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Numerical Analyses of a single-phase natural convection system for Molten Flibe using MARS-FLIBE code

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1. Introduction

The molten salt reactor (MSR) has been researched and developed extensively at Oak Ridge National Laboratory (ORNL) in the projects of the aircraft reactor experiment (ARE) and the molten salt reactor experiment (MSRE) from 1940s to 1960s [1,2]. These two projects establish the basic technologies for MSR, and demonstrate its main advances, including good neutron economy, inherent safety and on-line refueling, processing and fission product removal. These advantages make the MSR attractive and to be one of the six candidates for the Generation IV Reactor. Therefore, the researches related to the MSR are being conducted. To analyze the molten salt-cooled systems in the laboratory, this study generated the properties of molten salt using MARS-LMR. In this research, the implemented salts were Flibe (LiF-BeF_2) in a molar mixture that is 66% LiF and 34% BeF_2, respectively. Table 1 indicates the comparison of thermal properties of various coolants in nuclear power plants.

2. Generation of Flibe properties into MARS-LMR

Table I: Problem Description

Properties	Water (298K)	Gallium (305K)	Flibe (750K)	Hg (300K)
Melting temperature [K]	273.15	303.15	731.15	234.32
Boiling temperature [K]	373.15	2477	1431	629.88
Density [kg/m^3]	997.08	6090	2050	13529
Specific heat [J/kg·K]	4181	382	2386	139.3
Dynamic viscosity [kg/m·s]	0.001	0.00186	0.01733	0.00152
Thermal conductivity [W/m·K]	0.58	30	1.1	8.54
Prandtl number	7	0.0237	38	0.0248

The implementation of a Flibe is generally performed using a detailed equation of state to generate fluid properties [3]. MARS-LMR code for liquid metals uses the soft-sphere model based on Monte Carlo calculations for particles interacting with pair potentials [4]. Although MARS was originally intended for a safety analysis of light water reactor, Flibe properties were newly added to this code as so-called MARS-FLIBE, which is applicable for Flibe-cooled systems. To generate the Flibe property table by computer programs, it needs parameters of Helmholtz free energy equation and transport properties such as surface tension, thermal conductivity, and dynamic viscosity equation for Flibe as following [3,4].

$$A = NKT\left[-\ln\frac{Ve}{N\lambda^3} + C_n\rho^{n/3}\left(\frac{\varepsilon}{KT}\right) + \frac{1}{2}(n+4)Q\rho^{n/9}\left(\frac{\varepsilon}{KT}\right)^{1/3} - \rho^m\left(\frac{\varepsilon}{KT}\right)\right] + E_{coh} \quad (1)$$

$$\sigma_1 = 1.2\times10^{-4}\left(T-273.15\right)+0.26 \quad (2)$$

$$\mu = 1.16\times10^{-4}e^{3755/T} \quad (3)$$

$$k = 1.1 \quad (4)$$

where ρ is the normalized density, $N\sigma_2^{\,3}/\sqrt{2V}$.

To solve eq. (1), it needs parameters such as n, m, Q, C_n, ε, σ_2, for Flibe and ε, σ_2 could be gained by solving the pressure and energy equation like eq. (5) and (6).

$$P = -\left(\frac{\partial A}{\partial V}\right)_{N,T} \quad (5)$$

$$E = A - T\left(\frac{\partial A}{\partial T}\right)_{N,V} \quad (6)$$

Other parameters were obtained from the paper of Chen et al. [5] developing an equation of state for Flibe based on a soft-sphere model. By using these equations, the data of thermodynamic properties can get like specific volume, internal energy, thermal expansion, isothermal compressibility, specific heat, and entropy for each combination of temperature and pressure. Fig. 1-6 show the comparisons of generated thermodynamic table data with existing correlations for Flibe and most of them show good agreements and the discrepancies will be modified.

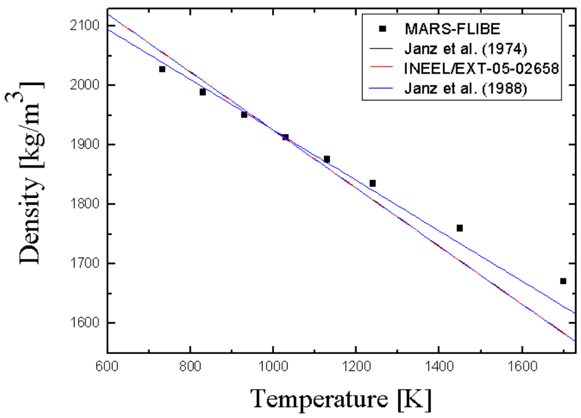

Fig. 1. Density comparison of generated thermodynamic table data with Janz et al. and INEEL/EXT-05-02658.

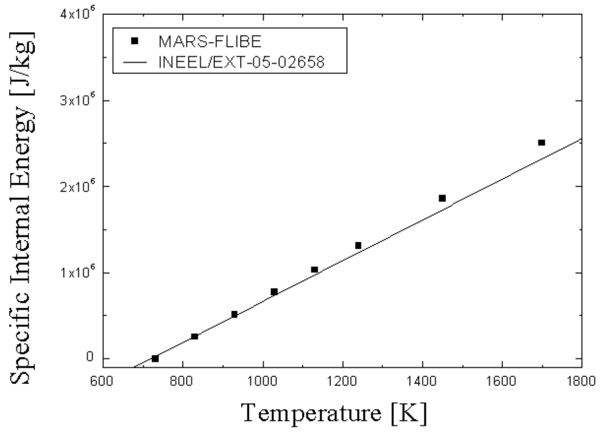

Fig. 2. Specific internal energy comparison of generated thermodynamic table data with INEEL/EXT-05-02658.

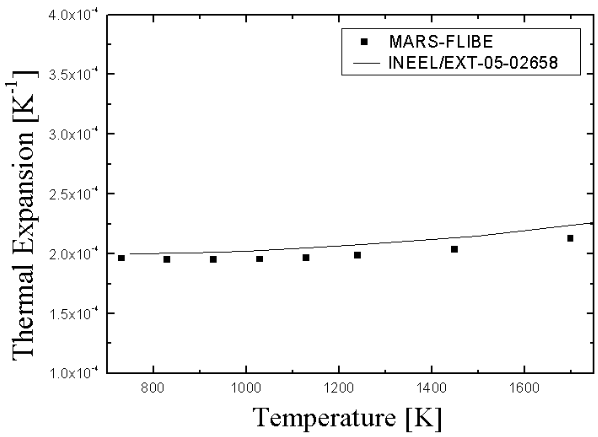

Fig. 3. Thermal expansion comparison of generated thermo-dynamic table data with INEEL/EXT-05-02658.

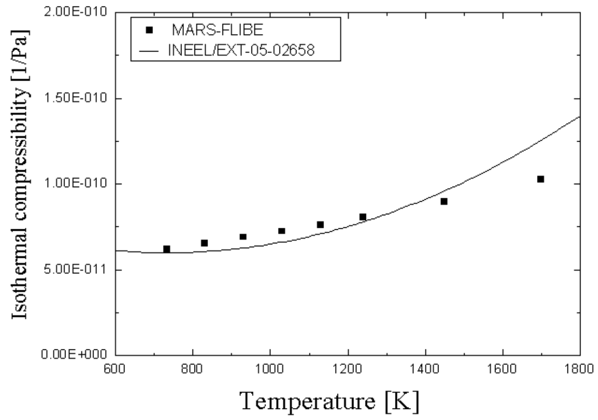

Fig. 4. Isothermal compressibility comparison of generated thermodynamic table data with INEEL/EXT-05-02658.

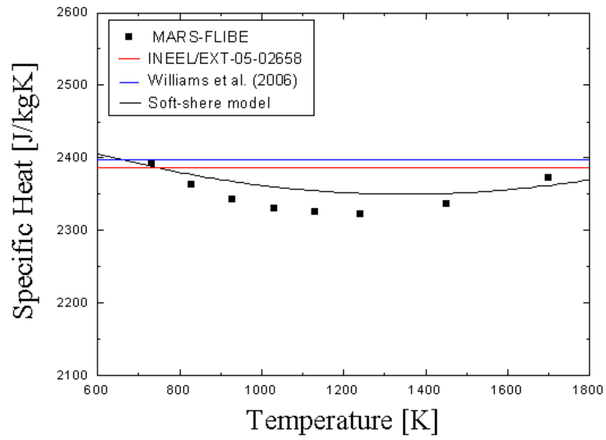

Fig. 5. Specific heat comparison of generated thermodynamic table data with INEEL/EXT-05-02658.

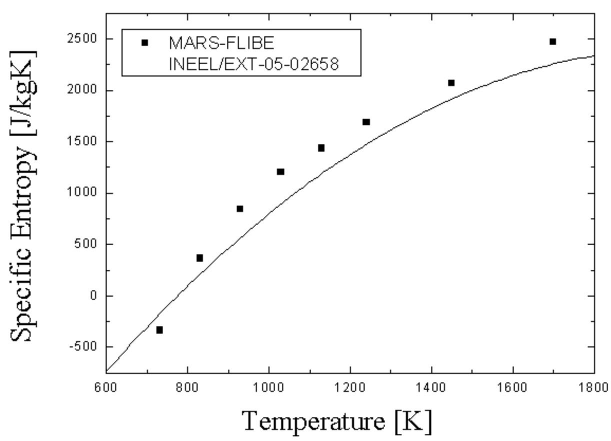

Fig. 6. Specific entropy comparison of generated thermo-dynamic table data with INEEL/EXT-05-02658.

3. Numerical analyses of molten salt-cooled systems using MARS-FLIBE

By using this thermodynamic property table file, the thermal hydraulic systems of Flibe can be simulated for numerical and parametric studies. In this study, the natural convection phenomena of Flibe were considered.

3.1 Numerical analysis of natural convection loop for Flibe

Fig. 7 indicates the nodalization of the natural convection loop. Under natural convection conditions, the Flibe operates without a pump and the flow is driven entirely by the buoyancy generated power. Fig. 8 and 9 indicate the temperature and the natural convection mass flowrate of Flibe. The maximum temperature and the mass flowrate of Flibe are about 1050K and 0.005kg/s, respectively. The initial conditions of this simulation are as shown in table II. The heat transfer coefficients of Flibe in natural convection loop can be calculated by adding the related heat transfer correlations in the MARS-FLIBE code.

Table II: The initial conditions (1)

Parameters	Value
Initial temperature [K]	815.15
Power [kW]	2.4
Height / Length / Diameter [m]	1.3 / 0.76 / 0.0127
Material	Stainless steel

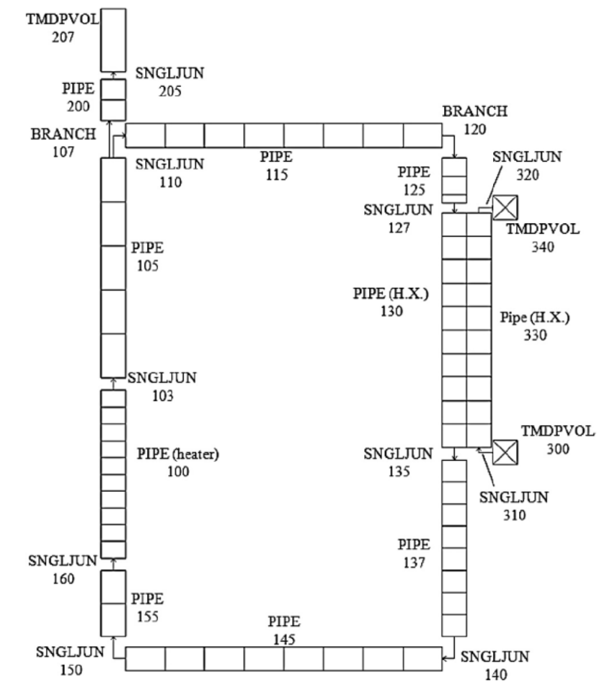

Fig. 7. Nodalization of the natural convection loop adopted for MARS-FLIBE

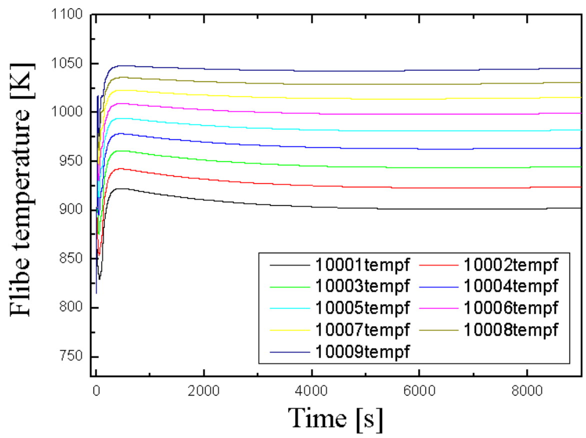

Fig. 8. Temperature distribution of Flibe in heater (component 100)

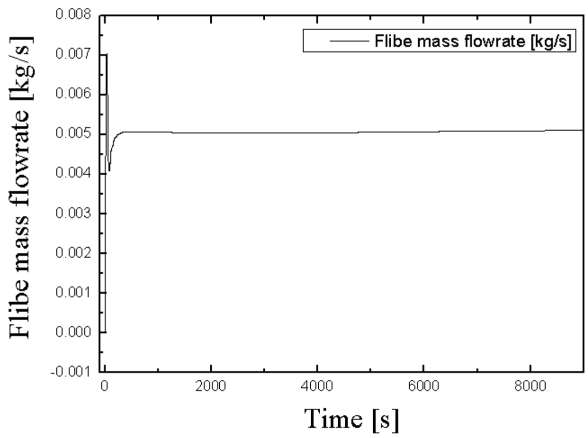

Fig. 9. Natural convection mass flowrate of Flibe

3.2 Numerical analysis of In-Vessel Retention for APR 1400 under Flibe-based External Reactor Vessel Cooling (IVR-ERVC).

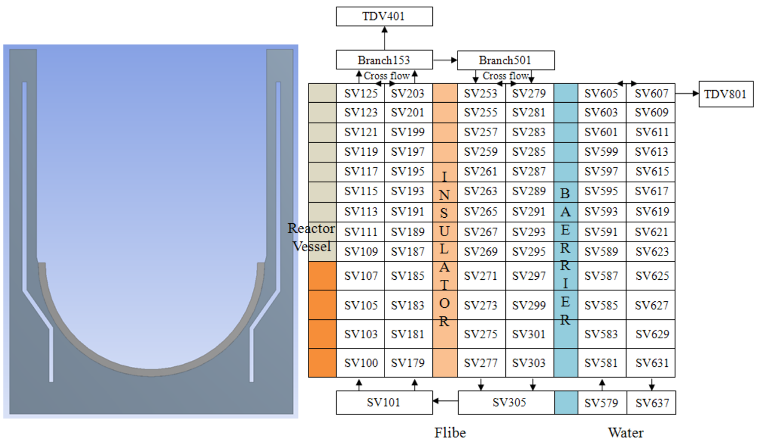

Fig. 10. Nodalization of the Flibe based IVR-ERVC

For the investigation on the effect of Flibe for IVR-ERVC, numerical simulation for severe accident in APR 1400 using MARS-FLIBE was performed. Fig. 8 shows the nodalization of the Flibe based IVR-ERVC

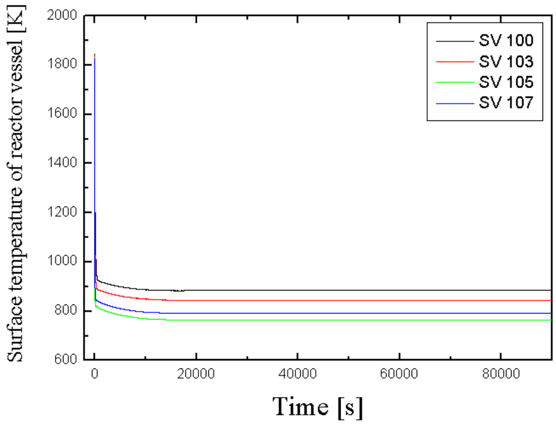

Fig. 11. Wall temperature distribution of reactor vessel

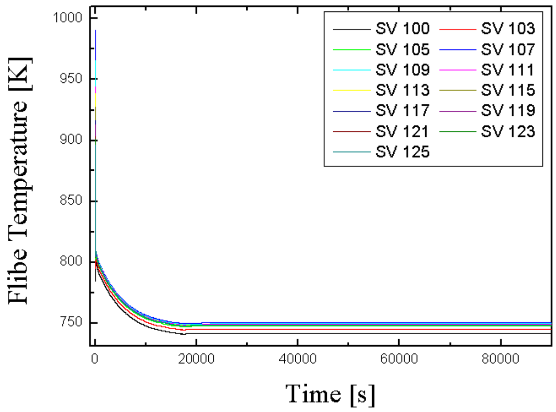

Fig. 12. Temperature distribution of Flibe

and ultimate heat sink is H_2O. The initial conditions of this simulation are as shown in table III. Fig. 11 and 12 show the temperature distribution of outer vessel wall and Flibe, respectively. The analysis was focused to examine the range of temperature for outer reactor vessel wall and Flibe. Unfortunately, the result related to Flibe based IVR-ERVC isn't positive. As shown in Fig. 11 and 12, the maximum temperatures of outer vessel wall and Flibe at steady state condition are 900K and 760K respectively. Although the maximum temperature of Flibe is below the boiling point of Flibe, the maximum temperature of outer reactor vessel is too high.

Table III: The initial conditions (2)

Parameters	Value
Height [m]	7.4
Radius of reactor vessel [m]	2.574
Thickness of reactor vessel [m]	0.165
Thickness of insulator [m]	0.114
Thickness of barrier [m]	0.1
Material of barrier	Stainless steel
Initial decay power [MW]	100
Initial temperature of Flibe [K]	805.15

4. Conclusions

Molten salt was added to the MARS-LMR code to support the analysis of Flibe-cooled systems. The molten salt includes LiF-BeF_2 in a molar mixture that is 66% LiF and 34% BeF_2, respectively. MARS-LMR code for liquid metals uses the soft sphere model based on Monte Carlo calculations for particles interacting with pair potentials. Although MARS was originally intended for a safety analysis of light water reactor, Flibe properties were newly added to this code as so-called MARS-FLIBE which is applicable for Flibe-cooled systems. Using transport equations and Helmholtz free energy equation, the thermodynamic property file of Flibe was generated. By using this thermodynamic property table file, the thermal hydraulic systems of Flibe can be simulated for numerical and parametric studies. In this study, the natural convection phenomena in the rectangular natural convection loop and IVR-ERVC in APR 1400 were simulated. Through the simulations in Flibe-cooled systems, the temperature distribution and mass flowrate of Flibe can be calculated and the heat transfer coefficients of Flibe in natural convection loop will be calculated by adding the related heat transfer correlations in the MARS-FLIBE code. MARS-FLIBE code will be used to predict and design of Flibe-cooled systems.

Nomenclature

C_n	fcc Madelung constant
Cp	specific heat [J/kg·K]
E_{coh}	cohesive energy [J/kg]
g	gravity [m/s^2]
H	height [m]
K	Boltzman constant [J/K]
k	thermal conductivity [W/m·K]
N	atomic weight [kg/mol]
n	constant
R	flow resistance parameter
Q	multiplier
q	total heat [W]
T	temperature [K]
V	specific volume [m^3/kg]

Greek symbols

ρ	density [kg/m^3]
μ	viscosity [kg/m·s]
λ	de Broglie wavelength [m]
ε	parameter [J/atom]
σ_1	surface tension [N/m]
σ_2	parameter [m^3/atom]
β	thermal expansion [K^{-1}]

REFERENCES

[1] E.S. Betties, R.W. Schroeder, G.A. Cristy, H.W. Savage, R.G. Affel, L.F. Hemphill, "The aircraft reactor experiment-design and construction", Nuclear Science and Engineering, vol. 2, p. 804-825, 1957.

[2] M.W. Rosenthal, P.R. Kasten, R.B. Briggs, "Molten-salt reactors-histroy, states, and potential", Nuclear Application & Technology, vol. 8, p. 107-117, 1970.

[3] C.B. Davis, "Implementation of Molten Salt Properties into RELAP5-3D/ATHENA", Idaho National Engineering and Environmental Laboratory Bechtel BWXT Idaho, LLC, 2005.

[4] D.A. Young, "A soft-sphere model for liquid metals", University of California, Livermore, California, 1977.

[5] X.M. Chen, P.F. Peterson, V.E. Schrock, "The equation of state of liquid Flibe", University of California, Berkeley, 1991.