the time integration is carried out by the Euler implicit discretization technique.

## 2. Neutronic and thermal models

The basic, elementary model for the description of a molten-fuel reactor with circulating fuel can be introduced adopting multigroup diffusion theory with one or more families of precursors. Considering for simplicity a one-dimensional slab reactor of thickness  $a$ , the neutronic

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equations read as [1]:

$$\left\{ \begin{array}{l} \left( \frac{1}{v^g} \partial_t - \partial_z D^g \partial_z + \Sigma_r^g \right) \Phi^g = \sum_{g' \neq g} \Sigma^{g' \rightarrow g} \Phi^{g'} \\ \quad + \chi_p^g (1 - \beta) \sum_{g'} (v \Sigma_f \Phi)^{g'} + \chi_d^g \sum_p (\lambda C)_p + S^g, \quad z \in (0, a), \quad t > 0 \\ \\ (\partial_t + \lambda_p + \partial_z) (u C_p) = \beta_p \sum_g (v \Sigma_f \Phi)^g, \quad z \in (0, a), \quad t > 0, \end{array} \right. \quad (1)$$

with boundary and initial conditions:

$$\left\{ \begin{array}{l} \Phi^g(0, t) = \Phi^g(a, t) = 0, \quad t > 0, \\ C_p(0, t) = e^{-\lambda_p \tau} C_p(a, t - \tau), \quad t > 0, \\ \Phi^g(x, 0) = \Phi_0^g(x), \quad z \in (0, a), \\ C_p(x, 0) = C_{p,0}(x), \quad z \in (0, a), \\ C_p(a, t) = C_{p,a}(t), \quad t \in (-\tau, 0). \end{array} \right. \quad (2)$$

A simple thermal model is now adopted, where the thermal field is characterized only by the average fuel and surrounding material temperatures. Hence, the two-temperature thermal model coupled with the neutronic equations is given by the following equations:

$$\left\{ \begin{array}{l} (\rho c V)_f \partial_t T_f = E_f \int_0^a \sum_{g'} (\Sigma_f \Phi)^{g'} dz - (\rho c A)_f 2u(T_f - T_{in}) - hp_f a(T_f - T_w), \quad t > 0, \\ \\ (\rho c V)_w \partial_t T_w = hp_f a(T_f - T_w), \quad t > 0, \end{array} \right. \quad (3)$$

where  $T_{in}(t)$  and  $T_{out}(t)$  denote the inlet and outlet temperatures,  $T_f(t) = (T_{out} + T_{in})/2$  is the average core temperature and  $\rho$ ,  $c$  and  $V$  stand for density, heat capacity and volume, respectively. The lower indices  $f$  and  $w$  refer to the molten fuel and to the surrounding material,  $h$  and  $p_f$  are the conductance between the fuel and the surrounding material and the length of the contact perimeter respectively.  $E_f$  is a proper energy generation coefficient for the fuel channel.

The feedback phenomenon is introduced with a modification on the absorption cross section, depending linearly on two feedback coefficients for the fuel and the moderator:

$$\delta \Sigma_a^g = \alpha_f^g (T_f - T_{f0}) + \alpha_w^g (T_w - T_{w0}). \quad (4)$$

Possible improvements in the thermal model should take into account the effects of the temperature modifications on the fission production and the presence of a delayed power source associated to the energy release in the graphite which may play an important role in many safety significant transients. These aspects rely within the development of the present work.

When passing to a multigroup transport model, the equations for neutrons (1) are substituted

by the following ones:

$$\left\{ \begin{array}{l} \left( \frac{1}{v^g} \partial_t + \mu \partial_z + \sigma_t^g \right) \phi^g = \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\mu) \sum_{g'} \sigma_l^{g' \rightarrow g} \phi^{l,g'} \\ \quad + \frac{\chi_p^g}{2} (1 - \beta) \sum_{g'} (v \Sigma_f \Phi)^{g'} + \frac{\chi_d^g}{2} \sum_p (\lambda C)_p + S^g, \quad z \in (0, a), t > 0 \\ (\partial_t + \lambda_p + \partial_z) (u C_p) = \beta_p \sum_g (v \Sigma_f \Phi)^g, \quad z \in (0, a), t > 0, \end{array} \right. \quad (5)$$

and the corresponding vacuum boundary conditions for the angular flux  $\phi^g(z, \mu, t)$  are introduced as:

$$\begin{aligned} \phi^g(0, \mu, t) &= 0, \quad \mu > 0, t > 0, \\ \phi^g(0, \mu, t) &= 0, \quad \mu < 0, t > 0, \end{aligned} \quad (6)$$

while the boundary conditions for delayed neutron precursors are left unchanged with respect to Eq. (2). The transport model is discretized adopting a discrete ordinates diamond differencing scheme. Since this method works on cell averaged values, discretization of the diffusion equation has been introduced in the cell-centered form.

The numerical code developed for this work is specifically suited for the solution of time-dependent problems in presence of non-linear phenomena, introducing perturbations of the cross sections and of the external source with various dependences on time. In a following section some results are presented for different configurations, evidencing the appearance of transport phenomena for optically small systems.

### 3. Numerical aspects

The equations of systems (1) and (5) are discretized in time and in space. For the steady-state case (eigenvalue or source problem), as well as for each time step in a time-dependent calculation, the non-linear coupling between the neutron-concentration equations and the temperature equations is resolved by a number of iterations. Each iteration starts with given temperatures, then the corresponding absorption cross sections are computed and fluxes and concentrations are determined; afterwards, new temperatures are determined and a convergence check is applied. At each iteration the solution of the flux equations requires a succession of external iterations over the fission source, starting from the solution for the delayed neutron precursor concentrations. An implicit scheme in time with constant step  $\Delta t$  is used. A region-wise constant mesh of width  $\Delta z_k$ , ( $k = 0, 1, \dots, N$ ), is used for the spatial discretization.

The solution of the transport model is based on discrete-ordinate diamond differencing [2]. To make a consistent comparison with diffusion, also the diffusion equation is discretized with a cell-centered scheme, leading to an algebraic problem for the cell-averaged flux with the following structure:

$$-l_k \Phi_{k-1}^g + d_k \Phi_k^g - l_{k+1} \Phi_{k+1}^g = \Delta z_k \widehat{S}_k^g. \quad (7)$$

The source term includes scattering and fission contributions, together with the term deriving from the previous time step in time-dependent calculations.

The concentrations equations are formulated on cell-edge values and the cell-averaged values are recovered as the average of the edge values, leading to a standard up-wind formulation of the problem for the convective term:

$$l'_k \widehat{C}_{p,k-1} + d'_k \widehat{C}_{p,k} = \widehat{S}_{p,k}, \quad (8)$$

where

$$l'_k = \frac{1}{2} \left( 1 + \frac{1}{\lambda_p \Delta t} \right) - \frac{u}{\lambda_p \Delta z_k}, \quad d'_k = \frac{1}{2} \left( 1 + \frac{1}{\lambda_p \Delta t} \right) + \frac{u}{\lambda_p \Delta z_k}. \quad (9)$$

The source term for the delayed concentrations includes the fission contribution and the term due to the discretization of the time derivative.

#### 4. Results

Preliminarily, some results concerning criticality calculations using both diffusion and transport for a simple homogeneous system in the one-group framework are presented. The geometry is characterized by a small optical dimension. In Table 1 the values of the multiplication constant  $k_{eff}$  are reported, showing the discrepancies connected to the use of different models for the solution of the eigenvalue problem. The differences are obviously enhanced by the use of the zero-flux boundary conditions in the diffusion model, as is shown in the first column of the results, where a large reduction of the value of  $k_{eff}$  is observed. However, the comparison is consistent only if Mark boundary conditions for diffusion are applied. In any case, large discrepancies are still clearly detected.

The effect of the fuel motion is also evidenced, as can be seen in Fig. 1, where the critical fluxes and the precursor distributions are plotted in both diffusion and  $S_8$  model for different flow regimes.

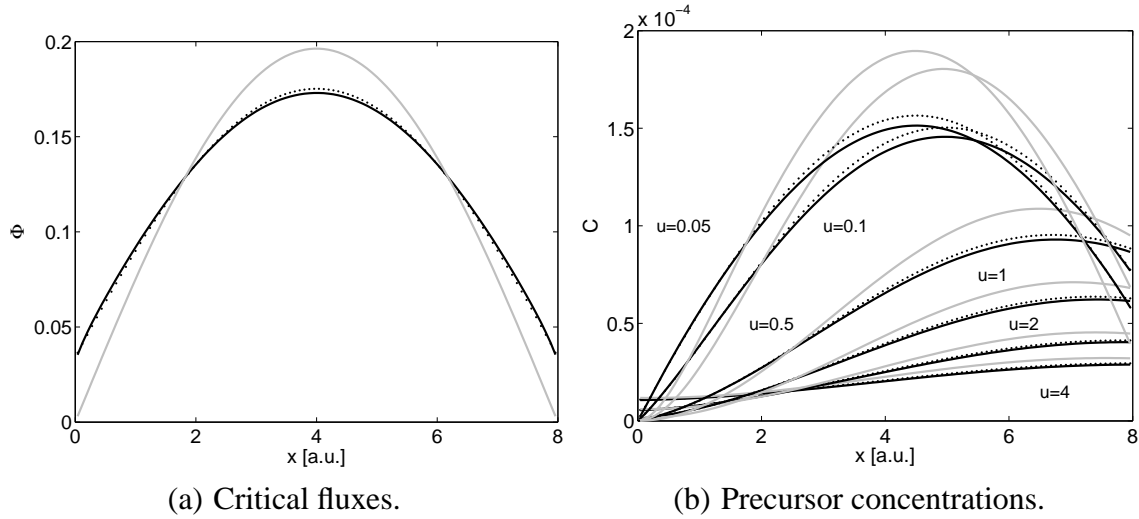
**Table 1:** Values of  $k_{eff}$  as a function of fuel velocity evaluated with diffusion and  $S_N$  models. Geometric dimension:  $H = 8$  mfp,  $c = 0.9$ ,  $\beta = 650$  pcm,  $\lambda = 0.1 \text{ s}^{-1}$ .

$u$ [mfp/s]	$\tau$ [s]	diffusion (zero BC)	diffusion (Mark BC)	$S_4$	$S_6$	$S_8$	$S_{16}$
0.05	800	0.90103	0.97871	0.99806	0.99931	0.99968	1.00000
0.1	400	0.90061	0.97831	0.99765	0.99891	0.99927	0.99959
0.5	80	0.89801	0.97560	0.99489	0.99615	0.99651	0.99683
1	40	0.89697	0.97442	0.99369	0.99495	0.99530	0.99562
2	20	0.89642	0.97379	0.99304	0.99430	0.99466	0.99498
4	10	0.89623	0.97357	0.99282	0.99407	0.99443	0.99475

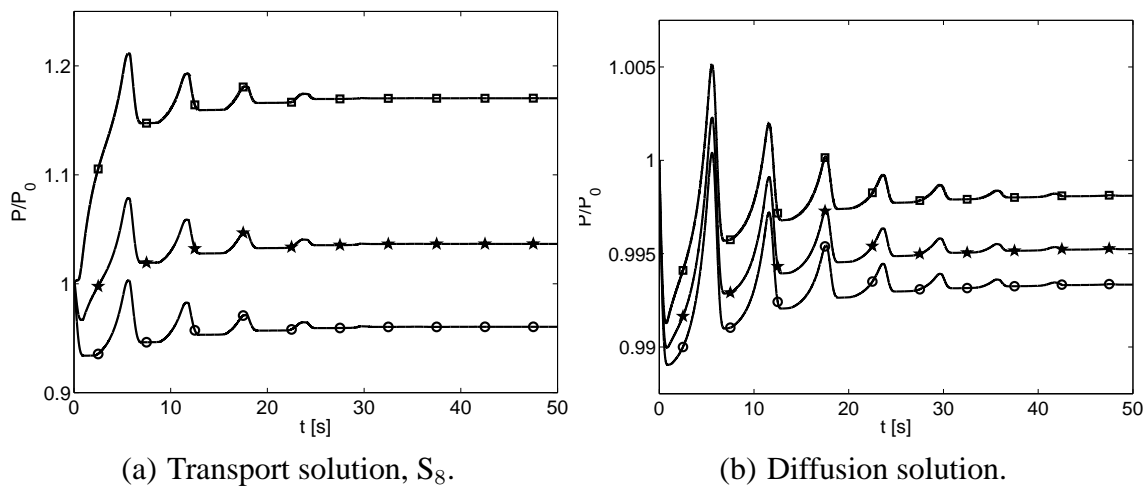
A time dependent calculation is then presented still for the one-group system previously defined in subcritical source-driven regime. A fuel velocity transient is considered, inducing the power evolutions drawn in Fig. 2. The fuel velocity is step-changed from 1 mfp/s to 8 mfp/s, reducing the total transit time in the circuit to 6 s. The initial effective multiplication constant takes the value 0.98000 in the  $S_8$  calculation, while it is only 0.88318 in diffusion. The equilibrium power and temperature values are rather different, due to the large  $k_{eff}$  difference, and have strong influence in the following transient. The oscillation observed in the graphs is due to the re-immission of precursors with a period equal to the circulation time in the primary circuit. The three graphs clearly show the effect and the importance of the feedback phenomenon.

A calculation is now performed using more realistic geometrical and material data, as typical of recent designs of fluid fuel reactors developed within the research activities on innovative

**Figure 1:** Critical configuration in diffusion (gray lines),  $S_{16}$  (black lines) models. The solution for diffusion with Mark boundary diffusion is also presented (dotted lines).



**Figure 2:** Fuel velocity transient in one-group framework. Circles: no feedback; stars:  $\alpha_f = \alpha_w = 2E - 6 \text{ cm}^{-1}\text{C}^{-1}$ ; squares:  $\alpha_f = \alpha_w = 5E - 6 \text{ cm}^{-1}\text{C}^{-1}$ . The two feedback coefficients correspond to a reactivity effect that, when evaluated at first order, is 5.4 pcm/C and 13.4 pcm/C, respectively.



systems for waste transmutation [3]. The MOSART concept [4], being a homogeneous structure with no moderator, is characterized by a harder energy spectrum and consequently the possible appearance of transport phenomena needs to be evaluated, both in steady state and in transient conditions. The two-temperature model takes into consideration in this case the fuel core and the reflector. A four-group cross section data set is used, with a fuel velocity of 50 cm/s and a recirculation time of 3.94 s, corresponding to a total transit time in the primary circuit of 11.94 s. The initial subcritical system is characterized by a multiplication constant of 0.98034 in  $S_8$  and 0.97999 in diffusion.

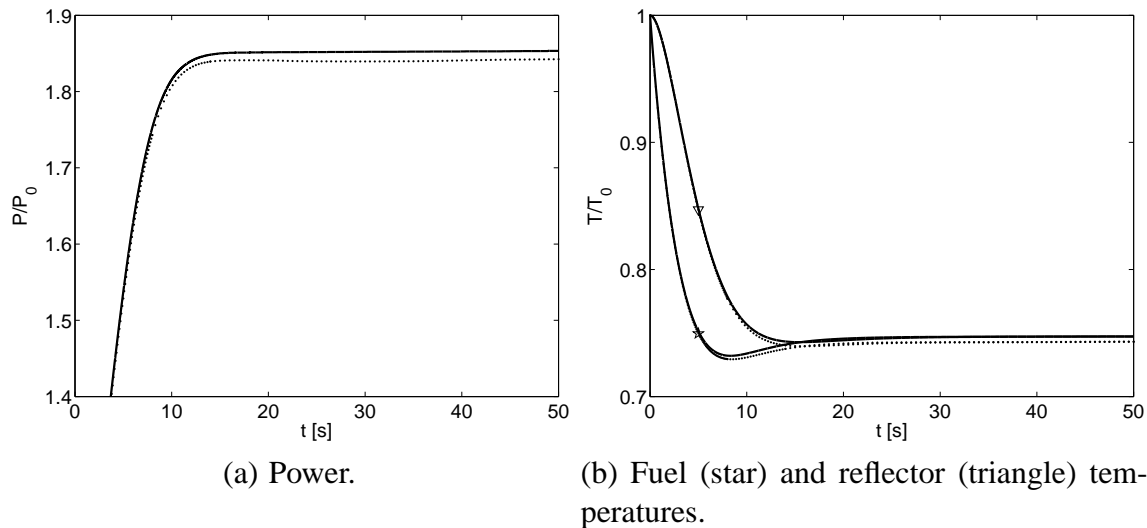
The two transients presented in the following concern evaluations typical for safety analysis, e.g. a fuel overcooling leading to a reduction of the core inlet temperature and a circulation pump coastdown.

A transient started by a reduction of the core inlet temperature from 600 C to 300 C is considered in Fig. 3. The final steady state effective multiplication constants are 0.98929 in  $S_8$  and 0.98893 in diffusion. The reactivity coefficient is assumed to be 2.3 pcm/C for both the fuel and the reflector.

A pump coastdown transient is studied in Fig. 4. The fuel velocity is reduced to one-fifth its initial value in 3 s, following the curve given in Fig. 4b. The final steady state effective multiplication constants are 0.96776 in  $S_8$  and 0.96742 in diffusion.

Although it appears that diffusion theory yields rather good results for these transients, the power prediction is on the side of unsafety. Also, the transients considered do not involve localized effects which may lead to more critical conditions for safety evaluations.

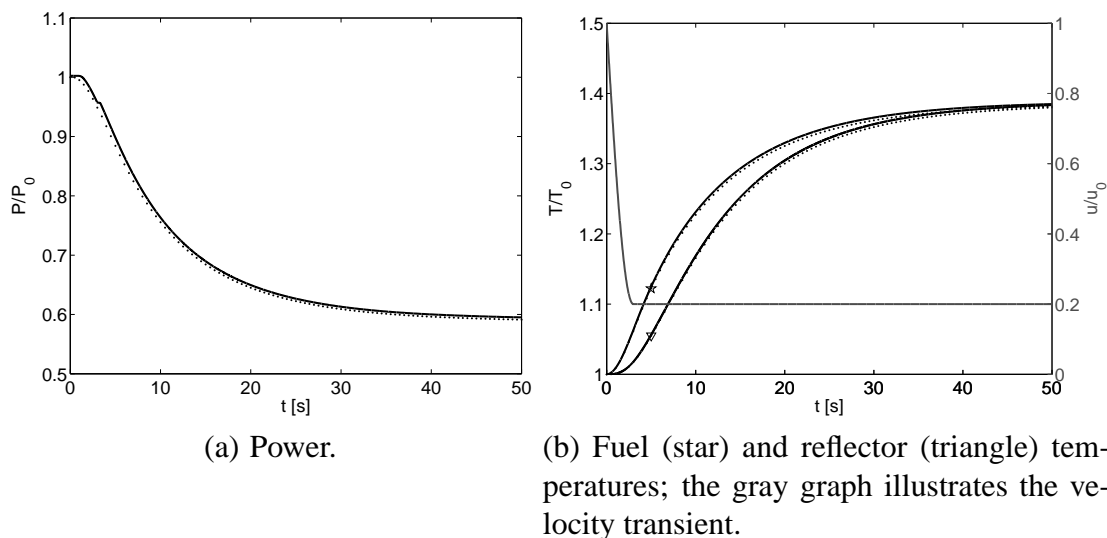
**Figure 3:** Transient induced by a reduction of the inlet temperature to one-half its initial value.  $\alpha_f^g = \alpha_w^g = 1E - 7 \text{ cm}^{-1} \text{ C}^{-1}$  in all four groups. Solid line:  $S_8$ , dotted line: diffusion.



## 5. Conclusion

A numerical solution for the non-linear dynamics of a circulating fuel reactor is presented, both in the frame of transport and diffusion theory. The results presented evidence the possibility of the appearance of significant transport effects in the time dependent simulation of

**Figure 4:** Transient induced by a reduction of the fuel velocity to 1/5 its initial value.  $\alpha_f^g = \alpha_w^g = 1e - 7 \text{ cm}^{-1} \text{ C}^{-1}$  in all 4 groups. Solid line:  $S_8$ , dotted line: diffusion.



small-size molten salt systems, which must therefore be properly accounted for in safety evaluations.

## References

- 1) R. Sanchez, B.D. Ganapol, S. Dulla, P. Ravetto, "Analysis of a Simplified Molten-Fuel Reactor," Proc. of the 18-th Int. Conf. on Transport Theory, 18ICTT, Rio de Janeiro, Brazil, July 20-25, 2003, 196-204 (2003).
- 2) E.E. Lewis, W.F. Miller, Jr., "Computational Methods of Neutron Transport," Wiley, New York,(1984).
- 3) W. Maschek, A. Stanculescu, "IAEA CRP on Studies of Advanced Reactor Technology Options for Effective Incineration of Radioactive Waste," Proc. of the Int. Conf. GLOBAL 2005, Tsukuba, Japan, Oct 9-13, 2005, Paper No. 010 (2005).
- 4) V. Ignatiev et al., "Integrated Study of Molten Na,Li,Be-F Salts for LWR Waste Burning in Accelerator Driven and Critical Systems," Proc. of the Int. Conf. GLOBAL 2005, Tsukuba, Japan, Oct 9-13, 2005 (2005).