Development of 1-D Freezing Model for Fuel Salt in Molten Salt Reactors and Implementation into Modelica Using TRANSFORM Library

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*Keywords : molten salt reactor, freezing, Modelica, TRANSFORM

1. Introduction

Molten salt reactors (MSRs) have recently gathered increasing global interest due to their unique advantages. Firstly, they offer high efficiency owing to their high operating temperatures while maintaining atmospheric operating pressure. Secondly, MSRs provide significant safety benefits. The molten fuel used in these reactors exhibits greater thermal expansion compared to conventional solid fuels, which enhances the inherent safety characteristics of the system. Additionally, the risk of a meltdown is inherently avoided since the fuel is already in a liquid state [1].

While MSRs generally exhibit strong safety characteristics, there remain some uncertainties that need to be thoroughly evaluated. In particular, the freezing of molten salt during transient conditions poses a significant risk to the overall safety of the reactor system. For instance, salt freezing in the pipe can cause sudden blockage of flow. Which can significantly reduce heat removal capacity, potentially leading to serious safety concerns [2].

Given the critical nature of these effects, several studies have focused on understanding and modeling salt freezing. For instance, Le Brun et al. developed a onedimensional (1-D) model of salt freezing, which was applied to the Direct Reactor Auxiliary Cooling System (DRACS) of the Fluoride-salt-cooled High-temperature Reactor (FHR) [3]. Similarly, Zeng developed a freezing model for FHR and coupled the model to ASYST code [4].

Although these studies have successfully simulated freezing phenomena and their associated effects, their primary focus has been on FHRs, where molten salt is used as a coolant rather than as a fuel. However, fuel salt differs significantly from coolant salt, particularly due to internal heat generation, which could lead to different outcomes. Therefore, it is crucial to develop a fuel salt freezing model that accounts for internal heat generation.

In this study, an analytical model for fuel salt freezing has been developed. This model has been implemented into Modelica language by modifying the TRANSFORM library. The details of the model and code structure will be explained, followed by simple simulations to demonstrate the model's behavior.

2. Methods

2.1 Analytical Model

The model geometry is assumed to be a circular pipe, as shown in Fig. 1, with the assumption that freezing occurs uniformly. The analysis domain is divided into a liquid domain and a solid domain, each of which solves its own set of conservation equations. The equations for each domain are presented in Table 1.



Fig. 1. Schematics of freezing pipe



(1)
$$\frac{\partial}{\partial t}(\alpha_l \rho) + \frac{\partial}{\partial z}(\alpha_l \rho u) = -\frac{\sigma_A}{A_T}$$

(2) $\frac{\partial(\alpha_l)(\rho u)}{\partial t} + \frac{\partial(\alpha_l)(\rho u u)}{\partial t} = -(\alpha_l)\frac{\partial p}{\partial t} - (\alpha_l)\rho u$

(2)
$$\frac{1}{\partial t} + \frac{1}{\partial z} = -(\alpha_l) \frac{1}{\partial z} - (\alpha_l) \rho g$$
$$-(\alpha_l) \frac{f}{2D_h} \rho u |u| - \frac{\sigma_A u}{A_T}$$

(3)
$$\frac{\partial}{\partial t} (\alpha_l \rho C_p T) + \frac{\partial}{\partial z} (\alpha_l \rho C_p T u) = -\frac{\sigma_A}{A_T} H_{l,Tm}$$

 $-\frac{q_l'' P_{h,l}}{A_T} + \alpha_l \dot{Q}_d$

$$(4) \quad \rho = \rho(p,T)$$

Solid Domain

$$(5) \quad \frac{\partial(\alpha_{s}\rho_{s})}{\partial t} = \frac{\sigma_{A}}{A_{T}}$$

$$(6) \quad \frac{\partial}{\partial t} \left(\alpha_{s}\rho_{s}C_{p}T_{s} \right) = \frac{\sigma_{A}}{A_{T}}H_{l,Tm} + \frac{q_{i}^{\prime\prime}P_{h,i}}{A_{T}} - \frac{q_{w}^{\prime\prime}P_{w}}{A_{T}}$$

$$+ \alpha_{s}\dot{Q}_{d}$$

$$(7) \quad \rho_{s} = \rho_{s}(p,T)$$

The conservation equations used are general, but several additional terms have been included. The term α_s is defined as the proportion of the solidified area to the total area. \dot{Q}_d and $H_{l,Tm}$ represents decay heat and latent heat respectively, as shown in equations (3) and (6).

The term σ_a represents the 'linear freezing rate' which has a unit of [kg/m-s]. Linear freezing rate is a key term that relates freezing phenomena to conservation equations.

Freezing rate is calculated based on the heat flux difference on freezing interface. As shown in Fig.2, there are two heat fluxes acting on freezing interface: one from the solid side (ϕ_a) and the other from liquid side (ϕ_b). On the liquid side, heat flux can be defined as equation (14). On the solid side, heat is transferred by conduction, requiring the temperature distribution to calculate heat flux.



Fig. 2. Cross-section of freezing pipe in r-direction

To calculate the temperature distribution, a quasisteady state is assumed for solidified layer. The conduction equation for the solidified layer is established in equation (8). And the temperature at the freezing interface is assumed to equal to the freezing temperature of salt, as shown in equation (9). From the conservation equation of solid domain, the average temperature (T_s) is known. Therefore, equation (10) can be derived.

(8)
$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dT}{dr}\right) + \frac{\dot{Q}_d}{k_s} = 0$$

(9) $T(\delta_l) = T_{frz}$

(10)
$$T_s = \frac{\int_A T(r) dA}{\int_A dA}$$

Using the above relations, the temperature distribution in the solidified layer can be derived as shown in equation (11).

(11)
$$T(r) = Cln\left(\frac{r}{\delta_l}\right) + T_{frz} + \frac{1}{4k_s}\dot{Q}_d\delta_l^2 - \frac{1}{4k_s}\dot{Q}_dr^2$$

(12) $C = \left[\frac{R^2 - \delta_l^2}{R^2 \ln\left(\frac{R}{\delta_l}\right) - \frac{R^2 - \delta_l^2}{2}}\right] \left[T_s - T_{frz} + \frac{\dot{Q}_d}{8k_s}(R^2 - \delta_l^2)\right]$

With temperature distribution, the heat flux can be calculated as shown in equation (13). The solidified layer growth rate (δ_s) is proportional to the heat flux difference as shown in equation (15), where Δe_s represents the heat of fusion.

(13)
$$\phi_a = -k \frac{dT(r)}{dr} \Big|_{r=\delta_l} = \frac{\delta_l \dot{Q}_d}{2} - \frac{k_s C}{\delta_l}$$

(14)
$$\phi_b = h_s (T_m - T_{frz})$$

(15)
$$\rho_s \Delta \mathbf{e}_s \dot{\delta}_s = \phi_a - \phi_b$$

Solidified layer growth rate (δ_s) is converted into the linear freezing rate (σ_a) through several modifications. First, the geometric relationship between the 'solidified layer growth rate (δ_s) ' and 'area growth rate (\dot{A}) ' is used, as shown in Fig. 3. This relationship is expressed in equation (16). Finally, the linear freezing rate is calculated by multiplying the density to the area growth rate as seen in equation (17).



Fig. 3. Relation of layer growth rate $\dot{\delta}_s$ and area growth rate \dot{A}

(16)
$$A = 2\pi \delta_l \delta_s$$

(17) $\sigma_A = \rho_s \dot{A} = \frac{2\pi \delta_l}{\Delta e_s} \left[\frac{\delta_l \dot{Q}_d}{2} - \frac{k_s C}{\delta_l} - h_s (T_m - T_{frz}) \right]$

2.2 Modelica Model

(10) i -

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Modelica is an object-oriented, equation-based programming language designed for multi-domain modeling and simulation of complex systems. Its flexibility and modularity make it well-suited for accurately simulating the dynamic behavior of systems across various engineering fields, including mechanical, electrical and thermal systems. As a result, Modelica has gained an increasing attention in nuclear research field as well [5,6].

Building on the strengths of the Modelica language, Oak Ridge National Laboratory has developed the TRANSFORM library and released it as open-source [7]. This library provides a comprehensive suite of tools specifically designed for the simulation and analysis of nuclear systems. TRANSFORM enables researchers and engineers to model a wide range of nuclear systems, including molten salt reactors and sodium fast reactors.

To leverage the advantages of Modelica framework, the analytical model derived in Section 2.1 was implemented into Modelica by modifying the TRANSFORM library. The Schematic of freezing model is shown in Fig.4. The 1-D pipe model and 1-D solid model are connected to each other, representing liquid salt and frozen salt respectively. The pipe geometry is circular, while the solid is annular.

As freezing occurs, the freezing rate is calculated by the 'freezeRate' model, represented by the blue rectangle in the upper left corner of Fig. 4. As a result of freezing, the diameters of the pipe and solidified layer change.



Fig. 4. Schematics of Modelica freezing model

'port_a' and 'port_b' provide connection points for external fluid components, while 'port_c' is a connection point for external thermal components. When this freezing model is used in an external model, it appears as a blue rectangular component, as shown in the lower part of Fig. 5. This blue component can be connected and used with other components, as seen in Fig. 5.

3. Results and Discussion

Two simple simulations were conducted to evaluate the behavior of the developed Modelica freezing model. The simulation setup is illustrated in Fig. 5. In this setup, the freezing pipe is connected to the pipe wall, which receives a boundary temperature condition from the outside. The details of the pipe and simulation setup are provided in Table II.

The first simulation demonstrates the sudden freezing of a pipe when the outside temperature drops from ambient temperature (20° C) to -196°C. In this scenario, the flow source provides a mass flow rate of 0.01 kg/s to the pipe, and decay heat is not considered.

Table II. Simulation setup

Fluid	Water
Pipe material	Copper
Inner radius (m)	0.00794
Outer radius (m)	0.01794
Pipe length (m)	0.5
Decay heat (kW/m^3)	500
Ambient temperature (°C)	20



Fig.5. Schematics of freezing pipe simulation

The results of this simulation are shown in Fig. 6. As the outside temperature rapidly decreases, freezing occurs, leading to a decrease in the liquid salt radius and an increase in the solidified layer radius. Eventually, the freezing results in complete blockage of the pipe. These results indicate that the developed freezing model effectively simulates the freezing phenomenon, capturing the key behaviors expected in such scenarios.



Fig. 6. Result of sudden freezing simulation

The second simulation examines the effect of decay heat during static freezing. In this scenario, the boundary condition temperature drops to -5°C, and no flow source is provided. This scenario simulates the conditions that might occur during a pump stop. The results with and without decay heat are compared.

As shown in Fig. 7, the presence of decay heat slows down the freezing process. At 80 seconds, the case without decay heat shows complete freezing of the pipe, whereas the case with decay heat does not reach full freezing. These results suggest that incorporating decay heat into the model provides a more accurate representation of the freezing process, especially in transient analyses where internal heat generation plays an important role. By accounting for decay heat, the model can offer improved predictions of system behavior.



Fig. 7. Result of static freezing simulation

4. Conclusions

A 1-D freezing model has been analytically developed and implemented in Modelica by modifying the TRANSFORM library. The simple simulations conducted successfully demonstrated the expected behaviors of the model. Validation of the model is currently underway, and once successfully validated, this model will be utilized for the safety analysis of molten salt reactors using the Modelica/TRANSFORM framework.

Acknowledgement

This work was supported by Korea Research Institute for defense Technology planning and advancement (KRIT) grant funded by the Korea government (DAPA(Defense Acquisition Program Administration)) (KRIT-CT-22-017, Next Generation Multi-Purpose High Power Generation Technology (Liquid Fueled Heat Supply Module Design Technology), 2022).

Also, this research was supported by a grant from the Endowment Project of "Study on Concept Design of Small Modular Reactor(SMR) powered Ships and Offshore Platforms(2520000281)" funded by the Korea Research Institute of Ships and Ocean Engineering.

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