

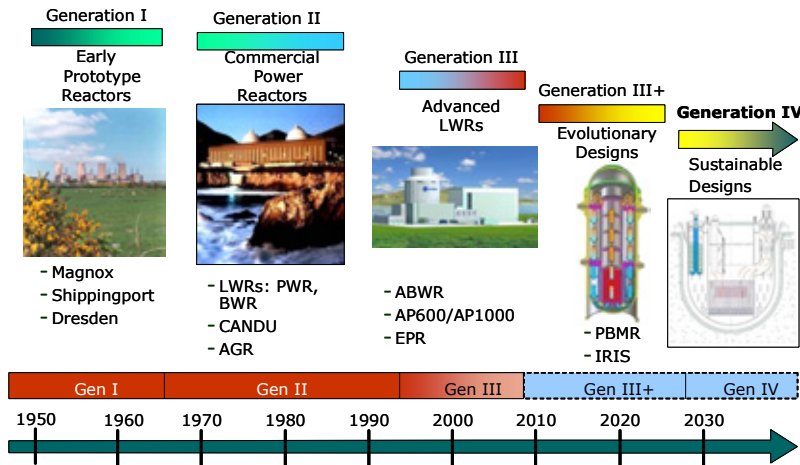


A Preliminary Approach to the Neutronics of the Molten Salt Reactor by means of COMSOL Multiphysics

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Generation IV Nuclear Energy Systems The technology roadmap

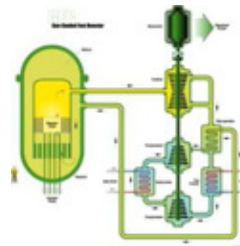


Goals for Gen-IV Nuclear Systems:

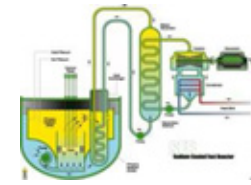
- Sustainability
- Safety and Reliability
- Proliferation Resistance and Physical Protection
- Economics

Reactor Types

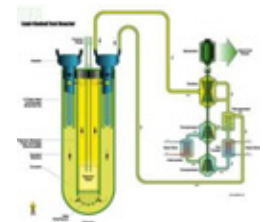
Gas Cooled Fast Reactor



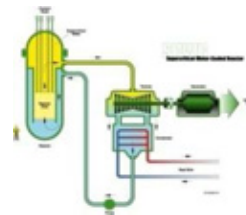
Sodium Cooled Fast Reactor



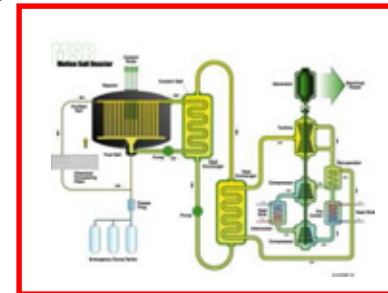
Lead Cooled Fast Reactor



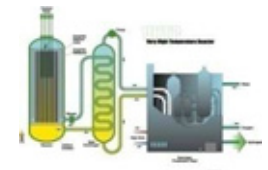
Supercritical Water Cooled Reactor



Molten Salt Reactor



Very-High Temperature Reactor



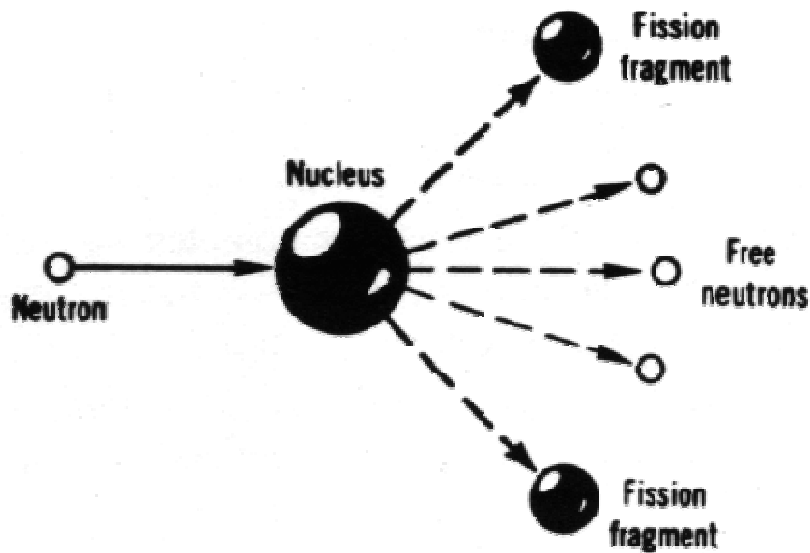
- To build a time-independent neutronic model of the representative core channel of a MSR based on two energy group diffusion theory with six group of delayed neutron precursors.

- Why COMSOL Multiphysics® ?

Given the unique feature of the molten salt, which simultaneously plays the role of fuel and coolant, the primary system presents a strong coupling between neutronics and thermo-hydraulics. COMSOL represents a powerful tool for the simulation of such multi-physics systems.

- Full validation of the model by means of the neutronic code **MCNP** (*Briesmeister, LA-13709-M*).

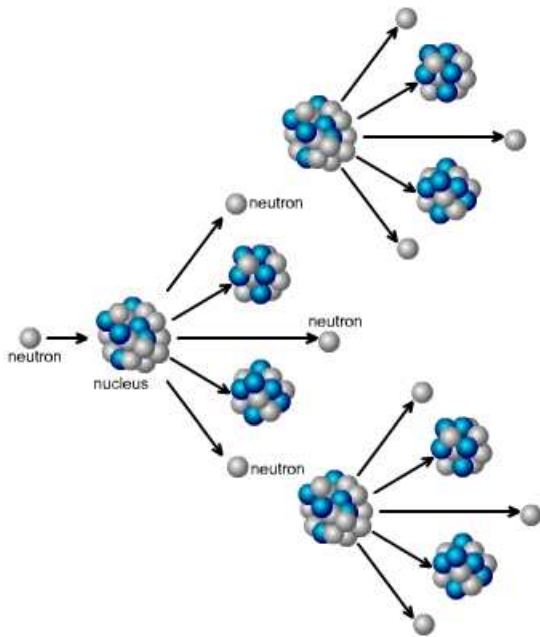
Fission reaction



Reaction Product	Energy (%)	Range	Time Delay
Kin. En. Fission Fragments	80	< 0.01 cm	instantaneous
Fast Neutrons	3	10-100 cm	Instantaneous
Fission Gamma Ray	4	100 cm	instantaneous
Fission Product decay	4	-	delayed
Neutrinos	5		delayed
Nonfission reactions due to neutron absorption	4	100 cm	delayed

- Fission reactions produce intermediate mass fragments, which are unstable and can decay by β emission. The daughter nucleus can decay via neutron emission (delayed neutrons). These fragments are the so-called “neutron precursors”.
- The neutrons emitted (prompt or delayed) can start a new fission reaction inducing a chain reaction.

Fission chain reaction



Not all the neutrons contribute the chain reaction because of parasitic capture and streaming out of the multiplying region, which can occur before a new fission reaction.

We can define the multiplication factor as follows:

$$k = \frac{P(t)}{L(t)}$$

$P(t)$ = rate of neutron production in reactor

$L(t)$ = rate of neutron loss in reactor (absorption plus leakage)

$$k \rightarrow \begin{cases} > 1 \Rightarrow \text{Reactor is supercritical and power increases} \\ = 1 \Rightarrow \text{Reactor is critical and power keeps constant} \\ < 1 \Rightarrow \text{Reactor is subcritical and power decreases} \end{cases}$$

Commonly the reactivity $\rho=(k-1)/k$, which measures the deviation of the system from critical configuration, is used.

The Single-Fluid Molten Salt Breeder Reactor (1)

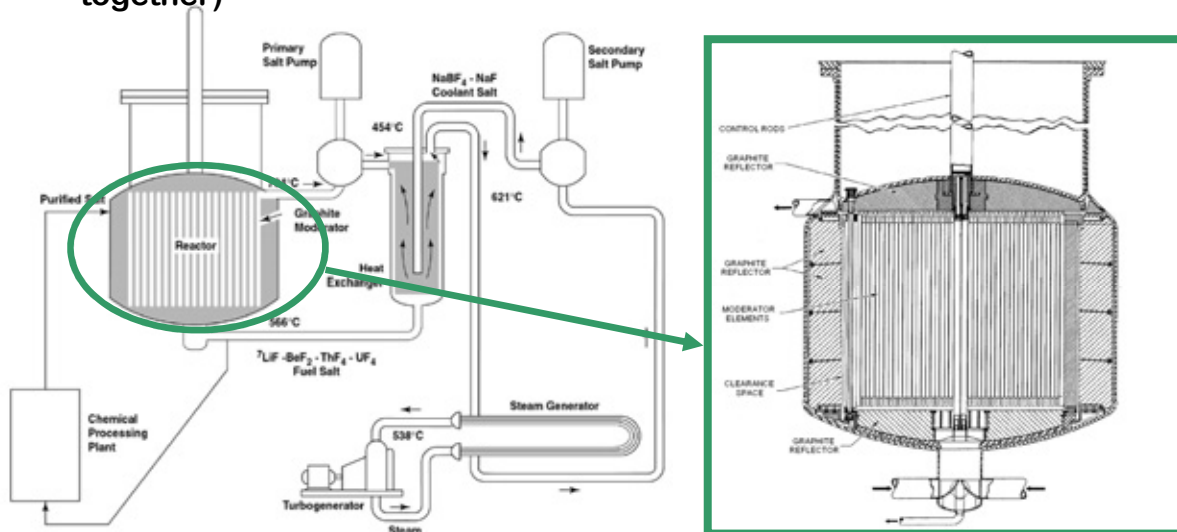
The Molten Salt Breeder Reactor concept, proposed by ORNL (*Robertson, ORNL-4541*) is a thermal reactor moderated by graphite and cooled by the liquid fuel.

Main Features

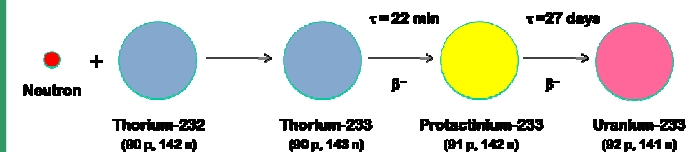
- 1000 MW of electric power
- Thermal neutron spectrum and Thorium fuel cycle
- The core is formed of square graphite blocks, each one with a central molten salt channel
- Fuel composition: ${}^7\text{LiF}$ (71.7 mol%), BeF_2 (16 mol%), ThF_4 (12 mol%) and ${}^{233}\text{UF}_4$ (0.3 mol%). Single primary fluid (fissile and fertile mixed together)

Design Parameters

Reactor power [MW _e]	2250
Average core power density [kW/l]	22.2
Fuel salt flow rate [kg/h]	$4.3 \cdot 10^7$
Core height [m]	3.96
Fuel salt velocity [m/s]	0.61-2.44
Inlet core temperature [°C]	566
Outlet core temperature [°C]	704

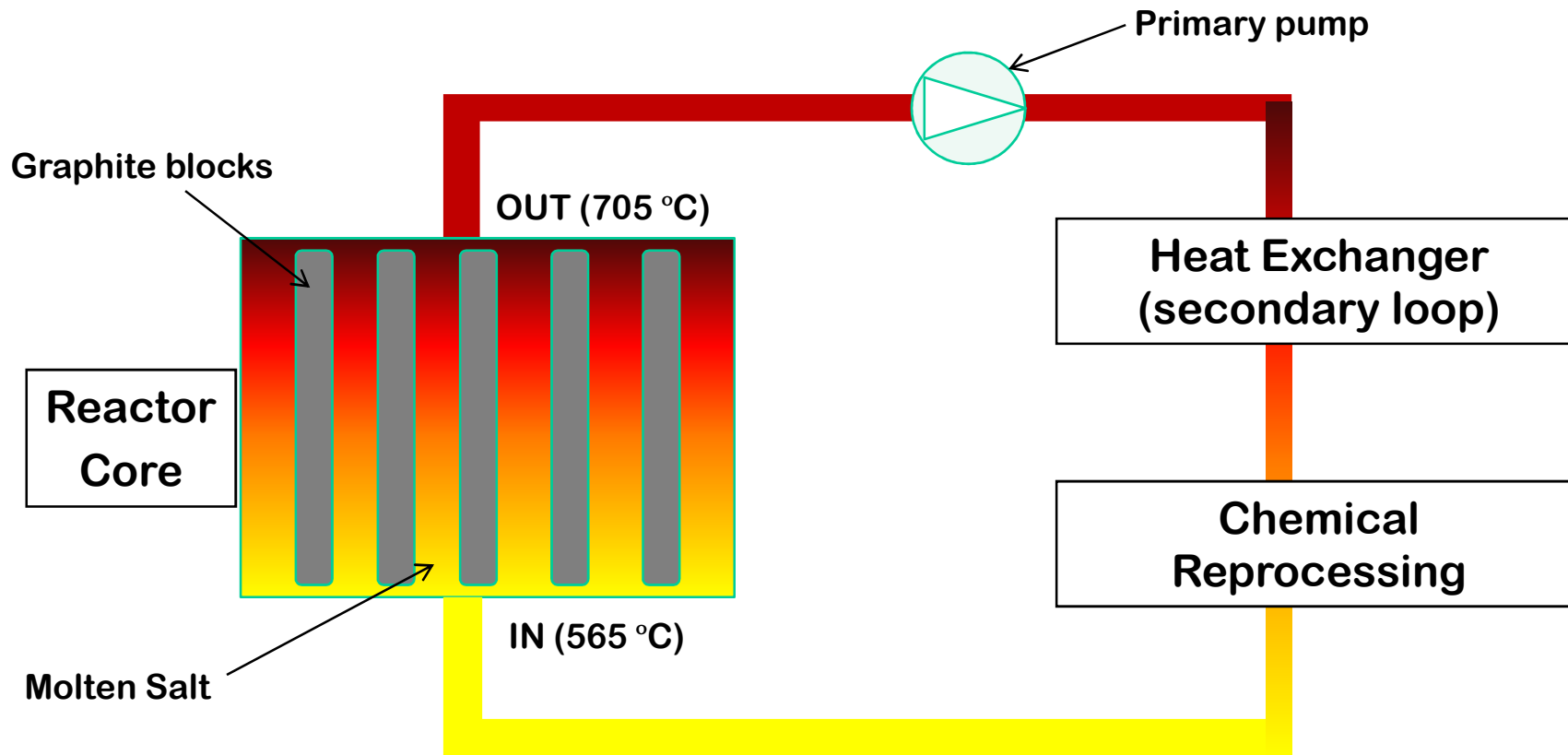


Uranium – Thorium Cycle (breeding)



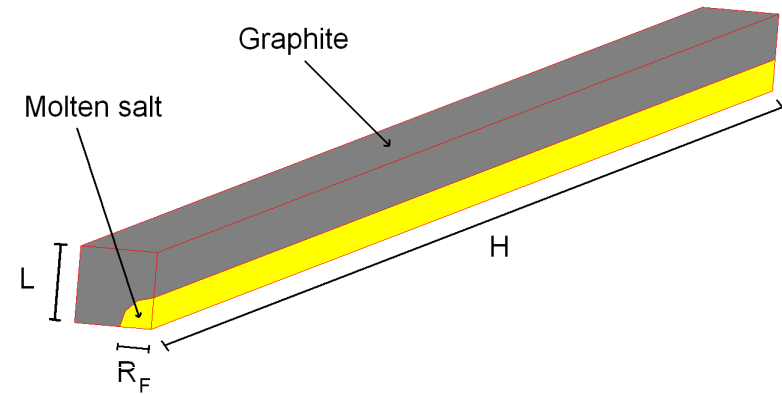
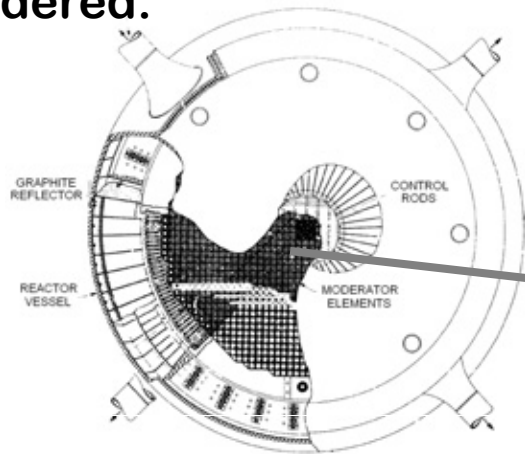
The Single-Fluid Molten Salt Breeder Reactor (2): how it works

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- The liquid fuel circulates through the core. When the fuel passes through the graphite blocks, neutrons are slowed down, fissions occur and the fuel heats up.
- When the fuel leaves the core, chain reaction ends. Neutron precursors exit the core too.
- Chemical Reprocessing for ^{233}Pa and bred ^{233}U removal.

A 3D model of $\frac{1}{4}$ of the representative channel of MSBR inner zone is considered.



Material

Constituent	Atomic density [atom·b ⁻¹ ·cm ⁻¹]
²³² Th	3.75·10 ⁻³
²³³ Pa	3.88·10 ⁻⁷
²³³ U	6.64·10 ⁻⁵
²³⁴ U	2.31·10 ⁻⁵
²³⁵ U	6.01·10 ⁻⁶
²³⁶ U	6.21·10 ⁻⁶
²³⁷ Np	8.59·10 ⁻⁷
²³⁸ Pu	6.10·10 ⁻⁶
²³⁹ Pu	1.29·10 ⁻⁷
²⁴⁰ Pu	6.83·10 ⁻⁸
²⁴¹ Pu	6.21·10 ⁻⁸
²⁴² Pu	1.23·10 ⁻⁷
⁶ Li	1.95·10 ⁻⁷
⁷ Li	2.24·10 ⁻²
⁹ Be	5.00·10 ⁻³
¹⁹ F	4.77·10 ⁻²
Graphite	9.51·10 ⁻²

Reference Data

L [cm]	5.08
H [m]	3.96
R _F [cm]	2.08
v _{in} [m·s ⁻¹]	1.47
T _{ref} [K]	900

Time-independent two-group diffusion equations *(Di Marcello, 2009)*

$$D_1 \nabla^2 \phi_1 - (\Sigma_{a1} + \Sigma_{1 \rightarrow 2}) \phi_1 + \Sigma_{2 \rightarrow 1} \phi_2 + \frac{(1-\beta)}{k_{\text{eff}}} (v_1 \Sigma_{f1} \phi_1 + v_2 \Sigma_{f2} \phi_2) + \sum_{i=1}^6 \lambda_i c_i = 0$$

$$D_2 \nabla^2 \phi_2 - \Sigma_{a2} \phi_2 + \Sigma_{1 \rightarrow 2} \phi_1 - \Sigma_{2 \rightarrow 1} \phi_2 = 0$$

$$\mathbf{u} \cdot \nabla c_i = \frac{\beta_i}{k_{\text{eff}}} (v_1 \Sigma_{f1} \phi_1 + v_2 \Sigma_{f2} \phi_2) - \lambda_i c_i = 0$$

$$\beta = \sum_{i=1}^6 \beta_i \quad c_i(z=0) = c_i(z=H) e^{-\lambda_i \tau_{\text{EL}}}$$

ϕ_1 is the fast neutron flux, $E_n \geq 1 \text{ eV}$

ϕ_2 is the thermal neutron flux, $E_n < 1 \text{ eV}$

c_i is the i -th precursor group concentration

τ_{EL} re-entering time of the fuel in the core

$D_i, \Sigma_{fi}, \Sigma_{ai}, \Sigma_{i \rightarrow j}$ are the group constants

\mathbf{u} is the fuel velocity (assumed constant)

β_i, λ_i are respectively the fraction and decay constant of the i -th precursor group

The system above represents an eigenvalues problem. To solve it one must find the eigenfunctions $(\phi_1, \phi_2, c_i)_\mu$ and the eigenvalues $k_{\text{eff}, \mu}$ which satisfies the system. The first eigenvalue corresponds to the so-called effective multiplication factor.

The model was implemented using the *Convection and Diffusion* application mode of **COMSOL** using eigenvalue solver. The group constants were calculated by means of the transport code **NEWT** of **SCALE5.1** package using ENDF/B-VI.7 nuclear library (*DeHart, ORNL/TM-2005/39*).

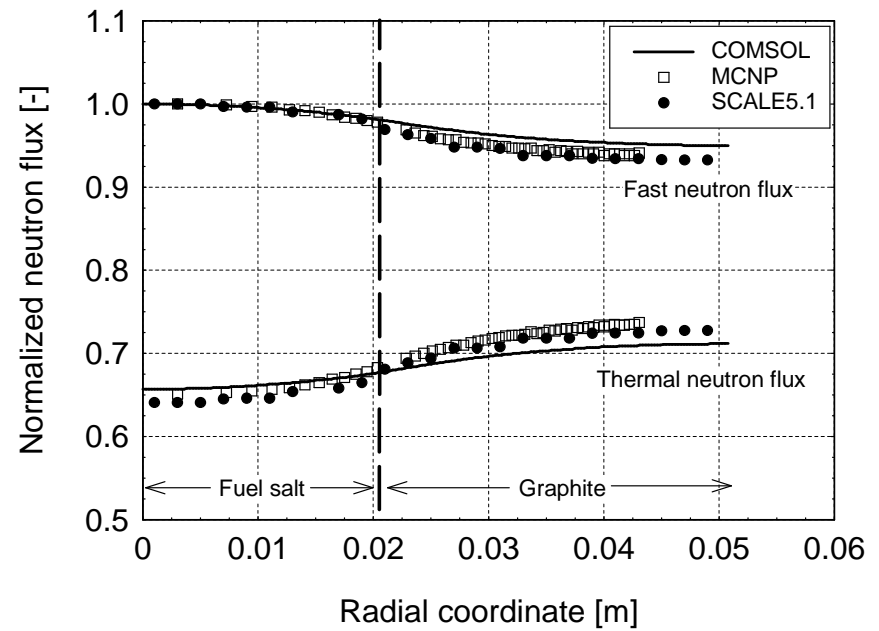
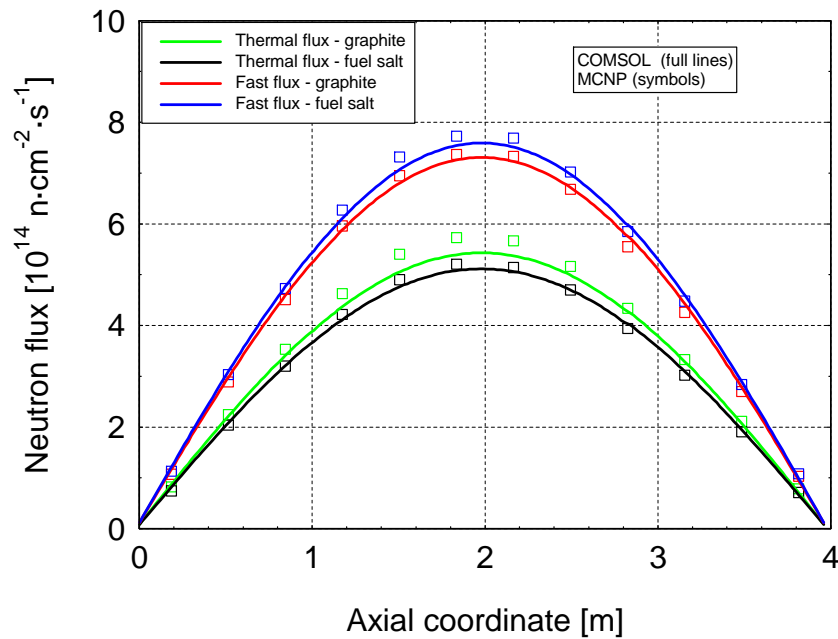
Moreover, a **MCNP** model using **JEFF31** library was used for the validation.

Group	$\nu\Sigma_f$ [cm ⁻¹]		Σ_C [cm ⁻¹]		Σ_{TOT} [cm ⁻¹]	
	Fast	Thermal	Fast	Thermal	Fast	Thermal
Fuel salt						
MCNP	6.22·10 ⁻³	4.23·10 ⁻²	6.86·10 ⁻³	1.62·10 ⁻²	3.10·10 ⁻¹	3.14·10 ⁻¹
SCALE5.1	6.00·10 ⁻³	4.43·10 ⁻²	6.96·10 ⁻³	1.71·10 ⁻²	3.17·10 ⁻¹	3.17·10 ⁻¹
Diff ^a [%]	-3.5%	4.7%	1.5%	5.6%	2.3%	1.0%
Graphite						
MCNP	-	-	1.18·10 ⁻⁵	1.37·10 ⁻⁴	3.95·10 ⁻¹	4.51·10 ⁻¹
SCALE5.1	-	-	1.32·10 ⁻⁵	1.49·10 ⁻⁴	4.07·10 ⁻¹	4.61·10 ⁻¹
Diff ^a [%]	-	-	12%	8.8%	3.0%	2.2%

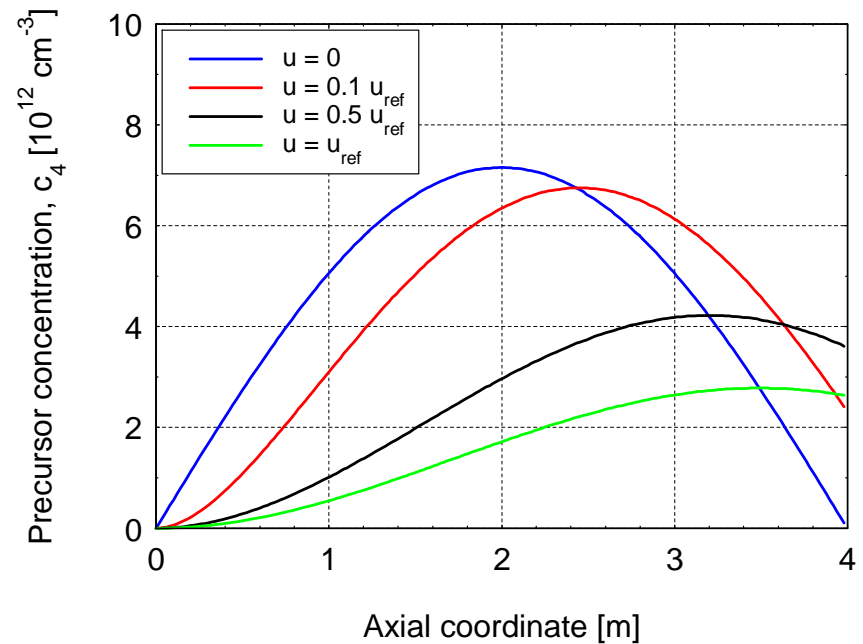
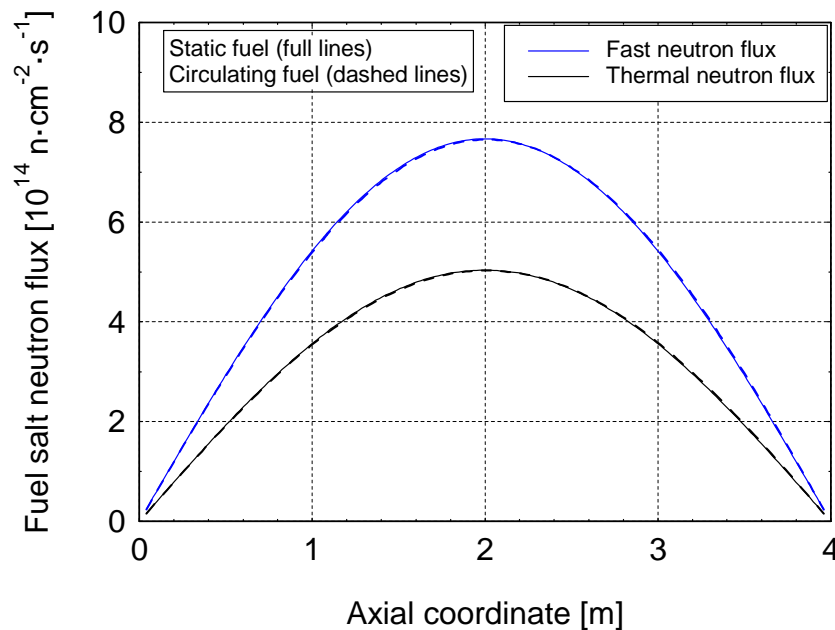
Multiplication Factor (k_{eff})

Code	k_{eff}
COMSOL	1.04216
MCNP	1.04745 ± 0.00079

Vertical and Radial Flux Profiles



Due to the flowing of the fuel through the primary loop, a certain amount of neutron precursors, depending on fuel velocity, can decay outside the core reducing the system reactivity differently from a solid fuel reactor.



The fuel velocity strongly affects the precursor concentration, whereas the effect is negligible on neutrons.

Comparison of COMSOL model with theoretical models. Two cases considered:

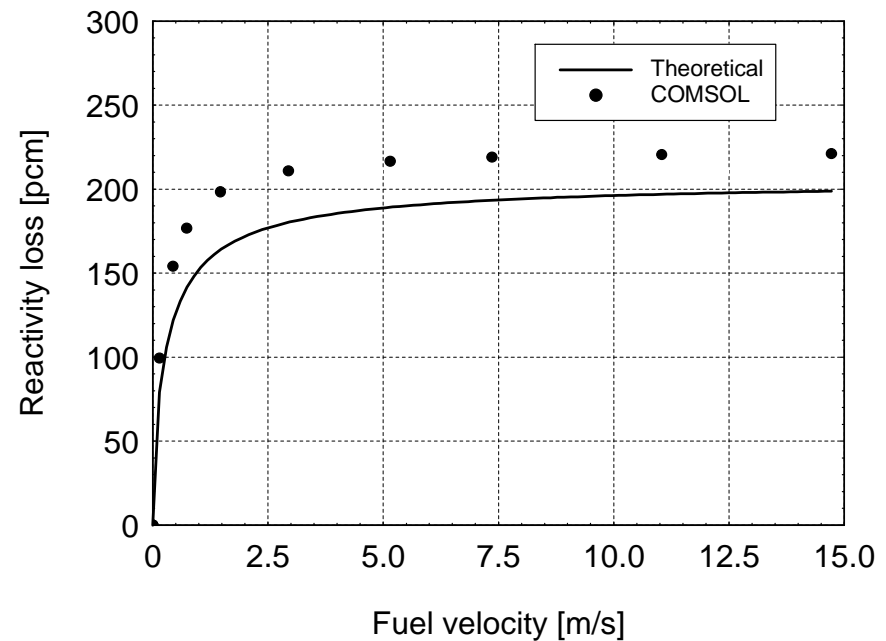
1. Closed primary loop (re-circulating fuel)

2. Infinite loop $\tau_{EL} \rightarrow \infty$

First Case

Zero-dimensional/theoretical reactivity loss is given by:

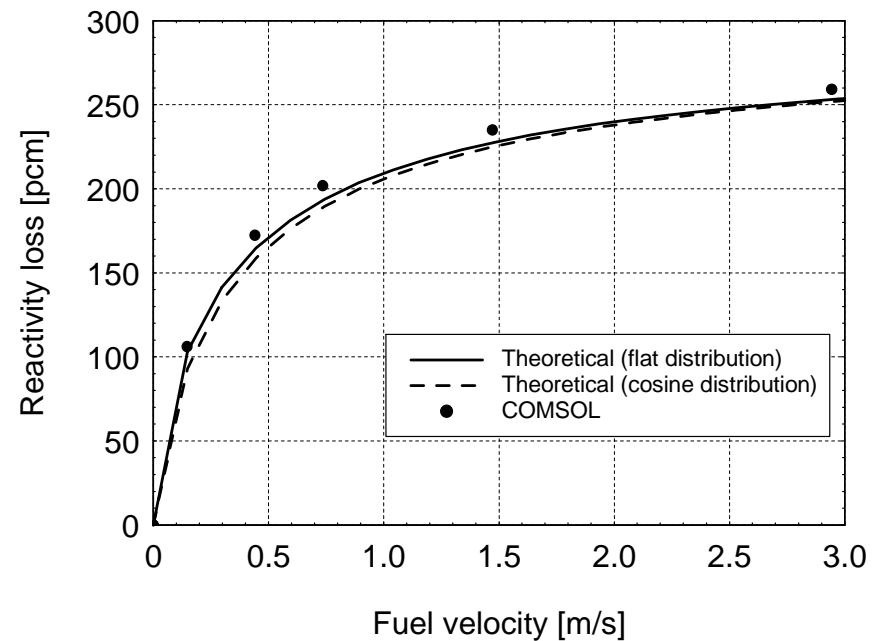
$$\Delta\rho = \beta - \sum_{i=1}^6 \frac{\beta_i \lambda_i}{\lambda_i + \frac{1 - e^{-\lambda_i \tau_{EL}}}{\tau_C}}$$



Second Case

One-dimensional theoretical model considering a flat (Kopphazi et al., 2003) and spatial cosine distribution of precursors. The reactivity loss for cosine distribution is given by:

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



A 3-D time-independent neutronic model of the representative MSBR channel was built in COMSOL.

The neutronic validation framework has shown that numerical results obtained by means of COMSOL and SCALE5.1 in terms of flux profiles reasonably agree with the MCNP results.

The encountered discrepancies can be considered acceptable from an engineering point of view.

The time-independent analysis permitted to evaluate the effect of fuel velocity on flux profiles, precursor concentration and system reactivity of MSBR channel.

All things considered, COMSOL revealed itself as a useful tool, able to treat the neutronics of a typical MSBR core channel, in prospect of analysing its dynamic behaviour.

The tested methodology for neutronic analysis with COMSOL supported by SCALE5.1 group constants calculation proved itself to be reasonable from an engineering point view. This confirmation will permit to extend the analysis to a more wide level which means:

- Refinements in the neutronic modelling of both the molten salt and the graphite, as well as of their "nuclear" interaction (temperature dependent cross section).
- Transient analyses oriented to the safety and the control strategy of the reactor, including neutronic thermo-hydrodynamics coupling in COMSOL.
- Adoption of more complex geometries.

- **Briesmeister, LA-13709-M**
J.F. Briesmeister, MCNP - A General Monte Carlo N-Particle Transport Code, Version 4C, LA-13709-M, Los Alamos National Laboratory (2000)
- **DeHart, ORNL/TM-2005/39**
M.D. DeHart, NEWT: A new transport algorithm for two-dimensional discrete ordinates analysis in non-orthogonal geometries, ORNL/TM-2005/39, Oak Ridge National Laboratory (2005)
- **Di Marcello, 2009**
V. Di Marcello, A Multi-Physics Approach to the Modelling of the Molten Salt Reactor, Proceedings of the 2nd International Youth Conference on Energetics 2009, Budapest, Hungary, June 5 (2009)
- **Kophazi et al., 2003**
J. Kophazi et al., MCNP based calculation of reactivity loss due to fuel circulation in molten salt reactors, Nippon Genshiryoku Kenkyujo JAERI Conference, 557-562 (2003)
- **Robertson, ORNL-4541**
R.C. Robertson, Conceptual design study of a single-fluid molten-salt breeder reactor, ORNL-4541 (1971)

Thank you for your kind attention