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ARTICLE

Preliminary Studies for a Molten-Salt Reactor with Fuel Elements

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In many molten-salt reactor designs, liquid fuel circulates through the core, heat exchanger, and pump. It may lead to an unstable reactivity level, influenced by fuel density variations due to irregularities in fuel flow. In this paper, we consider a design concept with multiple elements consisting of structures filled with liquid fuel salt and cooled by inert salt. This approach may help to avoid reactivity instabilities but may limit the power density and require salts with high solubility of actinides because of increased neutron absorption by the structures.

KEYWORDS: molten-salt reactor, Gen-IV, heat transfer, natural circulation, criticality

I. Introduction

Molten-salt reactor (MSR) concepts are now studied worldwide, for nuclear waste management and energy production. ENDURANCE[1)] and SAMOSAFER[2)] are current and recent MSR projects supported by EURATOM. Studies for SAMOSAFER show that the reactivity, in particular in MSRs with fast neutron spectrum, is influenced appreciably by fuel density variations due to irregularities in the fuel flow. The flow pattern in a large core is prone to small geometry modifications and temperature gradients in the salt can be locally large, leading to variations is local reactivity feedbacks.[3,4)] This may lead to instabilities in reactor power.[5)]

In this paper, we propose and investigate an MSR design with fuel-in-structure elements, referred to as MSR-ST. The considered currently elements are steel or Ni-alloy cylindrical, few-meter-high structures filled with liquid fuel up to their mid-height, with a gas plenum being located above the fuel. They are somewhat similar to fuel pins in reactors with solid fuel, but of larger diameter, so that we refer to the structure as can wall instead of clad in the following. Designs with elements of hexagonal, rectangular and other shapes in plane are considered currently as possible alternatives, we may study them later. The elements are immersed in a pool with inert salt, which flows upwards and cools them (**Fig. 1**). The inert salt flow is forced by pump(s) and circulates through the core, heat exchanger(s) and a downcomer with pump(s). A passive heat removal mode during normal operation is an option to study in the future.

A key feature of most MSR designs is the online fuel reprocessing, but we currently do not to consider it for MSR-ST. This may simplify the design and lower the construction cost. A possible drawback is a limited fuel cycle length, after which irradiated some elements are to be replaced by new ones, similar to reactors with solid fuel. An alternative is to introduce devices for discharging fuel from the elements and for filling them with fresh fuel.

MST-ST also offer other advantages as compared to conventional fast MSR designs. The reactivity is expected to be more stable during reactor operation. The fuel mass can be lower and the fuel flow is restricted by structures. A flow oscillation or irregularity in single element may lead to a minor variation of the core reactivity and therefore should not result in appreciable reactivity instabilities. Moreover, enclosing the fuel in the structures offers an additional safety barrier. An accident with a can wall rupture in one element would lead to fuel dispersion in the inert salt. Fissile content would be diluted in a large mass of the inert coolant, in and outside of the core region, and the reactivity of the core would go down.

In the paper, we consider relatively thick elements in plane, with the radius values from 2.5 to 10 cm, as we try to limit the structure volume fraction in the core and the related neutron absorption. The power density in the core is therefore may have to be reduced as compared to conventional MSR designs. In the following, we consider a MOSART reactor model - as studied in the past in an IAEA CRP[6)] for nuclear waste management - as the basis for the presented fluid-dynamics and neutronics studies. In the MOSART salt, the solubility of Plutonium and other transuranic isotopes (TRUs) at operating conditions is limited by a value of about 1 % Mol. In view of neutron absorption by structure, other salt types with higher TRU solubilities, may have to be considered in the future, after properties for new salts are introduced in the employed fluid-dynamics code, SIMMER-III.[7)]

In this paper, modelling uncertainties and ideas on their reduction are described first. Among these uncertainties, those related to natural circulation of fuel in structures are selected for the analysis, results of which are discussed. A model development for the SIMMER-III code is described. The results obtained with this and other codes are presented. The concept study is supported by a preliminary evaluation of the criticality and decay heat removal capacity.

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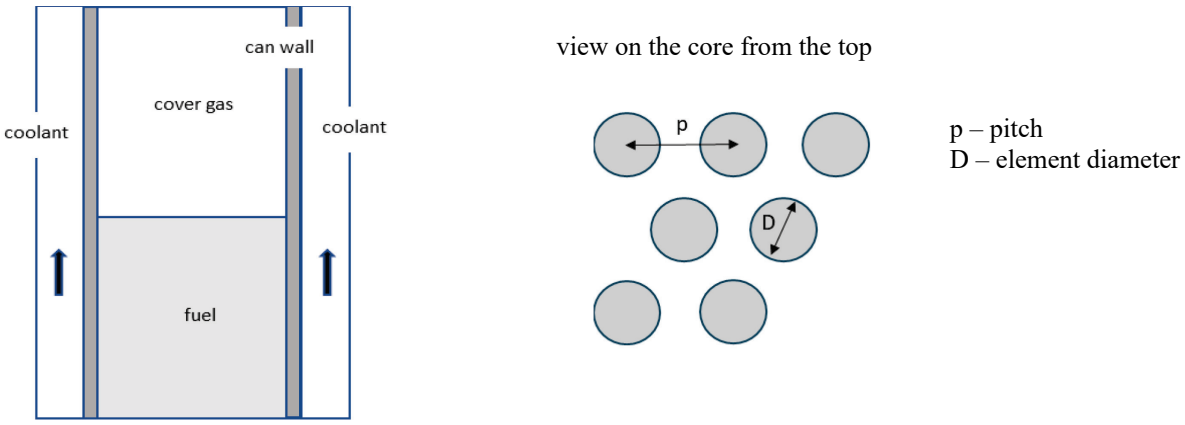

Fig. 1 Scheme of a single fuel salt element and 3D layout of the elements in the core

II. Methods

1. Fluid-dynamics Model

The SIMMER-III (Sn, implicit, multi-field, multi-component, Eulerian, recriticality) code is a tool for studies of hypothetical severe accidents in advanced nuclear reactors. It is a 2D fluid-dynamics code coupled with a structure module and, optionally, a time-dependent neutron transport code. The fluid-dynamics module, SIMMER uses a full formulation of the equation-of-state (EOS) model with coefficients of the equations fit for each material in three phases. In this paper, only the fluid-dynamics and structure modules were used. Neutronics calculations were done by another code.

In this paper, a SIMMER-III model is developed for the future analysis of the reactor with fuel elements and is not yet treated as a reference tool for core studies. In the analysis, for the fuel and inert salts, we employ equation-of-state (EOS) for the MOSART salt 14.85 LiF + 26.73 BeF_2 + 57.43 NaF + 0.99 PuF_3 (molar), developed for SIMMER earlier.[8)] For the inert salt, the density is the only property which is modified with respect to the fuel salt.

2. Modeling Simplifications and Uncertainties

The SIMMER-III model was prepared for a fuel element surrounded by inert salt in the R-Z geometry. The radial power profile in the fuel was assumed to be flat, the axial one was computed with a neutron transport model that is similar to that employed in SIMMER. Considering several SIMMER features and our modelling assumptions, we identify the following points being the largest sources of uncertainty:

- Originally, heat and mass transfer between fluids and structures in SIMMER is represented only by forced-convection correlations. For this study, a new heat transfer coefficient (HTC) had to be therefore implemented. It was the main objective of this analysis. The choice of the right HTC was not straightforward due to the lack of correlation applicable to this situation. The salt inside the cylinder has a Prandtl number in the mid-range (Pr=3-17), the Rayleigh number is very high (of order Ra~10^{13}-10^{18}). Cylinders are relatively high but with non-negligible width (aspect ratio AR=H/D between 10 and 40).

- There is no full EOS of any inert salt in SIMMER-III. The fluid used as a coolant is represented by the same set of thermophysical properties as the fuel salt with small modifications. Containing no heavy metals, the inert salt density should be smaller by a factor of ~2. Other parameters like heat capacity and viscosity are not adjusted yet. Assuming that the coolant mass flow rate is predefined, the coolant velocity forced by the pressure difference should be approximated by a correct order of magnitude.

- The heat exchanger detailed design does not exist. To study a post-accident situation, pressure losses in the heat exchanger were assumed to be approximately equal to the pressure losses along the fuel elements.

3. Heat Transfer Modelling Options

The SIMMER-III has its own models for heat transfer modelling in the laminar and turbulent conditions. Additionally, user-defined coefficients can be defined. By definition, a Nusselt number used for finding the heat transfer coefficient at every fluid-dynamics time step.

$$Nu = \frac{hD}{\lambda} \tag{1}$$

where: h - heat transfer coefficient [W·m^{-2}·K^{-1}], D – characteristic dimension [m], λ - thermal conductivity [W·m·K^{-1}].

The Nusselt number in SIMMER is defined by a usual correlation of this type for a forced convection:

$$Nu = a \cdot Re^b Pr^c \tag{2}$$

where Reynolds and Prandtl numbers:

$$Re = \frac{\rho v D}{\eta} \tag{3}$$

$$Pr = \frac{\eta c_p}{\lambda} \tag{4}$$

where: ρ – density [kg·m^{-3}], v – velocity [m·s^{-1}], η – viscosity [Pa·s], c_p – specific heat [J·kg^{-1}·K^{-1}], and coefficients a, b, c are defined for every combination of materials present in the SIMMER input. In this case, the heat transfer between the molten salt (fuel, material M=1) and the steel (structure material M=3) are defined. By default: $a = 0.023$, $b = 0.8$, $c = 0.3$.

In the natural convection conditions instead of the Prandtl number, this is usually the Rayleigh number present in the correlations, to take into account for the buoyancy and viscous

forces important to develop the natural circulation:

$$Ra_{\mathrm{i}} = GrPr = \frac{\rho g \beta \Delta T i^3}{\eta \alpha} \quad (5)$$

where: g – gravitational acceleration [m·s^{-2}], β – thermal expansion coefficient [K^{-1}], α – thermal diffusivity [m^2·s^{-1}], i – dimension [m].

Provided that we approximate the surface heat flux and heat generation as uniform, and the heat transfer through the horizontal surfaces is neglected, this equation can be written:

$$Ra_{\mathrm{R}} = \frac{\rho g \beta q''' \mathrm{R}^5}{\eta \alpha \lambda} \quad (6)$$

Correlations available in the literature for liquid metals very often concern low-Prandtl number fluids, like sodium[16] or solar salt in the heat pipes. The molten salt pools were investigated experimentally, usually for debris cooling, with heights comparable to diameters. Such a problem was proposed by Qian et al.[17] who numerically investigated an enclosure with molten salt of an AR= 1.0. Results have been obtained for three different conditions and the Rayleigh number ranges from 10^3 to 10^7 (when Ra exceeds 10^7 the flow will become unsteady and chaotic motion may occur). The Prandtl number was fixed at 11.6, which is a typical Prandtl number of molten salts. The authors stated that the influence of the Prandtl number is not large, following the findings of Jahn and Reineke.[18] They propose a condition of isothermal walls and the horizontal walls seem much less important even is a square cavity. Numerical studies by Arcidiacono et el. for cavities with AR= 0.25, 1.0 and 4.0 provide an idea of the results but do not propose a new correlation.[19-21] There is no single correlation which ideally matches all the criteria of this research and the closest to our modelling assumptions are shown in **Table 1**.

All the proposed experiments or formula refer to the bult properties of the fluid. Since SIMMER has a 'macroscopic' approach to heat transfer solver, it uses quasi 1D approach to the heat transfer calculation. It always uses the temperature and material properties from the cell in which a fraction of structure and liquid is present. The characteristic dimension is also the x-dimension of the cell. This has to be corrected in the new development. In order to model natural circulation, we have to involve several radial cells so the characteristic length must be given by the user. The temperature of a specific cell must be taken as 'bulk temperature'. This is the temperature of the cell near the axis in the R-Z geometry.

4. ANSYS Fluent

SIMMER-III represents a macroscopic approach to the flow modelling and in case of complex flows it should be always compared to a more precise tool. Additionally, in this case a new modelling strategy for heat transfer must be implemented in SIMMER. ANSYS Fluent is a computational fluid dynamics tool with two-phase flow and heat transfer modeling capabilities. Simplified salt properties were introduced to the solver and isothermal boundary condition was selected at the wall.

III. Results

Simulations were performed to find possible and optimal design options. The simulations were performed in ANSYS Fluent to find the key flow parameters: heat transfer coefficient (y+), velocity along the axis and velocity in the wall vicinity (before boundary layer). The maximum temperatures were compared.

In the first stage, geometry was studied for heat transfer capabilities from fuel to the coolant, and later the design was checked for loss-of-flow operation. Fuel salt options were verified in terms of criticality in selected geometries. Moreover, the preliminary safety analysis on the possibility of the passive heat removal has been confirmed.

1. ANSYS Fluent results

Simulation of the natural circulation in the cavity were performed in several series. The types of the wall boundary conditions were proposed: constant temperature boundary condition, and linear temperature profile with the temperature increment of 100 K. The flow pattern along the wall does not differ a lot in these setups. Therefore, a series of calculations was proposed for uniform flux only and the heat transfer coefficient vs. volumetric power plots were obtained for three different radii. The flow in the proposed MSR-ST cavity was very steady, typically for the medium-Grashof number-flows. Temperature stratification can be clearly observed.

Table 1 Selected correlations and experiments fulfilling some of the situation criteria

Conditions	Situation	Reference
$0.7 \le Pr \le 10^2$, $3\times10^3 < Re < 2\times10^5$	Flow in a pipe with internal source	Di Marcello et al.[9] with no-internal heat generation by Yu et al.[10]
$Ra_D = Ra_h = 1 - 4.5\times10^{13}$	Cavity, AR = 1-3 BAFOND experiment	Alvarez et al.[11]
$Ra = 5\cdot10^5 - 3\cdot10^{13}$, $Pr = 7$	Rectangular and semicircular cavities	Stainbrenner and Reineke[12]
$10^3 < Ra < 2\times10^{10}$, $Pr = 0.1\text{-}10$	Cylindrical and hemispherical cavities, AR=0.25-3	Bolshov et al.[13]
	Rectangular cavity	Sehgal[14]
$Ra = 5\cdot10^{13}$	Hemispherical cavity, AR = 0.2, 0.3, 1.0	Mayinger et al.
General formula	Cylindrical cavities	Filippov[15]

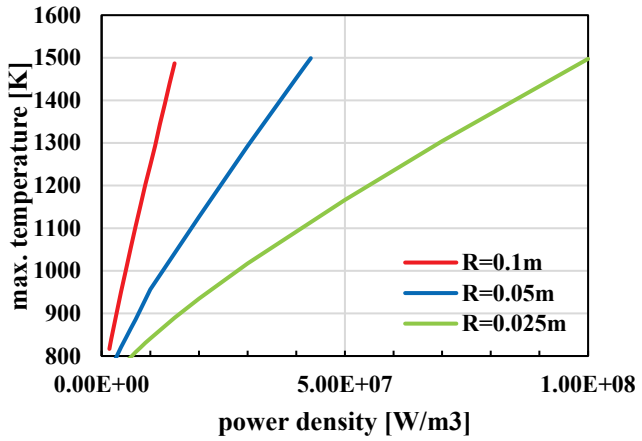

Fig. 2 Maximum salt temperature for radii R=2.5, 5.0 and 10.0 cm

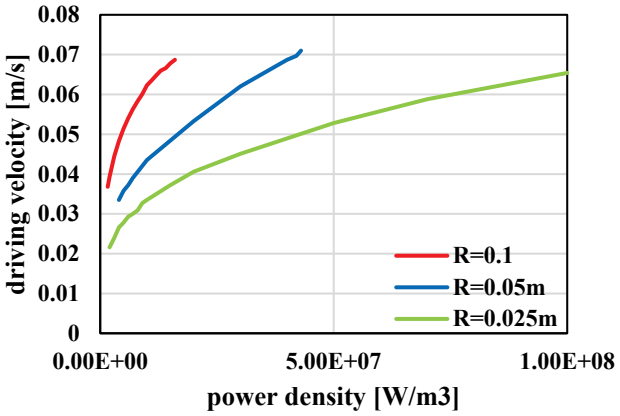

Fig. 3 Velocity along the axis for radii R=2.5, 5.0 and 10.0 cm

The maximum temperature is always located at the highest point in the cylinder, at the axis. This maximum temperature is a relevant safety parameter and is shown in **Fig. 2**. It can be seen that an increased height of the cylinder allows the flow to develop more efficient driving force and accelerate the flow (**Fig. 3**). It makes the heat exchange more efficient and allows more power density.

First, an attempt was done with the Steinberner-Reineke correlation to fit the heat transfer coefficient curve

$$\mathrm{Nu} = 0.85 \cdot \mathrm{Ra}_{\mathrm{R}}^{0.19} \qquad (7)$$

It occurred that the heat transfer coefficient is overestimated in every type of the geometry. Therefore, the correlation was adjusted to be closer to the ANSYS Fluent results. The 0.85 coefficient was replaced by 0.52. The improvement was significant for all the heights; however, it can be observed that the importance of this coefficient decreases with the radius increase (**Fig. 4**). The new correlation was introduced into the SIMMER-III source code.

2. SIMMER results

Until now, all the simulations were done for the isothermal is uniform flux conditions. In SIMMER-III a full subchannel is simulated in axisymmetry. The setup as on the left of the Fig. 1 was created with different dimensions: R= 5 and 10 cm.

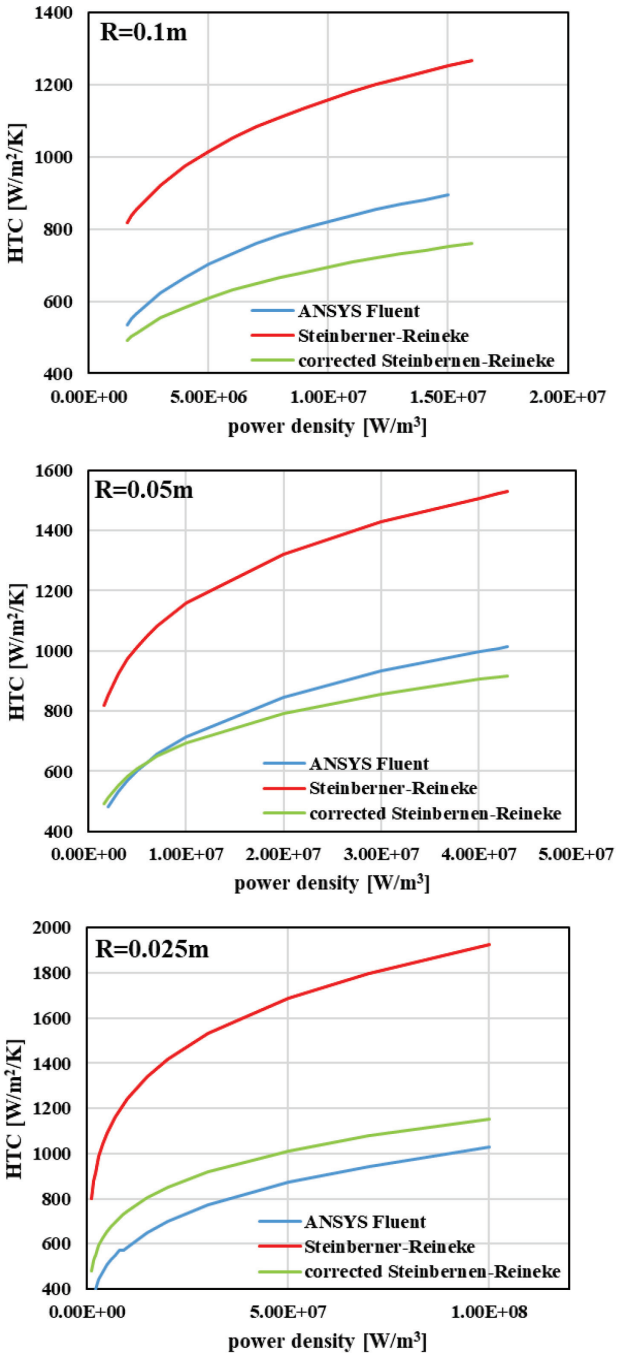

Fig. 4 Heat transfer coefficients obtained in ANSYS Fluent, by Steinberner-Reineke correlation and corrected for SIMMER-III development, (a) R=0.1m, (b) R=0.05m, and (c) R=0.025m

A can-wall thickness after the initial analysis was set as 3 mm. The pitch defines amount of the inert salt and the power density calculated for a subchannel. Narrower gap between the pins gives better heat transfer possibilities due to the more turbulent flow but imposes more pressure drop which is in particular relevant in the accident situation. Simulations were done for a half-gap equal to 2 and 1.5 cm. Increasing the internal heat transfer area is an attempt to enhance the heat transfer by the cost of the natural circulation driving force. In both fuel elements, the pitch does not bring a significant difference to the results (**Fig. 5** and **Fig. 6**), it can be therefore

decreased. The temperature in the fuel element increases almost linearly with the power density, until it reaches the plateau due to the balance between the buoyancy and friction.

This design is limited by the temperature on the can-wall, which should not exceed a value of about 1400 K, with a sufficient margin. For this reason, the Reference case was found significantly improved by decreasing the cylinder radius. In some cases, a decreased pitch can even improve heat transfer due to more turbulent coolant behaviour. The can wall was found to have little meaning on the result, with a major difference observed in the time needed to reach the steady state.

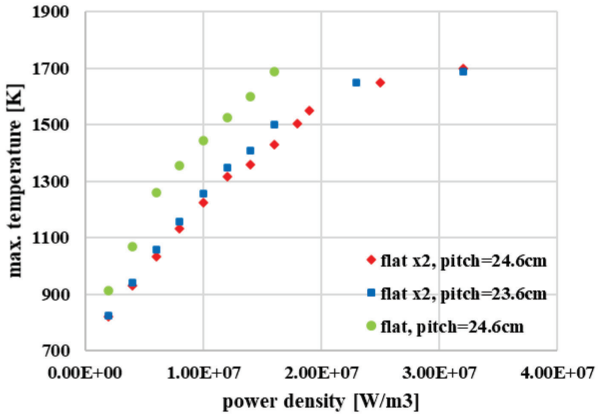

Fig. 5 Maximum fuel salt temperature in the system with R=10 cm. Calculated by SIMMER-III

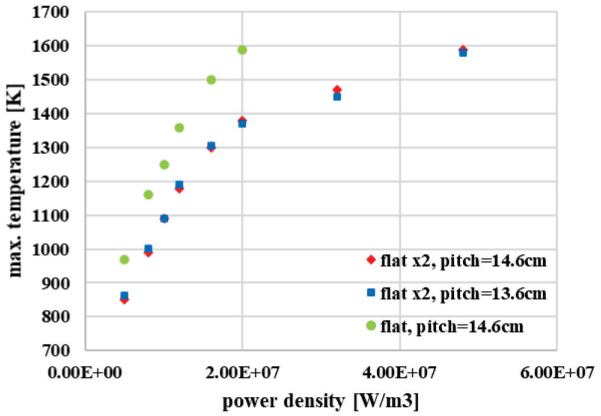

Fig. 6 Maximum fuel salt temperature in the system with R=5 cm Calculated by SIMMER-III

3. Emergency cooling

The chosen design is assumed to have undergone a loss-of-flow accident. In such a situation, power drops to ~5% in a few milliseconds[22] and coolant flow is induced only by its density variations. In the simulation, a secondary loop is attached to the cylinder, and the possibility of cooling by natural circulation is evaluated. In the simulation, we start from cold and static conditions, the result can be therefore assessed only for the steady state and not for the short-time transient when some temperature peaks are possible. The cooling loop has a height of 5 m. In geometry with R=10 cm, the coolant loop (1250 kg coolant) was enough to remove power density $3 \cdot 10^6$ W/m^3, while keeping the temperature below 1500 K, corresponding to 18.75% of the maximum allowable power. For R=5 cm, $2.6 \cdot 10^6$ W/m^3 can be safely removed due to smaller cooling mass and relatively more friction, at 8.1% of the maximum power for these dimensions.

4. Criticality

Several options of composition have been tested to prove which is the best for reaching criticality. Calculations were performed in the deterministic code with reflective boundary conditions.

The models were prepared based on data for the MOSART MSR[6] with a fluoride salt. This concerns the fuel salt and the structure materials. The isotopic composition for the fuel salt at the beginning of life was obtained by replacing all Pu and minor actinides in the MOSART salt with Pu. The composition of the inert salt was obtained by removing all actinides. The studies show a small sensitivity of the reactivity to the inert salt density and volume fraction, but a strong sensitivity to the volume fraction of solid structures.

For neutronics studies, we consider in particular a 2D R-Z cell model with vacuum axial and white (similar to reflective) radial boundary conditions. The height is 4 m. The model represents one element with 10 cm internal radius, 0.3 cm wall and 1 cm half-gap, the latter with inert salt. Plutonium is taken from spent LWR fuel after 60 GWd/t burnup, and 5 years of cooling (see[23]). The k-eff for this model, with radial reflective and vacuum axial boundary conditions for neutron transport, is about 1.21. Therefore, for the core containing a number of elements with the MOSART-like fluoride salt, the k-eff value can be close to 1 at the beginning of irradiation. Accumulation of FPs and MAs in the fuel limits the fuel cycle length, however. Thus, the concept appears to be feasible for fluoride salts also as concerns the criticality.

Currently, the main attention in EURATOM projects is on chloride salts, e.g. with the sodium chloride as the carrier salt. The Plutonium solubility limits are much higher, up to more than 40% in these salts. Therefore, the criticality is expected to be achievable at Pu contents in chlorides well below these limits. More studies are planned to confirm it.

IV. Conclusion

In this paper, we presented a new fast MSR design concept, MSR-ST, with fuel-in-structure elements. It appears to be feasible in terms of power density and reaching the criticality. In the future, we plan to study this concept in more detail and consider alternative fuel salts. In particular, chloride salts offer high TRU solubility (e.g. up to more than 40% of HM) that may offer more flexibility in developing different design options based on the proposed concept. The HTC selected for SIMMER-III extension was a choice between the best available correlations. They do not involve a factor related to the geometry with both meaningful dimensions. An extended study with both Ra_h and Ra_R should be proposed to find a correlation valid for wider range of ARs.

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