A Preliminary Approach to the Neutronics of the Molten Salt Reactor by means of COMSOL Multiphysics

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Abstract: The Molten Salt Reactor (MSR), proposed along with other five innovative concepts of fission nuclear reactor by the Generation IV International Forum (GIF-IV), represents a challenging task from the modelling perspective because of the strong coupling between neutronics and thermo-hydrodynamics due to liquid fuel circulation in the primary loop. In this paper COMSOL Multiphysics® is adopted to investigate the MSR neutronics, focusing on the steady-state core average conditions of the Molten Salt Breeder Reactor (MSBR) developed at Oak Ridge National Laboratory (ORNL). The results achieved by COMSOL, adopting a two energy group diffusion model and using group constants calculated by means of the deterministic code SCALE5.1, are compared with those achieved by the stochastic code MCNP for validation purpose. In particular, neutron flux profiles and integral quantities, like the effective multiplication factor and homogenized cross sections, are evaluated and discussed. The model implemented in COMSOL is then used to study the effect of the fuel velocity on the neutronic behaviour of the analysed MSBR core channel.

Keywords: Neutronics, Generation IV, Molten Salt Reactor.

1. Introduction

In 2002, the Generation IV International Forum (GIF-IV) [1] proposed six different reactor concepts aimed at a more sustainable nuclear energy progress. The Molten Salt Reactor (MSR) [2] is one of the candidates among the several designs studied within the GIF-IV program. The most attracting feature of this kind of reactor is represented by the liquid fuel, which consists of a molten salt mixture and also plays the role of coolant.

The MSR presents a strong coupling between neutronics and thermo-hydraulics due to the fact that the fuel is flowing through the primary loop; as a consequence, a certain amount of fission products (called neutron precursors), depending on the velocity field of the fuel salt, can decay outside the core emitting delayed neutrons, which strongly affect the neutron balance [3].

In this frame, COMSOL Multiphysics® [4] represents an interesting and promising tool to study the MSR system, as proved by the several studies performed at Politecnico di Milano [5,6,7,8] with the purpose to set up a suitable and reliable simulation environment and to study the physical behaviour of the nuclear components of interest. Since modelling of such complex and often non-linear systems requires qualified tools, the validation of numerical results is an important goal to be fulfilled: actually, great efforts have been spent on the heat transfer and fluid dynamics of molten salts [5,8,9,10].

In order to qualify the methodology here presented, based on the use of COMSOL for neutronic analysis of the MSBR core channel [11], a validation, including Monte Carlo calculation with MCNP [12], has been carried out by comparing the main neutronic parameters (multiplication factor, cross sections, flux profiles).

The present paper is organized as follows: in the second section, the particular reactor configuration and the analysed geometry are described; the third section deals with neutronics modelling; in the fourth section, the validation results are presented along with a preliminary study of the effect of the fuel velocity on the neutronic behaviour; the conclusions of this work are drawn in the fifth section.

2. System Description

Among the several Molten Salt Reactors concepts developed in the past and reconsidered in the last years [2], the MSBR was chosen as reference configuration for the analysis because of the large amount of data available from many conceptual design studies performed during 70s [11,13]. This reactor was designed to produce 1000 MW_e and is featured by a thermal neutron spectrum and thorium fuel cycle; the core is formed of square graphite-moderated blocks,

each one with a central molten salt fuel/coolant channel, as shown in Fig. 1.

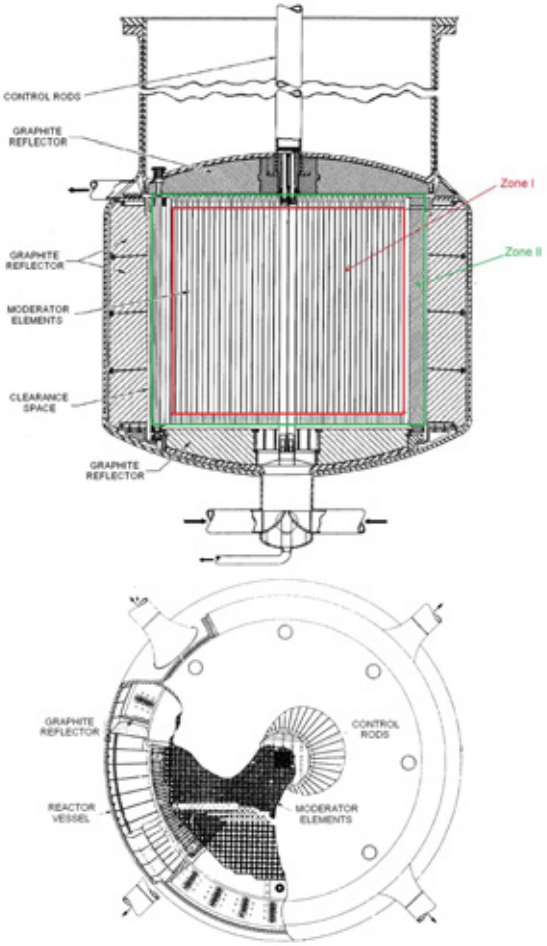

Figure 1. Longitudinal and horizontal sections of the MSBR core [11].

The reactor core has a central zone in which 13% of the volume consists of fuel salt (zone I), an outer, under-moderated region characterized by 37% of salt (zone II), and a reflector region containing about 1% of fuel. In the present work, ¼ of an equivalent core element, representative of the average conditions of zone I, has been adopted for the analyses (see Fig. 2), since the fission energy is mainly released in this region that extends over the major part of the core [11]. The channel radius, its height and the graphite element thickness are R_F = 2.08 cm, H = 396 cm and L = 5.08 cm, respectively.

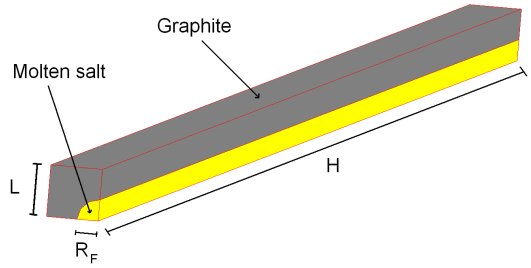

Figure 2. Geometrical representation of the analysed MSBR core channel (graphite is depicted in gray and fuel salt in yellow, respectively).

As concerns the fuel salt in the primary circuit, the main components are ^{7}LiF (71.7 mol%), BeF_2 (16 mol%), ThF_4 (12 mol%) and $^{233}UF_4$ (0.3 mol%); the equilibrium composition adopted in the present work is reported in detail in Table 1.

Table 1: Equilibrium composition of fuel salt and graphite

Constituent	Atomic density [atom·b^{-1}·cm^{-1}]
^{232}Th	$3.75\cdot10^{-3}$
^{233}Pa	$3.88\cdot10^{-7}$
^{233}U	$6.64\cdot10^{-5}$
^{234}U	$2.31\cdot10^{-5}$
^{235}U	$6.01\cdot10^{-6}$
^{236}U	$6.21\cdot10^{-6}$
^{237}Np	$8.59\cdot10^{-7}$
^{238}Pu	$6.10\cdot10^{-6}$
^{239}Pu	$1.29\cdot10^{-7}$
^{240}Pu	$6.83\cdot10^{-8}$
^{241}Pu	$6.21\cdot10^{-8}$
^{242}Pu	$1.23\cdot10^{-7}$
^{6}Li	$1.95\cdot10^{-7}$
^{7}Li	$2.24\cdot10^{-2}$
^{9}Be	$5.00\cdot10^{-3}$
^{19}F	$4.77\cdot10^{-2}$
Graphite	$9.51\cdot10^{-2}$

3. Neutronics Modelling

A preliminary model, based on the two energy group diffusion theory with six groups of neutron precursors, in steady-state conditions, was implemented using the *Convection and Diffusion* application mode of COMSOL, according to the following equations (symbols are defined in the Appendix) to be solved using the eigenvalue analysis:

$$D_1\nabla^2\phi_1 - (\Sigma_{a1} + \Sigma_{1\to2})\phi_1 + \Sigma_{2\to1}\phi_2 + \\ + \frac{(1-\beta)}{k_{eff}}(\nu_1\Sigma_{f1}\phi_1 + \nu_2\Sigma_{f2}\phi_2) + \sum_{i=1}^{6}\lambda_i c_i = 0 \quad (1)$$

$$D_2\nabla^2\phi_2 - \Sigma_{a2}\phi_2 + \Sigma_{1\to2}\phi_1 - \Sigma_{2\to1}\phi_2 = 0 \quad (2)$$

$$u\cdot\nabla c_i = \frac{\beta_i}{k_{eff}}(\nu_1\Sigma_{f1}\phi_1 + \nu_2\Sigma_{f2}\phi_2) - \lambda_i c_i = 0 \quad (3)$$

$$\beta = \sum_{i=1}^{6}\beta_i \quad (4)$$

The group constants of the diffusion equations (i.e., nuclear data, fission cross sections, absorption cross sections and diffusion coefficients) were evaluated by means of pin cell calculation performed with the code components NEWT/TRITON [14,15] of SCALE5.1 package. NEWT solves the two-dimensional multi-group neutron transport equation according to the "extended step characteristic method". The nuclear data used are based on ENDF/B version VI.7 library, available in SCALE5.1 as multi-group energy cross section libraries [16]. In the present work, the 238 energy group library was adopted. The reference temperature of 900 K was assumed for the fuel salt and graphite whose composition is reported in Table 1. The solution of the pin cell calculation was used to collapse the 238 group cross section library in the thermal and fast energy groups.

In order to choose an adequate spatial mesh for the SCALE5.1 model geometry, a sensitivity analysis was carried out evaluating the effective multiplication factor (k_{eff}) as a function of the number of the computational cells. The results (Fig. 3) show that k_{eff} is weakly dependent on the mesh size; it varies of less than 50 pcm (per cent mille) over three orders of magnitude; a good compromise between accuracy and computational time was reached by choosing a mesh structure of 590 cells.

The cut-off energy for the thermal group is usually chosen sufficiently high so that upscattering out of the thermal group can be neglected. In a typical Light Water Reactor (LWR) this value ranges between 0.5 and 1 eV, and up to 3 eV for high temperature gas cooled reactors [17]. In order to choose a reasonable value of the cut-off energy for the MSBR, the number of

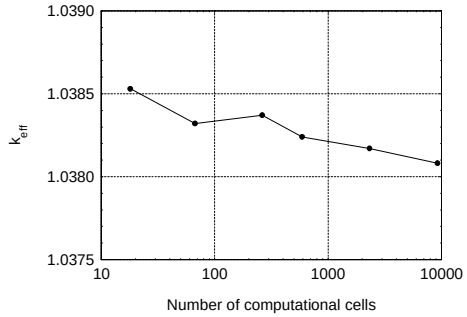

Figure 3. Results of the mesh sensitivity analysis for the SCALE5.1 pin cell model.

upscattering events per fission neutron source as a function of neutron energy was calculated by means of SCALE5.1. The curve is illustrated in Fig. 4 and shows that upscattering becomes negligible for neutron energy of about 1 eV. This value has been selected for the group constant calculation, whose results are briefly summarized in Appendix (see Table 4).

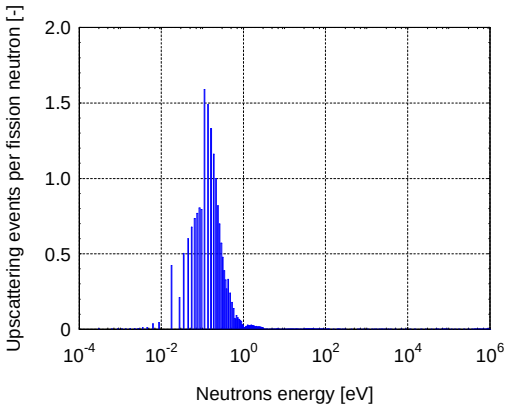

Figure 4. Number of upscattering events per fission source neutron vs. neutron energy calculated by SCALE5.1 (v6-238 cross section library).

4. Results and Discussion

In order to validate the COMSOL analysis results discussed in the present section, the MSBR pin cell geometry was modelled by means of MCNP using the JEFF3.1 cross section library [18]. This code permits to solve the neutron transport equation in integral form using continuous energy nuclear data with practically no approximation; therefore, it represents a valuable tool for such validation process when

experimental data are not available. A further analysis concerning the effect of fuel velocity on the system reactivity and flux profiles is presented.

4.1 Validation

A first assessment of the agreement between COMSOL, SCALE5.1 and MCNP is given by the multiplication factor calculation results reported in Table 2. This result can be considered acceptable for a preliminary evaluation of the rector core neutronics.

The difference between SCALE5.1 and MCNP, around 920 pcm, can be explained by the different nuclear data used, which are usually the main error source in neutronic calculations [19,20,21,22]. It is worth to remind that the SCALE5.1 model is based on energy multi-group approximation unlike MCNP, which uses continuous energy data as mentioned before. As far as COMSOL is concerned, the reason of the discrepancy can be found in the adopted diffusion theory approximation.

Table 2: Effective neutron multiplication factors

Code	k_{eff}
SCALE5.1	1.03824
COMSOL	1.04216
MCNP	1.04745 ± 0.00079

In Table 3 the macroscopic cross sections for the two energy groups calculated by SCALE5.1 and MCNP are given. As can be observed, the maximum difference (around 10%) occurs in the graphite and, more specifically, for the capture cross section.

In Fig. 5 the average axial flux profiles calculated by means of both COMSOL diffusive model and the MCNP model are shown[1], whereas in Fig. 6 the radial flux comparison is reported. In particular, fast and thermal neutron fluxes are plotted for the graphite and fuel salt materials.

[1] Being SCALE5.1, more specifically NEWT, a two-dimensional code, the axial profile cannot be calculated. However, the channel height (axial dimension equal to 396 cm) was used for a buckling correction to calculate neutron leakage normal to the plane.

Table 3: Comparison of the two energy group collapsed macroscopic cross sections

Group	$\nu\Sigma_f$ [cm^{-1}] Fast	$\nu\Sigma_f$ [cm^{-1}] Thermal	Σ_C [cm^{-1}] Fast	Σ_C [cm^{-1}] Thermal	Σ_{TOT} [cm^{-1}] Fast	Σ_{TOT} [cm^{-1}] Thermal
Fuel salt						
MCNP	$6.22\cdot10^{-3}$	$4.23\cdot10^{-2}$	$6.86\cdot10^{-3}$	$1.62\cdot10^{-2}$	$3.10\cdot10^{-1}$	$3.14\cdot10^{-1}$
SCALE5.1	$6.00\cdot10^{-3}$	$4.43\cdot10^{-2}$	$6.96\cdot10^{-3}$	$1.71\cdot10^{-2}$	$3.17\cdot10^{-1}$	$3.17\cdot10^{-1}$
Diff[a] [%]	-3.5%	4.7%	1.5%	5.6%	2.3%	1.0%
Graphite						
MCNP	-	-	$1.18\cdot10^{-5}$	$1.37\cdot10^{-4}$	$3.95\cdot10^{-1}$	$4.51\cdot10^{-1}$
SCALE5.1	-	-	$1.32\cdot10^{-5}$	$1.49\cdot10^{-4}$	$4.07\cdot10^{-1}$	$4.61\cdot10^{-1}$
Diff[a] [%]	-	-	12%	8.8%	3.0%	2.2%

[a] with respect to the MCNP values.

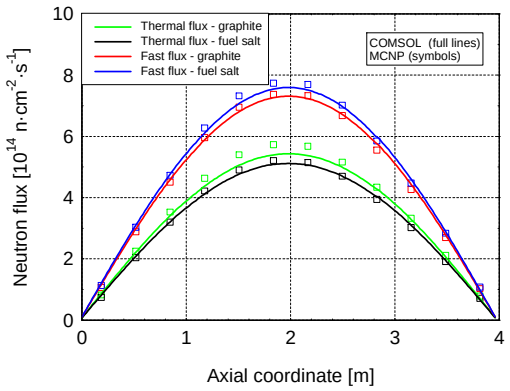

Figure 5. Comparison between COMSOL and MCNP average axial flux profiles.

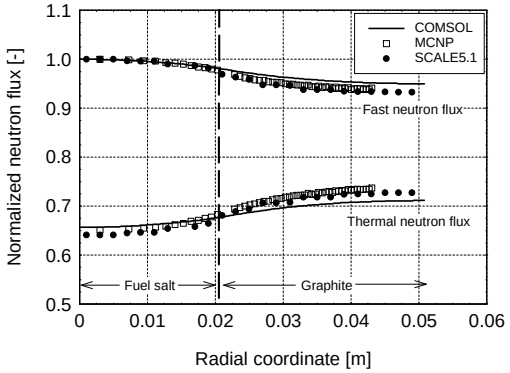

Figure 6. Comparison between COMSOL, SCALE5.1 and MCNP average radial flux profiles.

As can be noticed, COMSOL flux profiles are in accordance with those calculated by means of MCNP and SCALE5.1 within a maximum error of 7%. Nevertheless, the results show a slightly different behaviour of the COMSOL radial profile at the interface between fuel and

graphite (see Fig. 6), being the gradient lower. This discrepancy is mainly due to the diffusion theory approximation, adopted in the COMSOL simulation, which cannot properly describe the neutron transport near boundaries or where material properties change significantly [17].

Finally, a difference within 10% has been found for average and peak neutron fluxes between the COMSOL results and those ones reported by ORNL [11].

4.2 Fuel Velocity Effect

The neutronic behaviour of the system was studied by means of the COMSOL model as a function of fuel velocity, which is assumed uniform along the channel. Preliminary results are shown in Figs. 7, 8, 9 and 10, where the axial flux, the reactivity loss and the precursor concentration are reported. The axial fluxes calculated for circulating fuel (the normal operation values are adopted – i.e., $u = u_{ref} = 1.4$ m/s, and $\tau_{EL} = \tau^*_{EL} = 6$ s) are compared with the static fuel neutron fluxes. As expected, the profiles do not show any significant variations [3,5,23,24], proving that the assumption of static fuel represents an acceptable approximation.

The theoretical reactivity loss curve, based on space independent point reactor kinetics [25], calculated according to Eq. (5), is compared in Fig. 8 with the results obtained by means of the two energy group diffusive model adopted in COMSOL:

$$\Delta\rho = \beta - \sum_{i=1}^{6} \frac{\beta_i \lambda_i}{\lambda_i + \dfrac{1 - e^{-\lambda_i \tau_{EL}}}{\tau_C}} \qquad (5)$$

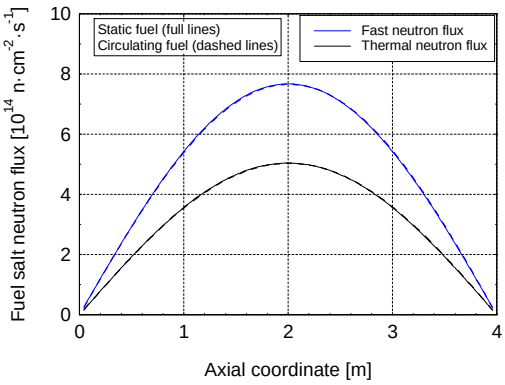

Figure 7. Effect of fuel velocity on axial flux profiles.

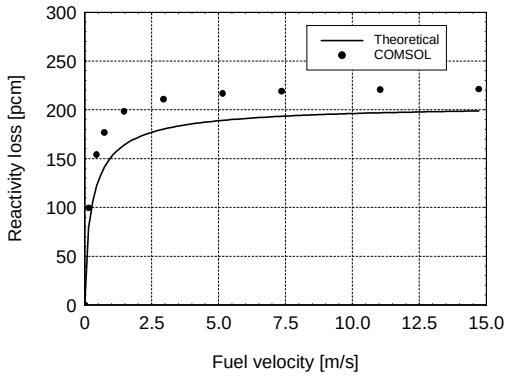

Figure 8. Comparison of COMSOL results with zero-dimensional theoretical reactivity loss as a function of the fuel velocity from Ref. [25].

The COMSOL reactivity variations calculated starting from a critical configuration, $k_{eff} = 1$, with the fuel velocity set to zero, are generally higher than the theoretical ones. This difference has to be found in the two different modelling approaches. In particular, the contribution to the reactivity of the delayed neutron precursors (DNP) at different axial positions of the channel is neglected in the theoretical model, which is based on a zero-dimensional geometry and, for this reason, is not able to catch the effect of the axial precursor distribution that is strongly affected by the fuel transport along the channel [24]. On the contrary, spatial effects are embodied in the COMSOL model, where the problem is also solved in the axial dimension.

In order to quantify the importance of the space dependency on the effective DNPs in the core, a calculation was performed using a simplified model of MSR that considers an infinite external loop (i.e., $\tau_{EL} \rightarrow \infty$). This means that all precursors leaving the core have no chance to re-enter it. In Fig. 9, the results are compared with the analytic reactivity loss based on a one-dimensional model in the case of cosine precursor distribution, Eq. (6), and flat distribution (see Ref. [26] for details):

$$\Delta\rho = \sum_{i=1}^{6} \beta_i \left[\frac{\pi^2}{2H^2 \left(\dfrac{\lambda_i^2}{u^2} + \dfrac{\pi^2}{H^2} \right)} \left(1 + e^{-\frac{\lambda_i H}{u}} \right) \right] \qquad (6)$$

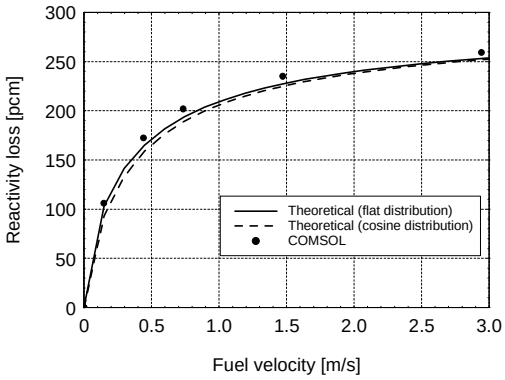

Figure 9. Comparison of COMSOL results with one-dimensional theoretical reactivity loss as a function of the fuel velocity.

As it can be noticed, the reactivity loss calculated by means of COMSOL is higher. This is straightforwardly explained by observing that the fuel transport causes the majority of the precursors to concentrate near the core exit (as depicted in Fig. 10, which shows the concentration of a precursor group for different values of velocity), where the probability for a precursor to decay outside the core becomes larger. Similar results were obtained by Kophazi et al. [26], where a modified version of MCNP was used for modelling the transport of DNPs. In summary, the COMSOL model permitted to take into account both the finite external loop and the space dependent effects.

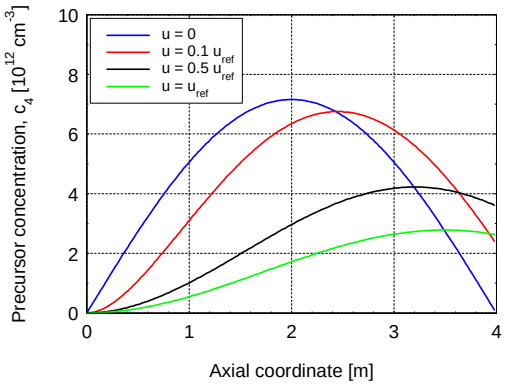

Figure 10. Precursor concentration of group 4 (c_4), achieved by means of COMSOL, as a function of the axial coordinate, for different values of fuel velocity.

5. Conclusions

A diffusive neutronic model of the average core channel of the MSBR was built in COMSOL, exploiting the deterministic code SCALE5.1 for the calculation of the group constants, with the purpose to assess the COMSOL capabilities for neutronic analyses.
To this end, a validation of the main neutronic quantities was performed in steady-state conditions by comparing the COMSOL results with those obtained by the stochastic code MCNP, which represents a reliable tool for neutronic analyses. In particular, criticality calculations were performed showing a good agreement of the flux profiles between COMSOL and MCNP models, based on diffusion and transport theory, respectively. The fact that the diffusion model is a mere approximation of the transport theory, necessarily affects the results of COMSOL. More precisely, the discrepancy is more evident at the interface between the fuel and graphite materials, where the diffusive flux gradients result lower than the values based on transport theory. Anyway, the overall agreement can be considered acceptable from an engineering point of view.

Moreover, COMSOL permitted to study the fuel velocity influence on the neutron flux and system reactivity. The flux profiles show no variations with the fuel velocity, proving that the assumption of static fuel for neutron distribution calculation represents an acceptable approximation. On the contrary, the system reactivity strongly depends on velocity: the calculated reactivity curve was compared with the theoretical one showing a significant difference due to the spatial distribution of DNPs accounted for in the diffusive model.

All things considered, COMSOL revealed itself as a useful tool, able to treat the neutronics of a typical MSBR core channel oriented to the description of its dynamic behaviour. Besides, COMSOL allowed to study the effects related to the fuel velocity, which represent a delicate aspect in the neutronic design and control of such systems.

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7. Appendix

The following nomenclature and units are used in the paper:

c_i concentration of the i^{th} precursor group [cm^{-3}]
D neutron diffusion coefficient [cm]
H core height [cm]
k_{eff} effective neutron multiplication factor
n neutrons
pcm per cent mille
R_F radius of the analysed core channel [cm]
u fuel velocity [$cm \cdot s^{-1}$]
u_{ref} reference fuel velocity [$cm \cdot s^{-1}$]

Greek symbols:

β total delayed-neutron fraction [-]
β_i delayed-neutron fraction of the i^{th} precursor group [-]
$\Delta\rho$ reactivity loss [pcm]
λ_i decay constant of the i^{th} precursor group [s^{-1}]
ν average number of neutrons per fission
Σ_a absorption cross section [cm^{-1}]
Σ_C capture cross section [cm^{-1}]
Σ_f fission cross section [cm^{-1}]
Σ_{TOT} total cross section [cm^{-1}]
$\Sigma_{1\to2}$ downscattering cross section [cm^{-1}]
$\Sigma_{2\to1}$ upscattering cross section [cm^{-1}]
τ_C circulation time in the core [s], { = H/u }
τ_{EL} circulation time in the external primary loop [s], { = $(u_{ref}/u)\ \tau^*_{EL}$ }
τ^*_{EL} circulation time at reference fuel velocity [s]
ϕ neutron flux [$n \cdot cm^{-2} \cdot s^{-1}$]

Subscripts:

F fuel salt
G graphite
1 fast neutron
2 thermal neutron

Table 4: Group constants calculated by means of SCALE5.1 at 900 K

Physical quantity	Value	Unit
$\nu_1\Sigma_{f1}$	$6.00 \cdot 10^{-3}$	cm^{-1}
$\nu_2\Sigma_{f2}$	$4.43 \cdot 10^{-2}$	cm^{-1}
$\Sigma_{a1,F}$	$9.36 \cdot 10^{-3}$	cm^{-1}
$\Sigma_{a2,F}$	$3.49 \cdot 10^{-2}$	cm^{-1}
$\Sigma_{a1,G}$	$1.32 \cdot 10^{-5}$	cm^{-1}
$\Sigma_{a2,G}$	$1.49 \cdot 10^{-4}$	cm^{-1}
$\Sigma_{1\to2,F}$	$1.62 \cdot 10^{-3}$	cm^{-1}
$\Sigma_{1\to2,G}$	$4.07 \cdot 10^{-3}$	cm^{-1}
$\Sigma_{2\to1,F}$	$3.68 \cdot 10^{-4}$	cm^{-1}
$\Sigma_{2\to1,G}$	$5.66 \cdot 10^{-4}$	cm^{-1}
D_{1F}	1.29	cm
D_{2F}	1.15	cm
D_{1G}	0.98	cm
D_{2G}	0.82	cm
λ_1	$1.258 \cdot 10^{-2}$	s^{-1}
λ_2	$3.364 \cdot 10^{-2}$	s^{-1}
λ_3	$1.367 \cdot 10^{-1}$	s^{-1}
λ_4	$3.227 \cdot 10^{-1}$	s^{-1}
λ_5	1.140	s^{-1}
λ_6	2.600	s^{-1}
β_1	$2.261 \cdot 10^{-4}$	-
β_2	$8.142 \cdot 10^{-4}$	-
β_3	$7.077 \cdot 10^{-4}$	-
β_4	$9.029 \cdot 10^{-4}$	-
β_5	$2.002 \cdot 10^{-4}$	-
β_6	$1.060 \cdot 10^{-4}$	-