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Liquid Metal Properties Using a Soft-Sphere Model

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1. Introduction

In recent years, the demands of new technologies for generation IV reactors (e.g., Liquid Metal Fast Breeder Reactor, High Temperature Gas Reactor) led to a great increase in research into properties of coolants over wide range. The predictive calculations relevant to the reactors will be performed using the Multi-dimensional Analysis for Reactor Safety (MARS) code in our country.

In this paper, we developed the properties that were used in MARS code by Young's Equation-of-State (EOS) model for the liquid metals (Sodium, and Lead-Bismuth Eutectic) which developed in 1977.

2. Equation of State Model

In 1977, Dave Young developed a semi-empirical Soft-sphere model for EOS and applied to the various Liquid metals [1]. The method made it possible to measure the thermodynamic characteristics of liquid metals along isobars up to 400 MPa and 7000 K.

The model basically uses the soft sphere model of Hoover [2] which is based on Monte Carlo calculations for particles interacting with pair potentials of the forms :

$$\phi(r) = \varepsilon\left(\frac{\sigma}{r}\right)^n, \qquad 4 \le n \le 12 \tag{1}$$

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

Eq. (2) represents the Helmholz free energy and in the brackets, the first term describes the kinetic energy, the second term is the static lattice potential energy, the third term is the thermal lattice potential correction, and the fourth term is the attractive potential energy. The last term of Eq. (2) means the molecular cohesive energy. λ is the deBroglie wavelength, ($h/\sqrt{2\pi mkT}$) and ρ is the normalized density, ($N\sigma^3/\sqrt{2}V$). Q is s multiplier to account for electronic effects on the heat capacity and Cn is the fcc Madelung constant.

Using the Eq. (2), the entropy, pressure, and internal energy may be found from Eqns. (3) ~ (5).

$$S = -\left(\frac{\partial A}{\partial T}\right)_{N,V} = \frac{E-A}{T} \tag{3}$$

$$P = -\left(\frac{\partial A}{\partial V}\right)_{N,T} = \frac{NkT}{V}\left[1 + \frac{1}{3}C_n\rho^{n/3}\left(\frac{\varepsilon}{kT}\right) + \frac{1}{18}n(n+4)Q\rho^{n/9}\left(\frac{\varepsilon}{kT}\right)^{1/3} - \rho^m\left(\frac{\varepsilon}{kT}\right)\right] \tag{4}$$

$$E = A - T\left(\frac{\partial A}{\partial T}\right)_{N,V} = NkT\left[\frac{3}{2} + C_n\rho^{n/3}\left(\frac{\varepsilon}{kT}\right) + \frac{1}{6}(n+4)Q\rho^{n/9}\left(\frac{\varepsilon}{kT}\right)^{1/3} - \rho^m\left(\frac{\varepsilon}{kT}\right)\right] + E_{coh} \tag{5}$$

The parameters σ, ε, n, m, Q would be adjusted according to the liquid metal. Above three correlations are fitted to the data of enthalpy, specific volume, and etc. from the experiments. Cohesive energy and Madelung Constant are specific values different to the liquid metals. The soft-sphere calculation first used chosen values of n, m, and Q and computes σ and ε by iteration scheme that solves the equations $P(V_m, T_m) = 0$ and $E(V_m, T_m) = H_m$. Here subscript 'm' means melting and H_m is the enthalpy at melt. Table 1 shows the experimental data used to produce the properties of 2 liquid metals.

Table 1. Experimental data for 2 liquid metals.

Metal	Atomic Weight (kg/mol)	Cohesive Energy (J/kg)	Melting Temp. (K)	Enthalpy at melt (J/kg)	Density at melt (kg/m^3)
Sodium	0.02299	4.659x10^6	371.0	2.067x10^5	927.0
LBE	0.208	7.11x10^5	397.7	7.627x10^4	10569.6

3. Sodium Properties

The soft-sphere fit to sodium data is shown in Figs. 1 and 2. The data were obtained from Golden et al.[3] As seen in the figures, the soft-sphere fit is adequate and the parameters used in soft sphere model are as follows :

$\sigma = 2.159746$ x 10^{-10} (m), $\varepsilon = 6.21332$ x 10^{-19} (J/atom)
$C_n = 6.3755$, $n=8$
$m=0.58$, $Q=0.95$

Eqns. (3) ~ (5) using above parameters and saturation equation, Eq. (6), are used to produce the sodium property table of MARS code. The applicable range of temperature is 371 to 2100 K and for the pressure is 10^{-5} to 11.2 MPa.

$$\ln P_s = 24.85 - \frac{12535.46}{T_s} - 0.35\cdot\ln(T_s) \tag{6}$$

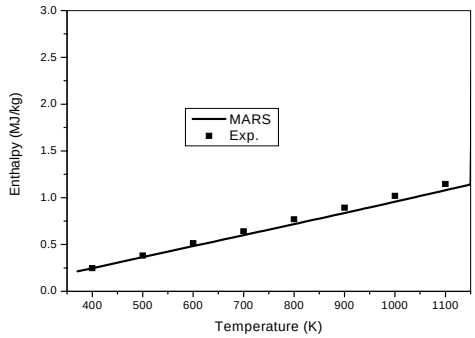

Fig. 1. Temperature vs. Enthalpy for sodium

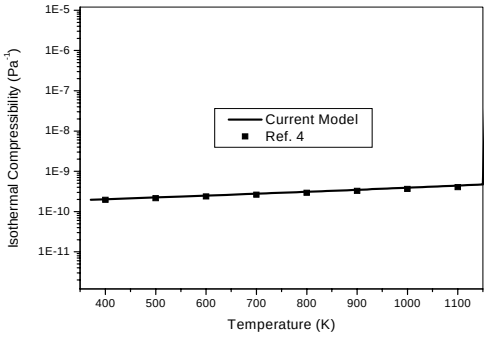

Fig. 2. Temperature vs. Compressibility for sodium

4. Lead Bismuth Eutectic (LBE) Properties

The soft-sphere fit to LBE data is shown in Figs. 3 and 4. The data were obtained from Benatomi et al.[4] The parameters used in soft sphere model are as follows :

$\sigma = 2.22822$ x 10^{-10} (m), $\varepsilon = 3.45799$ x 10^{-18} (J/atom)
$C_n = 5.9967$, $n=10.2$
$m=0.76$, $Q=1.5$

Currently, Madelung constant and other parameters for LBE are not known, thus, the Madeling constant of LBE was estimated from the Lead Data and cohesive energy and melting enthalpy at the table 1 were obtained from the fitting of experimental data.

$$\ln P_s = 35.77 + 2.80\times10^{-4}\cdot T_s - \frac{24053}{T_s} - 1.64\cdot\ln(T_s) \quad (7)$$

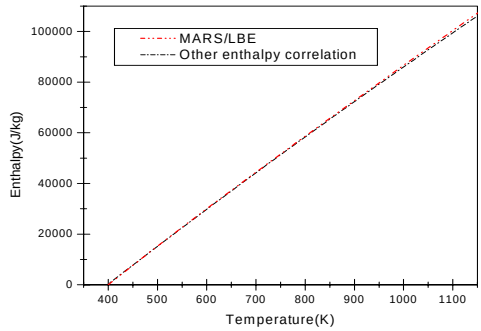

Fig. 3. Temperature vs. Enthalpy for LBE

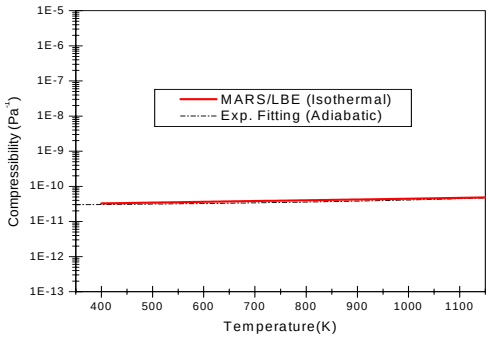

Fig. 4. Temperature vs. Compressibility for LBE

The range of the data of temperature is 400 ~ 3000 K and the pressure range is 10^{-10} ~ 9.0 MPa.

4. Conclusion

The thermodynamic property tables using soft sphere model for liquid metals of sodium and LBE were produced to apply the MARS program to Gen IV reactors. The produced data are well agreed with the other experimental data. The tables will be used in an analysis of sodium cooled fast reactor or LBE cooled accelerator driven systems.

ACKNOWLEDGMENTS

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