# Testing and Verification of Multiphysics Tools for Fast-Spectrum MSRs: The CNRS Benchmark

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## INTRODUCTION

Liquid fuel Molten Salt Reactors (MSRs) feature peculiar physical phenomena that are not present in solid fuel reactors. Some of these phenomena are not correctly resolved by legacy reactor physics tools, and require specific treatments. Recently, research activities within several collaborative projects related to MSRs design (e.g., see [1], [2]) lead to development of a number of different numerical tools for the coupled neutronics and thermal/hydraulics analysis of such systems. Unfortunately, especially in case of non-moderated, fast-spectrum MSRs, very few experimental data are available for an accurate process of verification and validation of the developed codes.

### Development of MSRs multiphysics tools and need for benchmarking and verification

The experience acquired within the EU EVOL Project highlighted the need to test and verify the multiphysics tools prepared for the Molten Salt Fast Reactor behavior simulation (e.g., [3], [4], [5], [6], [7]), in order to gain confidence in the phases of core design analysis and optimization. For this reason, code-to-code comparisons and benchmarking efforts were initiated among the different partners. In this phase, the peculiarities of circulating-fuel MSR governing phenomena, lead to the adoption of widely different solutions to the reactor physics modeling problems. In particular, multiphysics solvers were developed based on both Monte Carlo ([8]) and deterministic (e.g., [**?**], [**?**]) transport solvers. Moreover, different choices were adopted for what concerns the spatial discretization of the governing PDEs, focusing on both finite-volume and finite-element solvers. What is more, the challenging multiphysics coupling and time-integration issues were dealt with adopting solution that ranged from the simple, non-iterative, firt-order explicit coupling, to high-order, fully coupled implicit approaches.

Unfortunately, while the variety of the developed tools shed light on several circulating-fuel reactor physics issues, the differences arisen in the early phases of code-to-code comparisons were hardly explained and ascribed to a single defined modeling issue.

## THE CNRS BENCHMARK

### Motivation and goals

To overcome this issue, the development of a purpose-made benchmark was initiated at LPSC/CNRS/Grenoble. The main motivation behind this effort was not to "certify" that two codes are capable of giving the same answer to a given static or transient modeling problem. On the contrary, the main goal of the presented benchmark is to provide clear indications on the sources of the differences in the results of different multiphysics tools. Ideally, the CNRS benchmark is conceived in such a scalable way that, if followed from the first step on, both physical and numerical phenomena are introduce one at a time, and the difference between codes can be easily related to specific modeling issues.

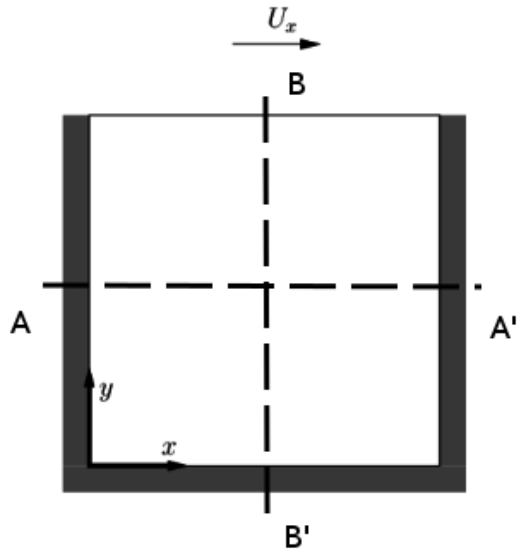


Fig. 1. 2D domain of the CNRS benchmark.

Moreover, since the available multiphysics tools for fast-spectrum MSR modeling present different degrees of complexity in terms of turbulence treatment (if any turbulence treatment is available at all!), geometry representation (2D or 3D), meshing capabilities, and coupling schemes, the CNRS benchmark is designed in order to allow the participation of virtually any code at the first phases and steps. At the same time, it was decided that all the "single-physics" phenomena not representing a peculiarity of liquid fuel reactors could and should be tested *before* dealing with a multiphysics benchmark. In this sense, turbulence treatment was removed from the benchmark and it was decided that the accuracy of the neutronics transport solution was not to be deeply investigated within this benchmark.[1]

The benchmark is divided in three phases: Phase 0 (single physics and one-way coupling verification), Phase 1 (steady-state benchmark), and Phase 2 (transient benchmark). The three phases are presented in the following sections. Here below, the geometry and material specifications of the CNRS benchmark are presented.

### Specifications

The CNRS benchmark involves a critical $2m \times 2m$ 2D square cavity of salt flowing under natural and forced conditions. Fig. 1 shows the considered domain and the $AA'$ and $BB'$ lines adopted to compare point-wise scores in the different steps.

The salt composition (reported in Table I) and geometry dimensions were selected to match the MSFR spectral indexes and dominance ratio, to provide a representative simplified case study.

[1] It is worth recalling that several high quality benchmark have been published on both subjects (e.g., see [**?**], [**?**]).

TABLE I. CNRS benchmark fuel isotopic composition.

| At. % | 2.11488 | 26.0836 | 14.0992 | 56.3969 | 1.30545 |
|---|---|---|---|---|---|
| Isotope | $^{6}$Li | $^{7}$Li | $^{9}$Be | $^{19}$F | $^{235}$U |

In order to catch the impact of natural circulation, fuel salt thermal expansion feedback, and delayed neutron precursors drift in a simple way, the laminar, incompressible formulation of the Navier-Stokes equations are considered, along with Boussinesq approximation, and using the following properties:

| | |
|---|---|
| Density | 2.0 g cm$^{-3}$ |
| Kinematic viscosity | 0.025 m$^2$s$^{-1}$ |
| Volumetric heat capacity | 6.15 10$^6$ J K$^{-1}$ m$^{-3}$ |
| Prandtl Number | 3.075 10$^5$ |
| Schmidt Number | 2.0 10$^8$ |
| Thermal expansion coefficient | 2.0 10$^{-4}$ K$^{-1}$ |

Fig. 2. Material properties.

The choice of the viscosity, Prandtl and Schmidt numbers were carefully optimized in order to highlight important physical phenomena and reduce, at the same time, the impact of numerical issues whose evaluation was beyond the scope of the present benchmark. In particular, the laminar Schmidt number ($Sc$, see Eq. 1) represents a trade off between reducing precursors diffusivity in order to enhance the impact of fuel motion of the effective delayed neutron fraction, and the need to cover the impact of the specific numerical diffusivity of different convection schemes.

$$-\nabla\left(\mathbf{u}c_i\right)+\nabla\cdot\frac{\nu}{Sc}\nabla c_i-\lambda_i c_i+q_i'''=0 \qquad (1)$$

$\mathbf{u}$ is the fuel velocity field and $\nu$ is the salt viscosity, $c_i$ is the $i^{th}$ family precursor concentration, and $q_i'''$ is the volumetric source of precursors.

The neutron data library JEFF-3.1 is prescribed, when possible, also for the availability of 8 groups delayed neutron emission data and spectra. The task of generating and collapsing few-groups cross sections for deterministic codes is left to the user. Nonetheless, precomputed group constants (along with diffusion coefficients and/or scattering matrices) are available upon request.

## PHASE 0: SINGLE PHYSICS AND ONE-WAY COUPLING VERIFICATION

The Phase 0 of the benchmark is aimed at the verification of the single physics capabilities of the codes, as a preliminary verification of the codes. Some of the results obtained in these steps will be adopted in Phase 1 for the normalization of the "observables", and are also provided as external input.

### Step 0.1: Velocity field

Solution: Fluid flow ($\mathbf{u}$ and $p$), o neutronics solution.
Fixed input: Velocity at top boundary ($U_x = U_{\mathbf{ref}}$).

*Description*

In this step, the solution of the steady state, incompressible flow in the 2D geometry is studied. At the wall boundaries *zero* velocity is imposed. The velocity at the top boundary is imposed ($U_x = U_{\mathbf{ref}}$). The thermophysical properties of the fluid are assumed constant in the whole benchmark.

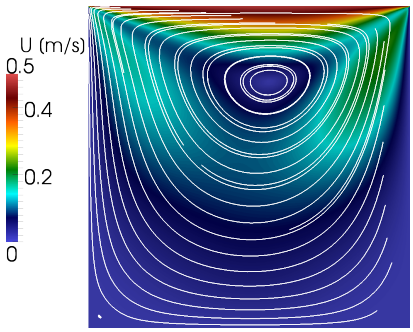


Fig. 3. Streamlines of the salt flow from the step 0.1.

*Function*

A correct solution of the fluid flow is mandatory to obtain a consistent multiphysics coupling. This step is aimed at the verification of the capability of the codes to obtain a correct velocity field.

Remarkable differences between the results obtained for this step are likely to affect further steps and should be investigated at this point.

"Observables":

- Velocity components along AA' ($u_x(x)$) and B'B ($u_y(y)$).
- Velocity in the 2D geometry ($u_x(\mathbf{r})$, $u_y(\mathbf{r})$).
- Flow streamlines, uniform seeds sampling in the B'B line.

### Step 0.2: Neutronics

Solution: Neutron flux ($\phi$) and delayed neutron precursors concentrations ($c_i$). No fluid flow ($\mathbf{u}(\mathbf{r}) = zero$)

Fixed input: Uniform reference temperature ($T(\mathbf{r}) = T_{\mathbf{ref}}$). Power normalization ($P = P_{\mathbf{ref}}$).

*Description*

In this step, the eigenvalue neutronic solution with static fuel is studied. At the walls, the vacuum boundary condition is applied. The neutron flux is normalized to have a total power $P = P_{\mathbf{ref}}$. The adoption of the same nuclear data library is suggested (e.g., JEFF-3.1), in order to avoid discrepancies coming from nuclear data. Group constants can be provided as input, to be adopted with deterministic codes. A correct evaluation of the effective delayed neutron fraction is of primary importance in the analysis of circulating-fuel reactors. The calculation of $\beta_{\text{eff}}$ is left as an option, here and in the following steps, for the codes capable of adjoint-weighted calculations.

*Function*

This step is aimed at the verification of the neutronics solution of the different codes in simple, static-fuel conditions. In order to proceed to further comparisons, fair agreement between the codes must be verified for the fission source distribution and the estimation of the effective multiplication factor. Minor differences in the $k_{\text{eff}}$ might arise from different approximations to the solution of the neutron transport equation. In this benchmark, the results related to the multiplication factor will be expressed as reactivity differences. For each code, the reactivity of this step is taken as reference ($\rho_{\mathbf{ref}}$).

A consistent calculation of $\beta_{\text{eff}}$ in circulating-fuel reactors in-

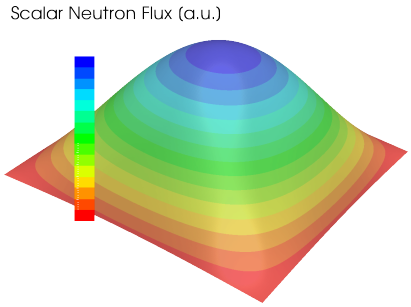


Fig. 4. Spatial distribution of the neutron flux from step 0.2.

volves the evaluation of both energy and spatial effects. The second (optional) function of this step is the verification of the correct importance weighting of the delayed neutrons. For the deterministic codes adopting one-group diffusion, a set of static effective delayed neutron fractions can be provided ($\beta_{\text{eff},i}$), accounting for the energy effects. In the following steps of the benchmark, the effective delayed neutron fraction will be expressed as fraction of the static (reference) value calculated in this step ($\beta_{\text{eff,static}}$).

"Observables":

- Fission rate density along AA' ($\int_E \phi\Sigma_f(x)$).
- Fission rate density in the 2D geometry ($\int_E \phi\Sigma_f(\mathbf{r})$).
- Effective multiplication factor / reactivity ($\rho_{\mathbf{ref}}$).
- Effective delayed neutron fraction ($\beta_{\text{eff,static}}$).

### Step 0.3: Temperature

Solution: Temperature ($T$) distribution with a given velocity field and heat source distribution.

Fixed input: Velocity field and heat source distribution from previous steps. Uniform volumetric heat removal coefficient $h$.

*Description*

In this step, the single physics analysis continues with the verification of the temperature distribution obtained by the different codes. Fixed velocity field and heat source distribution obtained in and are adopted. The heat is removed via an uniform artificial volumetric heat removal coefficient ($q'''(\mathbf{r}) = h(T(\mathbf{r}) - T_{\mathbf{ref}})$).

*Function*

In this step, the passive scalar transport capability of the codes is assessed separately and independently from the solution of the fluid flow and the neutron transport equation.

"Observables":

- Temperature distribution along AA' ($T(x)$) and B'B ($T(y)$).
- Temperature distribution in the 2D geometry ($T(\mathbf{r})$).

## PHASE 1: STEADY-STATE COUPLING

Phase 1 involves the steady-state multi-physics solution of the neutronics/thermal-hydraulic problem. The couplings between the physics are introduced one by one to facilitate the study of possible inconsistencies in the results.

For brevity, several steps of Phase 1 and Phase 2 are omitted from this manuscript.

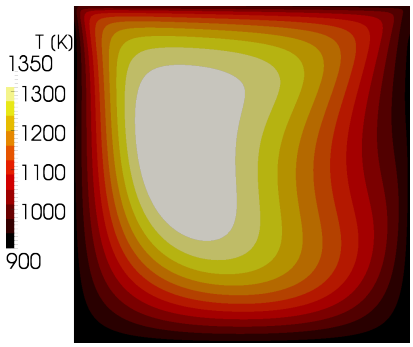


Fig. 5. Temperature distribution from step 0.3.

### Step 1.1: Circulating fuel (one-way coupling)

Solution: Neutron flux ($\phi$) and delayed neutron precursors concentrations ($c_i$)

Fixed input: Velocity field (from previous steps). Uniform reference temperature ($T(\mathbf{r}) = T_{\mathbf{ref}}$). Power normalization: $P = P_{\mathbf{ref}}$.

*Description*

This step involves the solution of the steady-state eigenvalue criticality problem, in presence of fuel motion, with a fixed velocity field and uniform fuel temperature.

*Function*

This step is aimed at the assessment of a correct evaluation of the effects of the fluid flow on neutronics. In particular, the consistency of reactivity loss due to fuel motion is to be verified. The evaluation of the $\beta_{\text{eff}}$ reduction is an optional function of this step. Results obtained in are adopted as references for $\rho$ and $\beta_{\text{eff}}$ normalization.

"Observables":

- Delayed neutron source along AA' ($\sum_i^i c_i\lambda_i(x)$) and B'B ($\sum_i^i c_i\lambda_i(y)$).
- Delayed neutron source in the 2D geometry ($\sum_i^i c_i\lambda_i(\mathbf{r})$).
- Reactivity change from ($\rho - \rho_{\mathbf{ref}}$)
- Normalized effective delayed neutron fraction ($\frac{\beta_{\text{eff}}}{\beta_{\text{eff,static}}}$)

### Step 1.5: Buoyancy

Solution: Neutron flux ($\phi$) and delayed neutron precursors concentrations ($c_i$). Temperature distribution ($T$). Flow field.

Fixed input: Total power ($P$). Zero velocity at the top wall ($U_x = zero$). Uniform volumetric heat removal coefficient $h$.

*Description*

In this step, the full neutronics/thermal-hydraulics coupling is analysed, without external source of momentum. The fuel flow is driven by the buoyancy effects due to the temperature gradients. The buoyancy is calculated assuming a constant volumetric expansion coefficient, and adopting the Boussinesq approximation (incompressible simulation).

*Function*

This step provides the easiest conditions for the analysis of the fully coupled multiphysics problem, without an external source of

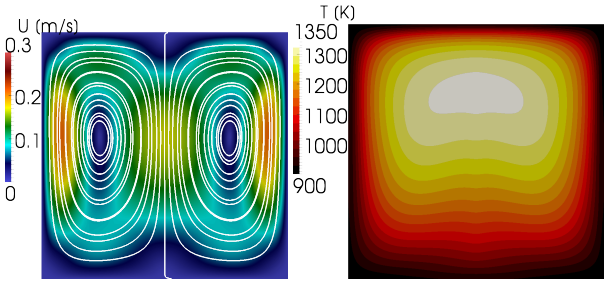


Fig. 6. Temperature flow distribution from step 1.5.

momentum. The main objective is to test the capability of the codes to predict the correct velocity field induced by the fission source. Most of the multiphysics coupling issued for steady-state eigenvalue problems are studied in and **??**. Possible discrepancies in the results obtained for the present step can be considered mainly related to the buoyancy effects. The buoyant flow moves some of the delayed neutron precursors from the center (higher neutron importance) to the top of geometry (lower neutron importance). The second (optional) function is to compare the evaluation of the reduction in $\beta_{\text{eff}}$ due to buoyancy effects.

"Observables":

- Velocity component along AA' ($u_x(x)$) and B'B ($u_y(y)$).
- Velocity in the 2D geometry ($u_x(\mathbf{r})$, $u_y(\mathbf{r})$).
- Flow streamlines, uniform seeds sampling in the AA' line.
- Temperature distribution along AA' ($T(x)$) and B'B ($T(y)$).
- Temperature distribution in the 2D geometry ($T(\mathbf{r})$).
- Delayed neutron source along AA' ($\sum^{i} c_i\lambda_i(x)$) and B'B ($\sum^{i} c_i\lambda_i(y)$).
- Delayed neutron source in the 2D geometry ($\sum^{i} c_i\lambda_i(\mathbf{r})$).
- Reactivity change from ($\rho - \rho_{\mathbf{ref}}$).
- Effective delayed neutron fraction ($\frac{\beta_{\text{eff}}}{\beta_{\text{eff,static}}}$)

## CONCLUSION

This manuscript presents a brief introduction of the CNRS benchmark developed for testing and comparisons of liquid fuel MSR multiphysics modeling tools. The focus of the present work is on the description of the motivation and the goals of the proposed benchmark. Only few steps are presented as example. Full details and specifications can be obtained from the authors.

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