

Fuel tap: a simplified breed and burn MSR

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ABSTRACT

Breed-and-burn Molten Salt Reactors are an interesting option of reactor design that allow high fuel utilization while operating on an open fuel cycle. Such reactors usually require specialized codes in order to model its fuel cycle and the flowing fuel in an unmoderated core. In this work, we propose a design and perform a preliminary analysis of a homogeneous chloride salt single-fluid design. The fuel cycle is analyzed using the EQL0D tool in order to model reactor start-up and transition into an equilibrium state. Core simulation is performed using ATARI, an OpenFOAM-based multiphysics code developed at PSI. Results show that the core size for such a reactor is quite big and that it can be easily started with high-assay LEU. In addition, the core has been designed to promote a quasi-1D flow, opening the possibility of modeling the core with legacy codes in the future.

KEYWORDS: Breed-and-burn, Chloride, Fuel cycle, Multiphysics

1. INTRODUCTION

Interest in MSRs has increased significantly this decade, with multiple parties proposing different reactors based on either the MSRE legacy design or new ones. Of the new designs some stand out for proposing a fast reactor core. Usually these fast cores are completely clear, with only the homogeneous fuel flowing freely inside. One of the potential advantages of fast MSRs is the possibility of operating on breed-and-burn mode (BNB), achieving high fuel utilization with an open cycle.

In light of this potential, we explore the conceptual design of a single fluid, molten chloride fast reactor operating on a breed-and-burn mode. Studies presenting the fuel-cycle of such reactors in a more detailed way are available [1]. The main driver for a single fluid design is the simplicity and resistance to proliferation that such design offers. Multi-fluid designs compromise on these in exchange for a different set of advantages. A study on the fuel-cycle of a multi-fluid design entitled "Simulation of breed and burn fuel cycle operation of a molten salt reactor in batch-wise refueling mode" by Raffuzi V. is present in this conference for more details on the subject.

One of the challenges of these fast open-cavity reactors is that legacy tools are not capable of modelling such free flow. Therefore, modelling of these reactors use frameworks that are primarily designed for computational fluid dynamics (CFD) in the context of nuclear reactor multiphysics. [2–5]

This approach presents challenges, because the computational requirements of CFD are much higher than legacy tools. If there is a need to model accurately the flow inside such reactors for safety demonstration, particularly if uncertainty quantification is needed, significant time and resources are likely to be required. Considering this, we will explore the possibility of shaping the flow using baffles hoping to attain a quasi-1D flow that could be modelled by legacy tools while still preserving the necessary neutron economy for BNB operation.

In the spirit of open and collaborative research, all input files and additional information related to this study, such as CAD geometry, are publicly available at GitHub *. Anyone is free and welcome to contribute to the development of the study or fork the repository and use it for their purposes.

2. METHODOLOGY AND SPECIFICATIONS

The Serpent Monte Carlo code [6] and the MATLAB-based EQL0D procedure [1, 7] were used to obtain critical dimensions and few-groups cross-sections for the equilibrium fuel composition of a Breed-and-Burn cycle chloride-fueled MSR.

EQL0D is a fuel cycle procedure dedicated to MSRs, simulating fuel evolution using a point-like representation of the fuel. Continuous removal of volatile and insoluble fission products and refueling operations are simulated using user-input removal rates.

Multiphysics modelling of the core is performed using ATARI, an open-source OpenFOAM-based [8] code developed at PSI whose presentation paper is under preparation. For the scope of this paper, fluid dynamics is modelled using the traditional Reynolds-averaged Navier-Stokes equations supplemented by the k-ε turbulence model and neutronics is modelled using neutron diffusion approximation with delayed neutron precursors convection.

2.1. Materials and Properties

Considering that this is only a conceptual study, accurate values for properties are not fundamental. The proposed fuel used is 60-40 mol % NaCl and UCl₃ with ²³⁵U enriched to 10.7% and 100% ³⁷Cl as a starting point [1, 9]. Table I shows the parameters used for the fluid, which are on the ballpark of molten salt values but not particular of any. Of these, the most important estimate was of density, since it would also impact neutron transport simulations with Serpent, the estimation of the critical core size and ultimately, the CAD geometry. The density value was taken as a molar % linear combination of the pure salts [10]. Density variation is modelled using a Boussinesq approximation considering the salt to have an expansion coefficient of $2 \times 10^{-4} \text{ K}^{-1}$ at 923 K.

*More information at <https://github.com/deOliveira-R/MCBR>

Table I: Fluid properties

Parameter	Value
Density	3640 kg m^{-3}
Specific heat capacity	$1500 \text{ J kg}^{-1} \text{ K}^{-1}$
Dynamic viscosity	0.025 Pas
Prandtl number	15

Structural materials in the core are given the properties of Hasteloy-N without further consideration at this stage. The core reflector used is PbO; a choice that will be justified in section 3.2.

2.2. Core Geometry and Meshing

Figure 1 shows the proposed geometry for the reactor core. It does not look much different than a typical reactor, having a cylindrical vessel of 4.8 m diameter as base with a 2:1 height-to-diameter ratio (HDR) after critical core size calculations with Serpent. As can be seen on the Serpent geometry, it also includes a 1 m thick reflector (shown in "PbO yellow") that was not included in the CAD geometry to limit the number of cells. This choice of aspect ratio was made to allow the addition of a heat exchanger above the middle level of the core, promoting natural circulation during postulated accident scenarios in a planned future work.

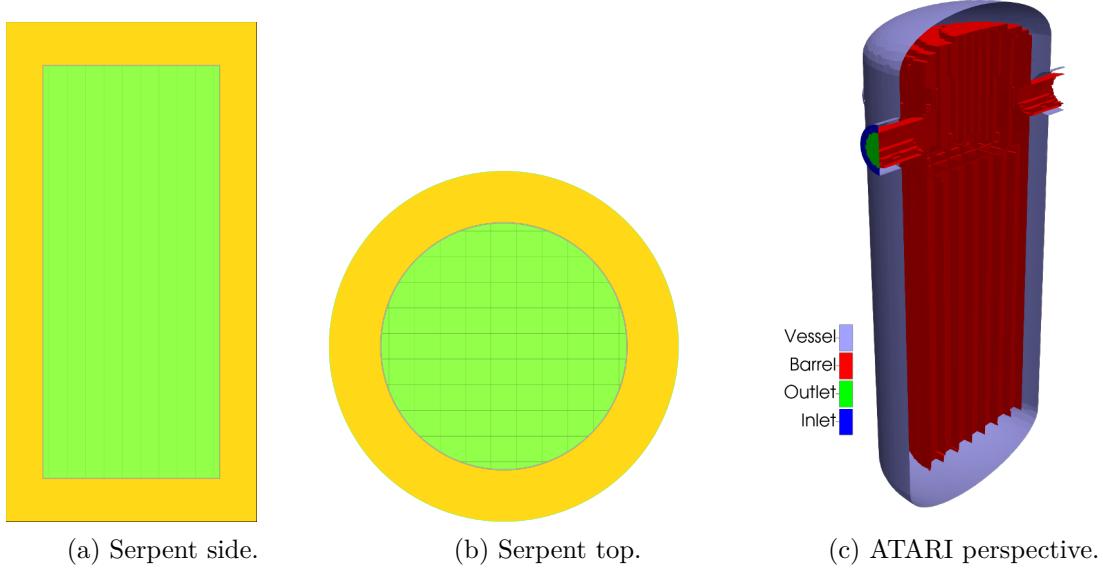


Figure 1: Core geometries with barrel and baffles.

The design borrows some old concepts and introduce new ones. The concentric pipe and core barrel are present in high temperature gas reactors, which should allow the temperature of external walls to be close to inlet temperature. The addition of flow baffles in a fast MSR,

instead of a clear core is, at least, atypical if not new.

In order to mesh the CAD geometry, the standard OpenFOAM mesher was used called "snappyHexMesh" (SHM).

2.3. Boundary Conditions

In Serpent, vacuum boundary conditions are applied after the reflector. In ATARI, vacuum boundary conditions are applied directly after the vessel walls due to Serpent not generating albedos for cylinders. In addition, an integral power of 3 GW is given for eigenvalue calculations as a starting point considering the reactor size.

The boundary conditions for fluid dynamics are presented on table II. Zero gradient boundary conditions means that the gradient normal to the surface is zero. The mass flow rate boundary condition uses the fluid density to calculate the appropriate fluid velocity normal to the inlet surface.

Table II: Fluid dynamics boundary conditions

Field	Inlets	Outlets	Walls
Pressure	zero gradient	1 bar	zero gradient
Velocity	mass flow rate 3200 kg s^{-1}	zero gradient	no slip
Energy	temperature 923 K	zero gradient	zero gradient
k and ϵ	zero gradient	zero gradient	standard wall functions

3. RESULTS AND DISCUSSION

3.1. Fuel Cycle Study

Simulation of the breed-and-burn cycle equilibrium was first performed using the EQL0D procedure. The starting point were results obtained previously in terms of burn-up, fuel salts, and reflector materials [9].

Table III: Candidate chloride fuel salts considered and their properties, adapted from [9].

Composition (mol%)	Density (kg m^{-3})	T_{melt} (K)	Discharge BU (%FIMA)	Critical radius (m)
NaCl–UCl ₃	68–32	3320	793	33.6
NaCl–UCl ₃	60–40	3640	863	33.8
NaCl–UCl ₃ –UCl ₄	70–15–15	3640	773	35
NaCl–UCl ₃ –ThCl ₄	50–25–25	3160	773	35.8

Providing adequate performance, the NaCl–UCl₃ mixture (60–40 mol %) with 100% enrichment in ³⁷Cl was selected as the most feasible based on critical radius (or inventory) and the lack of UCl₄, which has a low boiling point. A discharge burn-up of 33%FIMA was also selected because it leads to minimal critical dimensions at equilibrium.

3.2. Reflector and baffles

The possibility of using different reflectors materials was investigated using a 0.92 HDR (optimum according to diffusion theory) and assuming a 1 m thick reflector of a given material.

The critical radius of the core at equilibrium of the breed-and-burn cycle with fixed discharge burn-up was compared for several high-temperature candidate reflector materials. PbO was selected as a reflector material due to its acceptable performance and higher melting point than the molten salt.

Table IV: Reflectors considered at equilibrium

Reflector	Critical radius (m)	T_{melt} (K)
Lead (reference)	2.50	601
Lead monoxide	2.60	1161
Barium chloride	3.00	1235
Barium oxide	3.25	2196
No reflector	3.50	-

The impact of the baffles on the neutronics was evaluated, leading to a choice of square lattice of 1 mm thin baffles with 50 cm side.

Finally, the case using PbO reflector, baffles and 2:1 HDR was used to generate 8-group cross-sections and 6-group delayed neutron precursor data for core simulation.

3.3. Clear and Baffled Cores Comparison

In figure 2 we can see the effect that the insertion of baffles has on the flow. Using the eddy viscosity as a measure of turbulence, this design choice reduced the values of this parameter by at least an order of magnitude. Fluid flow has a quasi-1D behaviour as expected. Other fields do not show a significant difference, at least during steady state.

In the figure, it is possible to appreciate the impact of the mesh on the results. Due to the blocky rough mesh at the inlet, a region of extremely high velocity, turbulence and Courant number is present. Using SHM there are 2 known approaches to mesh the geometry and include the barrel and baffles as internal boundaries. One is to mesh the geometry without the internal boundaries and add them after meshing with the help of the "topoSet" and "createBaffles" utilities. This approach works, but results in the rather blocky barrel shown in figure 1c. Another approach would be to generate the mesh with internal boundaries directly. This approach does generate a mesh that is smooth and resolves the curvature of the barrel, however this mesh also results in a floating point exception during solution of the pressure equation. At the moment, only the first method has been successfully applied. Meshing in SHM is not straightforward, debugging even worse.

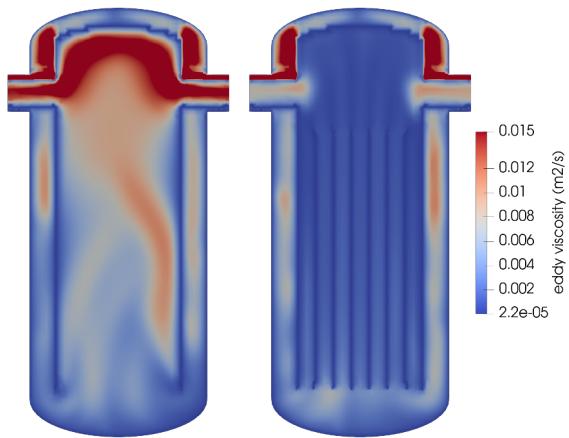


Figure 2: Eddy viscosity in clear (left) and baffled (right) cores.

3.4. Steady State Results

Figure 3 shows the converged flux (group 1) and volumetric power fields. It is immediately noticeable that they look the same, as they should since convection of decay power is not being modelled at the moment. ATARI calculated a k_{eff} of 0.97640 whereas Serpent a value of 0.97876 for the unreflected core (and 1.00391 ± 0.00039 for the reflected one). A difference of 236 pcm is considered acceptable and expected at this stage where the few-group energy structure has not been optimized.

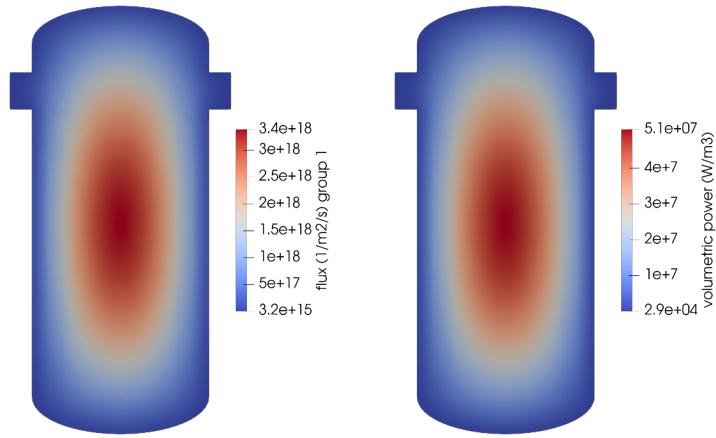


Figure 3: Flux in group 1 and volumetric power in the core.

Figure 4 shows the flow velocity in the core, which is rather slow at mostly below 1 m s^{-1} giving this reactor a significant leeway to increase mass flow rate and power. We can also see that the delayed neutron precursors are drifted from their place of origin and that the temperature field shows that the vessel walls stay close to inlet temperature. Mesh defects

again impacts the inlets, affecting the velocity field locally and consequentially the convection of delayed neutron precursors.

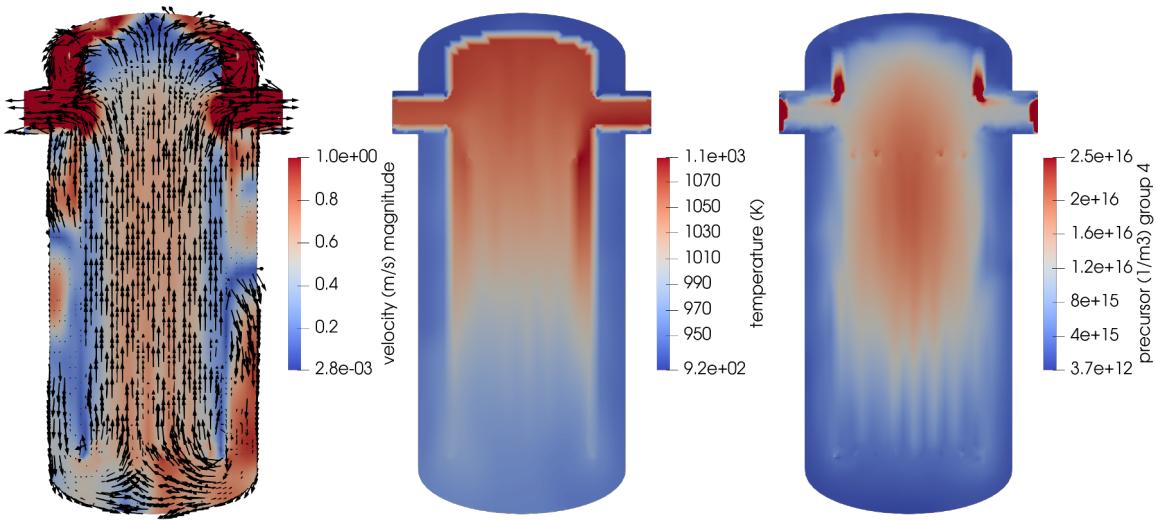


Figure 4: Velocity and velocity-dependent fields of temperature and delayed neutron precursor in group 4.

4. CONCLUSIONS

Neutronics calculations show that the integration of baffles and the improvement of core geometry for the purpose of improved natural circulation are possible in a Breed-and-Burn reactor, at the cost of a slightly higher inventory due to increased salt volume.

Fluid dynamics simulation confirms the expectation of a quasi-1D flow in a baffled configuration, opening the possibility to model this core using fast running legacy tools in the future. In case of concerns regarding channel blockage events, engineered passages can be designed to allow desirable cross-flow.

Multiphysics simulations demonstrate that the external wall temperature is close to inlet temperature as designed. The results also show the expected behaviour for the simulation including k_{eff} close to criticality, axially elongated flux and volumetric power fields, drift of delayed neutron precursors and the temperature rise in the core.

The simulations with ATARI still presents some issues. From a fluid dynamics aspect, the mesh show problems close to the inlets. This is seen as one of the biggest deficits of the present work and generating a smooth mesh with internal boundaries directly should be a focus of future developments. From a neutronics aspect, imposing vacuum boundary conditions at the walls is seen as the main issue and proper albedo coefficients must be generated. In order to circumvent Serpent limitations regarding albedos in a cylinder, we envision simplifying the problem to a 2D approximated one or finding the cylinder-equivalent square prism for the case. A criteria for equivalency however is not yet decided.

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