NENE 2018
September 10-13
PORTOROŽ
SLOVENIA
27th International Conference Nuclear Energy for New Europe

# A Multiphysics Model for Analysis of Inert Gas Bubbles in Molten Salt Fast Reactor – Part 1: Numerical Modelling

**Parikshit Bajpai**
Politecnico di Milano
Via La Masa, 34
20156, Milan, Italy
parikshit.bajpai@mail.polimi.it

**Carolina Introini, Antonio Cammi, Stefano Lorenzi**
Politecnico di Milano
Via La Masa, 34
20156, Milan, Italy
carolina.introini@polimi.it, antonio.cammi@polimi.it, stefano.lorenzi@polimi.it

## ABSTRACT

The Molten Salt Fast Reactor (MSFR) is the reference circulating fuel reactor under the framework of Generation IV reactors and is currently being developed under the HORIZON2020 SAMOFAR project. Prediction of dynamic behaviour of Molten Salt Fast Reactor poses multiple challenges arising from the peculiar characteristics of the MSFR which are substantially different from other reactors including the Molten Salt Reactor Experiment (MSRE). However, among the models developed in the past for molten salt reactors, most are focussed on thermal reactors such as the MSRE. In the MSFR, the fast neutron spectrum, and consequently the absence of graphite, leads to broad changes and makes the models developed for thermal systems unfit for use with MSFR. Prediction of MSFR requires a model with a tight coupling between neutronics and thermal-hydraulics. The two-phase mixture of fuel salt and inert gas bubbles present in the MSFR further complicates the modelling the MSFR.

In this paper, we present the model equations to describe the thermal-hydraulics and neutronics of MSFR and to predict the void reactivity feedback associated with the inert gas bubbles. The model equations are based on coupling two-phase computational fluid dynamics (CFD) models with neutronic equations for circulating fuel. In MSFR, the flow of fuel salt and gas bubbles mixture can be classified as a dispersed bubbly flow for which the thermal-hydraulics has been modelled using an Euler-Euler two-fluid approach. Furthermore, for small volume fraction of the dispersed phase, i.e. for small bubble fraction, the two-fluid model has been further simplified by combining the momentum and continuity equation of the two phases and adding a gas-phase transport equation to track the void fraction. The prompt neutron flux has been modelled adopting the one-group diffusion approximation and the DNP transport equation has been implemented for delayed neutron precursor (DNP) concentration. Reactivity insertion for small changes in the void fraction has been computed through a first order perturbation theory approach.

## 1 INTRODUCTION

Molten Salt Fast Reactor (MSFR) is the circulating-fuel system selected by the Generation-IV International Forum. This reactor concept was initially studied under the EURATOM EVOL project, and is currently being developed under the H2020 SAMOFAR project [1, 2]. In MSRs, a molten fluoride salt acts as both the fuel and coolant. While this peculiar feature offers several advantages over solid fuelled reactors, it also poses a challenge in reactor design and modelling. The delayed neutron precursors (DNPs) drift along with the fuel salt and as a consequence the fuel salt velocity has a significant impact on the distribution DNPs thus affecting the reactor kinetics and resulting in a tightly coupled multiphysics problem. Moreover, for on-line removal of fission products, a bubbling system has been proposed in the MSFR design. In addition to its primary objective, the bubble injection can also be seen as a reactivity control method by exploiting the highly negative void feedback coefficient of MSFR. However, such an application requires development of multiphysics model capable of evaluating the impact of bubbles on the thermal-hydraulics and neutronics of MSFR. At present, most of the models available in literature approximate the two-phase mixture of fuel salt and gas bubbles as a single phase flow by merging the void feedback effect with density feedback. However, as the spatial distribution of the bubbles is expected to impact the void feedback, such a modelling approach is not suitable for the case of evaluating the feasibility of bubbling as a method of reactivity control. Moreover, while the density feedback mechanism is an intrinsic property of fuel salt, essentially related to fuel expansion with change in temperature, void feedback is exogenously related to the decrease in localised fuel concentration by insertion of bubbles. Therefore, the bubbling system of MSFR requires careful modelling to accurately predict thermal-hydraulic and neutronic influence of gas bubbles.

In Section 2, the two-fluid model for gas-bubbles mixture is presented followed by a simplified bubbly flow model. In Section 3, the diffusion approximation for the prompt neutron flux and the transport equation for the delayed neutron precursors (DNPs) is presented. In Section 4, a bubbling feedback coefficient has been defined to quantify the the impact of inert gas bubbles on reactor thermal hydraulics and neutronics.

## 2 TWO PHASE FLOW MODELLING

Traditionally, two-phase flows have been classified into three main classes based on geometry of the interfaces, namely, separated flows, mixed or transitional flows and dispersed flows and the three classes of flow can be subdivided into different regimes [3, 4]. The existence of flow in a particular flow regime is determined by the geometry of the system and the thermophysical properties of the phases, such as viscosity and surface tension and these flow regimes strongly affect the interfacial exchanges of mass, momentum, and energy. In the MSFR, bubbly flow regime is encountered in which the discrete phase consists of gas bubbles immersed in the fuel salt.

Two-phase flows are modelled using two main approaches - the Eulerian-Lagrangian approach, and the Eulerian-Eulerian approach. The Eulerian-Lagrangian approaches track the individual bubbles or clusters of bubbles through the carrier liquid by solving an appropriate equation of motion while the two-fluid Eulerian-Eulerian approach describe the motion of bubbles in a macroscopic sense by taking phase ensemble averages of the microscopic flow equations [5]. In the two fluid model, each phase, controlled by its own conservation equations which include the phase interaction terms, moves and develops independently. Several correlations appear in the model to account for loss of information associated with the aver-

aging and additional closure relations must be added. This model, however, suffers from a loss of characteristics of the interfaces. This loss of topological information is not a shortcoming for application to the present work, since, in context of the present work, just an averaged description of the two-phase is sufficient to predict the impact of bubbles on fluid-flow and subsequently on neutronics. In fact, the better computational efficiency compared to Lagrangian particle tracking and the predictive capabilities of this approach makes it the preferred choice in the present work.

### 2.1 Two Fluid Model

The two-fluid model is expressed in terms of two sets of conservation equations governing the balance of mass, momentum and energy in each phase. The degree of coupling between the phases is decided by the interfacial interaction terms which, therefore, have a strong influence on the transfer processes. The transfer processes of each phase can be expressed by their own equations and without the interfacial exchanges the two phases are essentially independent. With the liquid phase as continuum and the gaseous phase (bubbles) as dispersed phase, the equations written in non-conservative form [6] have been presented below.

The momentum equations can be written as

$$\begin{aligned}
\frac{\partial \rho_l \alpha_l \vec{u_l}}{\partial t} + \rho_l \alpha_l \vec{u_l} \nabla \cdot (\vec{u_l}) &= -\alpha_l \nabla p + \alpha_l \rho_l \vec{g} \\
&\quad + \nabla \cdot \alpha_l (\vec{\tau_l} + \vec{\tau_l^T}) + (\Gamma_{lg} \vec{u_g} - \Gamma_{gl} \vec{u_l}) + \vec{M_{lg}} + \alpha_l \vec{F_{V,l}} \\
\frac{\partial \rho_g \alpha_g \vec{u_g}}{\partial t} + \rho_g \alpha_g \vec{u_g} \nabla \cdot (\vec{u_g}) &= -\alpha_g \nabla p + \alpha_g \rho_g \vec{g} \\
&\quad + \nabla \cdot \alpha_g (\vec{\tau_g} + \vec{\tau_g^T}) + (\Gamma_{gl} \vec{u_l} - \Gamma_{lg} \vec{u_g}) + \vec{M_{gl}} + \alpha_g \vec{F_{V,g}}
\end{aligned} \tag{1}$$

The continuity equations take the following form

$$\begin{aligned}
\frac{\partial}{\partial t} (\rho_l \alpha_l) + \nabla \cdot (\rho_l \alpha_l \vec{u_l}) &= \Gamma_{lg} \\
\frac{\partial}{\partial t} (\rho_g \alpha_g) + \nabla \cdot (\rho_g \alpha_g \vec{u_g}) &= -\Gamma_{lg}
\end{aligned} \tag{2}$$

where, $\vec{u}$ is the velocity of each phase, $p$ is the pressure, $\alpha$ represents the phase volume fraction, $\rho$ is the density of each phase, $\Gamma$ represents mass transfer rates, $\tau$ denotes the viscous stress tensor, $\tau^T$ denotes the Reynolds stress tensor, $\vec{g}$ is the vector of gravitational acceleration, $\vec{M}$ is the interfacial force, and, $\vec{F_V}$ denotes any other volume force term . Subscripts $l$ and $g$ denote liquid and gas phase respectively. Subscript $lg$ denotes transfer from liquid to gas and vice-versa for subscript $gl$.

The heat transfer equations can be written as follows

$$\begin{aligned}
\frac{\partial}{\partial t} (\rho_l \alpha_l H_l) + \nabla \cdot (\rho_l \alpha_l \vec{u_l} H_l) &= \nabla \cdot [\alpha_l \lambda_l^e \nabla T_l] + (\Gamma_{lg} H_g - \Gamma_{gl} H_l) + Q_l \\
\frac{\partial}{\partial t} (\rho_g \alpha_g H_g) + \nabla \cdot (\rho_g \alpha_g \vec{u_g} H_g) &= \nabla \cdot \left[\alpha_g \lambda_g^e \nabla T_g\right] + (\Gamma_{gl} H_l - \Gamma_{lg} H_g) + Q_g
\end{aligned} \tag{3}$$

where $T$ denotes the temperature of each phase, $\lambda^e$ is the effective thermal conductivity, $H$ is the enthalpy and $Q$ denotes the heat source density. For gas-liquid bubbly flows without interfacial transfer, the mass transfer rates $\Gamma_{lg}$ and $\Gamma_{gl}$ are taken as zero.

The neutronics affects the thermal hydraulics through the heat source term $Q$. The source term can be given as the sum of the fission heat and the decay heat from DNPs. Therefore, the heat source term directly couples the neutronics and thermal-hydraulics.

## 2.2 Bubbly Flow Model

While the system of equations discussed as part of the two-fluid model provide the most accurate results for all kinds of bubbly flows, their advantages are overweighed by the computational requirements in case of flows with small void fraction. In such cases the equations for each phase can be combined into a single equation representative of both the phases. Such equations normally account for the flow in terms of the continuous phase and a gas phase transport equation is added to track the volume fraction of the dispersed phase.

The bubbly flow model simulated in this work is a simplification of the Euler-Euler model discussed in the previous section. The bubbly flow model is based on the assumptions that the gas density is negligible compared to the liquid density, the motion of the gas bubbles relative to the liquid is determined by a balance between viscous drag and pressure forces, and, the two phases share the same pressure field. The momentum and the continuity equations for the two phases can then be combined and a gas phase transport equation can be added to keep a track of the volume fraction of the gas bubbles. This results in the following system of equations

$$\alpha_l \rho_l \frac{\partial \vec{u_l}}{\partial t} + \alpha_l \rho_l \vec{u_l} \cdot \nabla \vec{u_l} = -\nabla p + \nabla \cdot \left[ \alpha_l (\mu_l + \mu_T) \left( \nabla \vec{u_l} + \nabla \vec{u_l^T} - \frac{2}{3} (\nabla \vec{u_l}) \vec{I} \right) \right] + \alpha_l \rho_l \vec{g} + \vec{F} \quad (4)$$

$$\frac{\partial}{\partial t} (\rho_l \alpha_l + \rho_g \alpha_g) + \nabla \cdot (\rho_l \alpha_l \vec{u_l} + \rho_g \alpha_g \vec{u_g}) = 0 \quad (5)$$

where $\vec{u_l}$ is the velocity of liquid phase, $p$ is the pressure, $\alpha$ denotes the phase volume fraction, $\rho$ is the density, $\vec{g}$ is the gravity vector, $\vec{F}$ is any additional force per unit volume, $\mu_l$ denotes the dynamic viscosity of liquid, and $\mu_T$ represents the turbulent viscosity.

For the case wherein there is no mass transfer between the two phases, the gas phase transport equation can be written as

$$\frac{\partial \rho_g \alpha_g}{\partial t} + \nabla \cdot (\rho_g \alpha_g \vec{u_g}) = 0 \quad (6)$$

Furthermore, at low void fractions, the role of bubbles in heat transfer is only through bubble induced turbulence and the temperature field can be well approximated by the energy equation for liquids as follows

$$\rho_l c_P \frac{\partial T}{\partial t} + \rho_l c_P \nabla \cdot (\vec{u_l} T) = \nabla \cdot [\lambda_l^e \nabla T] + Q \quad (7)$$

The power source density $Q$ in the above equation couples the neutronics and the thermal hydraulics using through the following equation

$$Q = (1 - \beta) E_f \Sigma_f \Phi + \beta \lambda_{heat} C \quad (8)$$

where $E_f$ represents the energy produced per fission, $\Sigma_f$ represents the macroscopic fission cross section, $\beta$ represents DNP fraction, $\lambda_{heat}$ represents the decay heat constant, $\Phi$ represents the neutron flux, and $C$ represents the DNP concentration.

# 3 NEUTRONICS

## 3.1 Neutron Flux

An exact model for the neutronic analysis requires the complete neutron transport equation. However, the one energy group neutron diffusion approximation [7] is capable of capturing the complexity of coupled neutronic and thermal-hydraulics in MSFR and has been adopted in this work to reduce the required computation time. As the neutrons are not affected by the molten salt motion because of the much shorter life span with respect to the characteristic time of the fuel circulation, the neutron diffusion equation takes the following form

$$\frac{1}{v_n}\frac{\partial \Phi}{\partial t} = \nabla \cdot (D\nabla\Phi) - \Sigma_a\Phi + \lambda C + (1-\beta)\nu\Sigma_f\Phi \tag{9}$$

where $\Phi$ is the neutron flux, $C$ denotes the delayed neutron precursor concentration, $v_n$ is the average velocity of neutron population, $\Sigma_a$ and $\Sigma_f$ represent the macroscopic absorption and fission cross-sections respectively, $D$ is the neutron diffusion coefficient, $\beta$ is the fraction of fission neutrons emitted by precursors, $\nu$ is the average number of neutrons emitted per fission reaction, and $\lambda$ is the decay constant of the precursors. The macroscopic cross-sections and their temperature dependencies can be calculated by means of SERPENT Monte Carlo code [8] employing the JEFF-3.1 library [9].

The gas bubbles present in reactor core act as voids from the point of view of neutrons and have an impact on the nuclear data of MSFR fuel. The bubbles alter the effective volume of fuel and thereby alter the macroscopic cross-sections. This effect can be accounted by weighting the cross-section by the volume fraction of fuel.

$$\Sigma = \alpha_l\Sigma_l + \alpha_g\Sigma_g \approx \alpha_l\Sigma_l \tag{10}$$

Thermal feedback on neutronics can been accounted by employing a simple logarithmic temperature dependence using cross-sections at 900 K and 1200 K for the interpolation. The cross-sections are assumed to be proportional to local density and also to local volume fraction of the fuel [10].

$$\begin{aligned} \Sigma(T,\rho,\alpha_l) &= \alpha_l\left(\frac{\rho}{\rho_0}\right)\left[\Sigma_0 + \alpha_\Sigma \log\left(\frac{T}{T_0}\right)\right] \\ D(T,\rho,\alpha_l) &= \frac{1}{\alpha_l}\left(\frac{\rho_0}{\rho}\right)\left[D_0 + \alpha_D \log\left(\frac{T}{T_0}\right)\right] \end{aligned} \tag{11}$$

where $T_0$ is the fuel reference temperature and $\rho_0$ is the fuel density at the reference temperature.

## 3.2 Delayed Neutron Precusor (DNP) Transport

In the MSFR, the delayed neutron precursors drift along with the fuel salt. This DNP drift plays an important role in reactor dynamics of molten salt reactors and the equation for precursor concentration must account for the effect of fuel mobility. The velocity field of the fuel is taken into account by introducing convection and diffusion terms in the balance equation of DNP [11, 12, 13]

$$\frac{\partial C}{\partial t} + \vec{u_l}\cdot\nabla C - \nabla\cdot\left(\frac{\mu_T}{\rho Sc_T}\nabla C\right) = \beta\nu\Sigma_f\Phi - \lambda C \tag{12}$$

where $C$ is the precursor concentration, $\vec{u_l}$ is the fuel velocity, $\mu_T$ represents the turbulent viscosity, and $Sc$ is the turbulent Schmidt number which is equal to 0.85 [14, 15].

## 4 BUBBLING FEEDBACK COEFFICIENT

The effect of nonuniform perturbations on reactor performance can be estimated by a multigroup calculation where perturbations are represented by appropriate space-dependent group constants. However, such localised perturbations inherently require a multigroup calculation in at least two dimensions resulting in a high computational cost. If the perturbations are not so large as to distort substantially the flux in the neighbourhood of the perturbation, *perturbation theory* can be employed to determine such effects. In case of small void fractions, the change in core multiplication caused by the bubbles is sufficiently small to be treated as a perturbation and therefore the original criticality calculation can be avoided [16].

The bubble induced perturbations in the core parameters, as compared to single-phase flow, can be represented in terms of the gas void fraction as follows

$$\begin{aligned} \delta\Sigma_f &= -\alpha_g \Sigma_f \\ \delta\Sigma_a &= -\alpha_g \Sigma_a \\ \delta D &= \frac{\alpha_g D}{(1-\alpha_g)} \end{aligned} \tag{13}$$

where $\alpha_g$ is the bubble void fraction computed from the gas phase transport equation.

The reactivity change, based on the first order perturbation theory, can be expressed as

$$\Delta\rho = \frac{\int_\Omega \left[\Phi' \left(\nu\delta\Sigma_f - \delta\Sigma_f\right)\Phi - \nabla\Phi'\delta D\nabla\Phi\right] d\Omega}{\nu \int_\Omega \Phi'\Sigma_f \Phi d\Omega} \tag{14}$$

where $\Phi'$ and $\Phi$ represent the perturbed and the unperturbed flux respectively. The perturbed flux is associated to changes in macroscopic cross-sections and diffusion length due to the effect of gas bubbles.

The reactivity feedback provided by the inert gas bubbles can be quantified in terms of the bubbling feedback coefficient. This coefficient is defined as the average reactivity inserted per unit gas void fraction in the core and takes the following mathematical form

$$\alpha_{bubbling} = \frac{\Delta\rho}{\frac{1}{\Omega}\int_\Omega \alpha_g d\Omega} \tag{15}$$

where the reactivity insertion due to bubbles $\Delta\rho$ can be computed by equation 14.

## 5 CONCLUSIONS

This paper presents a detailed mathematical model of different physics required for the description of two-phase flow in the MSFR reactor. The fluid-flow was modelled using an Euler-Euler two-fluid model, and, a number of simplifying assumptions, such as low-void fraction hypothesis, helped in further simplification of fluid-flow description to a simplified bubbly flow model. Heat transfer, neutron diffusion and transport of delayed neutron precursors equations for the two-phase flow in MSFR have been presented based on the bubbly flow model, neutron diffusion approximation and DNP transport equation. To quantify the effect of inert gas bubbles on the reactivity of the MSFR, a bubbling feedback coefficient has also be defined as the average reactivity inserted per unit gas void fraction in the core.

The model presented in this work serves as a starting point for the development of two-phase multiphysics models for MSFR. The multi-physics approach is most suitable for complex problems of this kind with a high degree of coupling between various variables such as velocity,

temperature, etc. The model presented accounts for the reasonable case of two-phase flow with a non-uniform distribution the bubbles within the core and can be directly implemented to simulate the steady-state thermal hydraulic behaviour using CFD and heat transport equation and to compute the neutrons flux and feedback effect of the bubbles.

## REFERENCES


[1] E. Merle-Lucotte, D. Heuer, M. Allibert, M. Brovchenko, N. Capellan, and V. Ghetta. "Launching the Thorium fuel cycle with the molten salt fast reactor". Proc. Int. Cong. Advances in Nuclear Power Plants '11, Nice, France, May 2-5, Societe Francaise d'Energie Nucleaire (SFEN), 2011, pp. 842–851.

[2] M. Brovchenko, D. Heuer, E. Merle-Lucotte, M. Allibert, V. Ghetta, A. Laureau, and P. Rubiolo. "Design related studies for the preliminary safety assessment of the molten salt fast reactor". Nuclear Science and Engineering, 175 (3), 2013, pp. 329–339.

[3] G. B. Wallis. One-dimensional Two-phase Flow. McGraw-Hill, New York, NY, 1969.

[4] M. Ishii. "Thermo-fluid dynamic theory of two-phase flow". In Collection de la Direction des Etudes et Recherches d'Electricite de France, Eyrolles, Paris, 1975, No. 22.

[5] R. T. Lahey Jr. and D. A. Drew. "On the development of multidimensional two-fluid models for vapor/liquid two-phase flows". Chemical Engineering Communications, 118 (1), 1992, pp.125–139.

[6] M. Ishii and T. Hibiki. Thermo-Fluid Dynamics of Two-Phase Flow. Springer-Verlag, New York, 2006.

[7] J. J. Duderstadt and L. J. Hamilton. Nuclear Reactor Analysis. John Wiley and Sons, New York, 1976.

[8] J. Leppänen, M. Pusa, T. Viitanen, V. Valtavirta, and T. Kaltiaisenaho. "The serpent Monte Carlo code: Status, development and applications in 2013". Annals of Nuclear Energy, 82, 2015, pp. 142–150.

[9] A. Koning, R. Forrest, M. Kellett, R. Mills, H. Henriksson, Y. Rugama. The JEFF-3.1 nuclear data library. Technical Report NEA–6190, Organisation for Economic Co-Operation and Development, Nuclear Energy Agency - OECD/NEA, Issy-les-Moulineaux, France, 2006.

[10] C. Fiorina, M. Aufiero, A. Cammi, C. Guerrieri, J. Krepel, L. Luzzi, K. Mikityuk, and M. E. Ricotti. "Analysis of the MSFR core neutronics adopting different neutron transport models". Proc. Int. Conf. on Nuclear Engineering '12, Anaheim, USA, July 30 - August 3, American Society of Mechanical Engineers (ASME), 2012.

[11] A. Cammi, V. Di Marcello, L. Luzzi, V. Memoli, and M. E. Ricotti. "A multi-physics modelling approach to the dynamics of molten salt reactors". Annals of Nuclear Energy, 38 (6), 2011, pp. 1356–1372.

[12] A. Cammi, C. Fiorina, C. Guerrieri, and L. Luzzi. "Dimensional effects in the modelling of MSR dynamics: Moving on from simplified schemes of analysis to a multi-physics modelling approach". Nuclear Engineering and Design, 246, 2012, pp. 12–26.

[13] E. van der Linden. Coupled neutronics and computational fluid dynamics for the molten salt fast reactor. Master's thesis, Technical University of Delft, Netherlands, 2012.

[14] L. Y. Jiang and I. Campbell. "Reynolds analogy in combustor modeling". International Journal of Heat and Mass Transfer, 51 (5), 2008, pp. 1251–1263.

[15] Y. Tominaga and T. Stathopoulos. "Turbulent Schmidt numbers for CFD analysis with various types of flow field". Atmospheric Environment, 41 (37), 2007, pp. 8091–8099.

[16] D. G. Cacuci. Sensitivity and Uncertainty Analysis, Volume 1 - Theory. Chapman and Hall/CRC, New York, 2003.