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Computational Fluid Dynamics (CFD) Problems in Molten Salt Reactors

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1. Introduction

Molten Salt Reactors (MSRs) represent an innovative advancement in nuclear energy technology, offering numerous benefits such as improved safety, fuel flexibility, and a significant reduction in nuclear waste [1]. These reactors utilize molten salts as both coolant and fuel, which allows for higher operating temperatures and enhanced thermal efficiency compared to conventional reactors [1]. However, the unique thermal-hydraulic properties of molten salts, combined with the intricate geometries of MSR cores, introduce significant challenges in accurately predicting flow and heat transfer behaviors within these systems.

It is expected that three-dimensional Computational Fluid Dynamics (CFD) modeling will become an imperative method for design optimization of MSRs. This is because the fuel is in a fluid form which means that the uncertainty in the fluid flow has to be resolved better than in the case with solid fuel. The uncertainty in fluid fuel will impact reactor efficiency, safety margins, and operational stability. The unique properties of molten salts, including their high Prandtl numbers, heat generation characteristics, and complex thermophysical behavior, present challenges that existing Reynolds averaged Navier-Stokes based turbulence models may not fully capture [2].

This issue will become more pronounced when accident progressions have to be predicted, where phenomena such as salt freezing, fouling/plate-out, and natural convection play crucial roles in determining the overall behavior of the reactor. Addressing these phenomena is essential to ensure the reliability of CFD simulations in MSRs. This study is to summarize a few identified issues in CFD analysis of MSR so far and try to address how these issues can be resolved in the future.

2. Uncertainties in MSR CFD

Applying CFD to industrial problems with well-known fluids such as water and air is becoming more and more standardized process. However, utilizing CFD to unfamiliar or not well studied fluid flow will always have issues especially in verification and validation although visually appealing simulations of fluid processes can be readily generated **[3]**. Ensuring the quality and accuracy of these simulations remains uncertain. The conventional sources of CFD uncertainties shown in the following **[4]** will still be present for MSR CFD.

- ✓ Numerical Uncertainty:
  Arising from the discretization of equations, numerical schemes, and solver settings used in the simulations.
- ✓ Model Uncertainty:
  Directly related to the physics of the phenomena being simulated, such as turbulence, multiphase flow, and heat transfer.
- ✓ User Uncertainty:
  Occurring due to incorrect input parameters, boundary conditions, or modeling choices made by the user.
- ✓ Software Uncertainty:
  Due to bugs or limitations in the CFD software itself.
- ✓ Application Uncertainties:
  Involving uncertainties related to the physical properties of materials, operating conditions, and other external factors.

Among the source of uncertainties, model uncertainty is of particular concern in MSRs because of the unique and complex behavior of molten salts. The MSR Thermal-Fluid Phenomena reports from BNL/NRC highlight several factors that make validating turbulence models for MSR accident analysis especially challenging **[5]**:

- ✓ Fouling / Plate-out:
  This refers to the precipitation and accumulation of contaminants on heat exchanger surfaces, originating from corrosion, fission products, and fissile material. The extent of fouling is dependent on time, location, and operational conditions. During an overcooling accident, changes in wall deposition can alter flow conditions along the walls, introducing significant variability in heat transfer and fluid dynamics.
- ✓ Salt Freezing:
  This concerns the temperature at which the molten salt solidifies, which is composition-dependent. In overcooling accidents, partial solidification within the primary system can significantly affect the molten salt flow characteristics, leading to localized changes in flow patterns, heat transfer rates, and pressure drops.

The challenges associated with fouling/plate-out and salt freezing exist during accident scenario simulations, where the behavior of molten salt can deviate significantly from normal operating conditions. Understanding these phenomena is important for improving the accuracy of CFD simulations and ensuring the safety of MSRs.

Fouling can directly impact the solid composition within molten salt. The severity of overcooling increases the possibility of solid presence within the molten salt, which can alter surface conditions and, consequently, turbulence prediction **[6]**. Such changes can lead to uncertainties in turbulence models. It has been reported that turbulence changes due to cumulative surface damage significantly impact mean velocity deficits at the wall. Even minor surface damage can induce substantial turbulence, emphasizing the importance of this phenomenon in accident analysis. In MSRs, the degree of corrosion varies with the type of salt used, and the dynamic nature of flow surfaces can affect the validation of CFD models during accident scenarios.

During accident analysis, the influence of solidified molten salt within the primary system becomes increasingly significant. This necessitates the consideration of frozen salt suspensions in the flow, resulting in a three-phase flow behavior as seen in Fig.1, especially near the wall degradation spot or overcooled finite volumes when external force disappears.

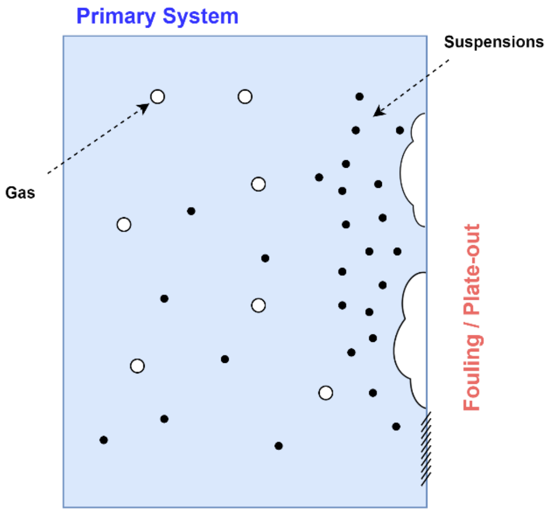

Fig 1. Molten salt three-phase flow concept near the surface degradation

If the consequence of such particulate flow has high impact on accident analysis, the colloidal fluid and its associated fluid flow phenomena will inevitably necessitate non-Newtonian fluid flow simulation approach. Such non-Newtonian fluid flow simulation will require to capture physical process such as high yield stress, caking, and sphere-formation **[1]**. High yield stress can dampen turbulence, cause tube plugging, and complicate fluid mixing. Caking can lead to tube plugging, mechanical imbalance in pumps, and a dramatic reduction in heat transfer. These issues contribute to model uncertainties in three-phase fluid flow modeling, which will significantly impact CFD calculation. In Fig.2, the concentrations of suspensions like colloidal particles lead to difference of yield stress, which affect the onset critical velocity of turbulence transition **[1]**. Depending on the concentration of suspension, the viscosity changes in each control volume, and as a result, during overcooling accident, where the concentration of colloidal particles becomes important, it is necessary to deal with the issue of inhomogeneous turbulence. Furthermore, extensive experimental campaigns will be needed to address each physical phenomenon if the phenomenon is important to the consequence of the accident. For example, analysis codes such as MELCOR and the MELCOR Accident Consequence Code System (MACCS) consider transport of colloidal particles. While these are not CFD code, its ability to integrate colloidal properties enhances the physical consistency of analysis results involving radionuclides during accident scenarios **[7]**. In addition, there are also numerical studies that reflect the deposition of noble metals in molten salt **[8] [9]**.

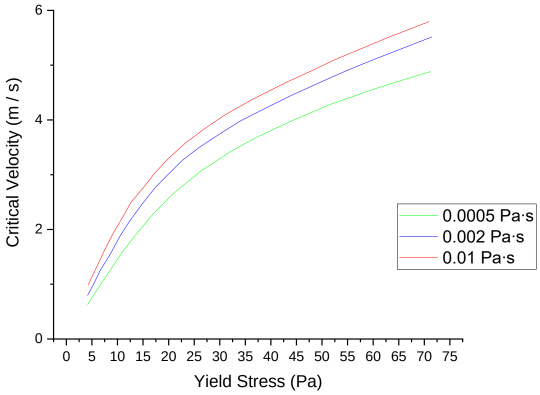

Fig 2. Effect of slurry physical properties on onset of turbulence, $\rho_{fluid} = 1602\ kg/m^3$

Unfortunately, non-Newtonian fluid flow was not important in the conventional nuclear systems, since non-Newtonian fluid was not often used as a coolant for the nuclear solid fuel cooling. Therefore, nuclear industry does not pertain abundant experience in this field, and the capacity building in this area will become essential.

Additionally, factors such as the entrainment of cover gas, thermal expansion, and the interaction between different phases (solid, liquid, and gas) contribute to the complexity of modeling molten salt behavior. **[5]** These factors are uniquely relevant to liquid-fuel molten salts, where traditional CFD models may not fully capture the intricate multiphase dynamics involved. Therefore, these elements require special attention when validating CFD models for transient and accident conditions in MSRs.

3. Addressing Issues in MSR CFD Simulations

To enhance the reliability and accuracy of CFD simulations in MSRs, particularly if CFD approach becomes imperative for accident analysis, several strategies can be suggested to address the identified issues:

- ✓ Experimental Validation:
  Conducting experimental studies to validate CFD models under operating molten fuel salt is needed for ensuring the accuracy of CFD method. This includes experiments such as separate effect test as well as integral effect test that can replicate the thermal-hydraulic conditions of MSRs, while covering the full range of thermal hydraulic variables during transients and accidents.
- ✓ Advanced Turbulence Modeling:
  Developing and validating advanced turbulence models that account for the unique properties of molten salts is necessary. These models should consider the high Prandtl numbers, concentration gradient effect, internal heat generation, and complex thermophysical behavior of molten salts, as well as the impact of dynamic surface degradation and solidification on flow dynamics.
- ✓ Multiphase Flow Modeling:
  Accurate modeling of multiphase flows, including the interaction between liquid, solid, and gas phases, will become essential for capturing the full range of phenomena that may occur during accidents. This includes the development of models that can simulate the effects of salt freezing, cover gas entrainment, and the formation of colloidal suspensions.
- ✓ Uncertainty Quantification:
  Implementing robust uncertainty quantification techniques can help identify and mitigate the sources of error in CFD simulations. By systematically analyzing the impact of various uncertainties—such as material properties, boundary conditions, and model parameters—greater confidence in simulation results can be achieved.
- ✓ Inter-disciplinary Collaboration:
  Collaboration between CFD experts, material scientists, and nuclear engineers is going to be very important for addressing the complex challenges associated with MSR design and safety evaluations. By leveraging expertise across multiple disciplines, more comprehensive and accurate models that account for the full range of physical phenomena involved in MSRs have to be developed.

4. Summary

Molten Salt Reactors represent a promising advancement in nuclear energy, but their unique thermal-hydraulic behavior poses significant challenges for CFD modeling with high confidence. Furthermore, in order to evaluate the MSR design and safety, it is expected that the three-dimensional CFD approach will become inevitably important which will be very different from the development process of conventional reactor development.

In this study a few challenging issues for applying CFD methods to MSRs were identified and discussed. Addressing these challenges requires a thorough understanding of the factors that contribute to model uncertainties. The full range of physical parameters during accidents where phenomena like fouling/plate-out and salt freezing play a critical role are not clear yet. However, it is foreseen that MSRs may require non-Newtonian fluid flow simulation to accurately represent important physical phenomena, which the nuclear industry does not have abundant experience within. These phenomena are expected to become very important for modeling MSRs with CFD methods, and therefore a good strategic planning to address these issues seem to be necessary.

By advancing turbulence and multiphase flow models, implementing uncertainty quantification techniques, and conducting experimental validation, the accuracy and reliability of CFD simulations can be significantly improved. These efforts are essential for ensuring the safety, efficiency, and viability of MSRs as the next-generation nuclear energy technology.

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