Modeling of LiF-NaF-KF ternary fluoride salt for calculation of Density, Viscosity and Thermal Conductivity

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Introduction

- LiF-NaF-KF salt is used in molten salt reactor
- Molten salts are used for thermal energy storage and transfer applications
- Accurate determination of thermo physical property data of molten salt is required to understand heat transfer characteristics.
- Experimentation is complex due to material interaction at high temperature
- Modeling of data can be done to predict the thermophysical properties
- Geometric model is most used to calculate density and viscosity when binary data is well known but ternary properties of system is not available
- Unit cell model is used to calculate thermal conductivity

Objectives

•To study Density, Viscosity and thermal conductivity properties.
•To develop computerized model which can be evaluated in excel.
•To compare this model with experimental data.

Methodology

•To study Density, Viscosity and thermal conductivity properties.
•To study equations required for GSM and Unit cell
•To develop computerized model which can be evaluated in excel.
•To compare this model with experimental data.

General Solution Model

•The properties of a ternary system can be expressed as a combination of the properties of all binary systems with an assigned probability weight
•Absolute property of ternary mixture

$$Y = Y^E + \sum_{i=1}^{m} xi \times Yi$$

- Excess property, Y^E

$$Y^E = \sum_{i,j=1}^{m} W_{ij} \times Y_{ij}^E$$

- W_{ij} is the weight probability of the binary system property

$$W_{ij} = \frac{xi * xj}{xi(ij) * xi(ij)}$$

- Where, x_i, x_j and x_k are the ternary mole fractions for the system 'i-j-k' while $X_{i(ij)}$ and $X_{j(ij)}$ are the mole fractions of the components 'i' and 'j' in the sub-binary system 'i-j', which are given by:

$$X_{i(ij)} = x_i + \sum_{k=1; k\neq i,j}^{m} x_k \xi^k_{i(ij)}$$

- $\xi^k_{i(ij)}$ is the similarity coefficient of component 'k' to component 'i' and 'j'

$$\xi^k_{i(ij)} = \frac{n(ij,ik)}{n(ij,ik)+n(ji,jk)}$$

- n (ij, ik) is a function called the sum of deviation of squares,

$$n(ij,ik) = \int_0^1 (Y_{ij}^E - Y_{ik}^E)^2 dX_i$$

- Excess properties can be calculated using following equation

$$Y_{ij}^E = (\sum_{i=1}^{m} xi \times Yi) - Y_{ij}$$

Unit Cell Model

•It is assumed that the mixing of ternary salts is complete and it behaves like a uniform phase.
•The component having the largest mass fraction is assumed to be the continuous phase, where the other two components are dispersed uniformly so as to appear as shown in Fig.
• In the current context of ternary salt mixtures (A–B–C), component A is considered as the continuous phase while B and C components are the dispersed phases if *XA*>*XB*>*XC*, where *X* is the mass fraction of the components.

•Thermal Conductivity $\lambda_e = X + Y + Z$
•Where,

$$X = \lambda_A \left(1 - \left(\frac{b}{a}\right)^2\right)$$

$$Y = \frac{\left(\left(\frac{b}{a}\right)^2 - \left(\frac{c}{a}\right)^2\right)\lambda_A\lambda_B}{\left(2\lambda_B - \frac{b}{a}(\lambda_A - \lambda_B)\right)}$$

$$Z = \frac{2\left(\frac{c}{a}\right)^2 \lambda_A\lambda_B\lambda_C}{\left(2\lambda_B\lambda_C - \frac{b}{a}(\lambda_A\lambda_C - \lambda_B\lambda_C) + \frac{c}{a}(\lambda_A\lambda_B - \lambda_B\lambda_C)\right)}$$

•It can be observed that the thermal conductivity is influenced by the densities and thermal conductivities of the individual components.

Results

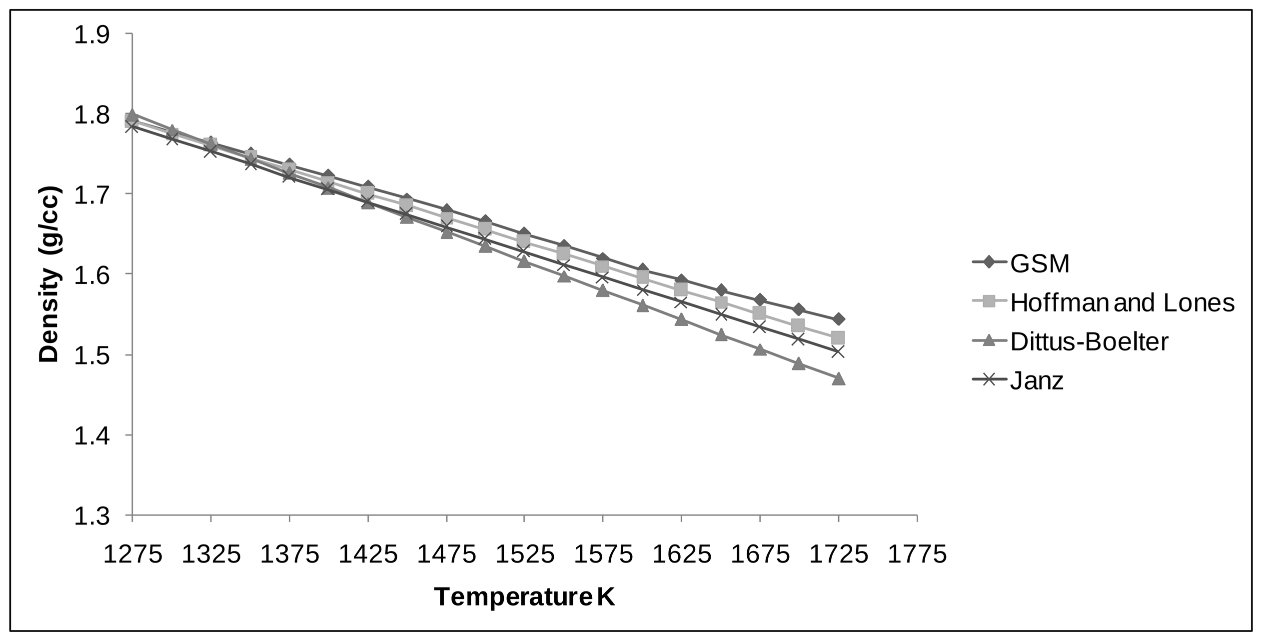

Figure. 1 Comparison of GSM with calculated density of FLiNaK with literature data.

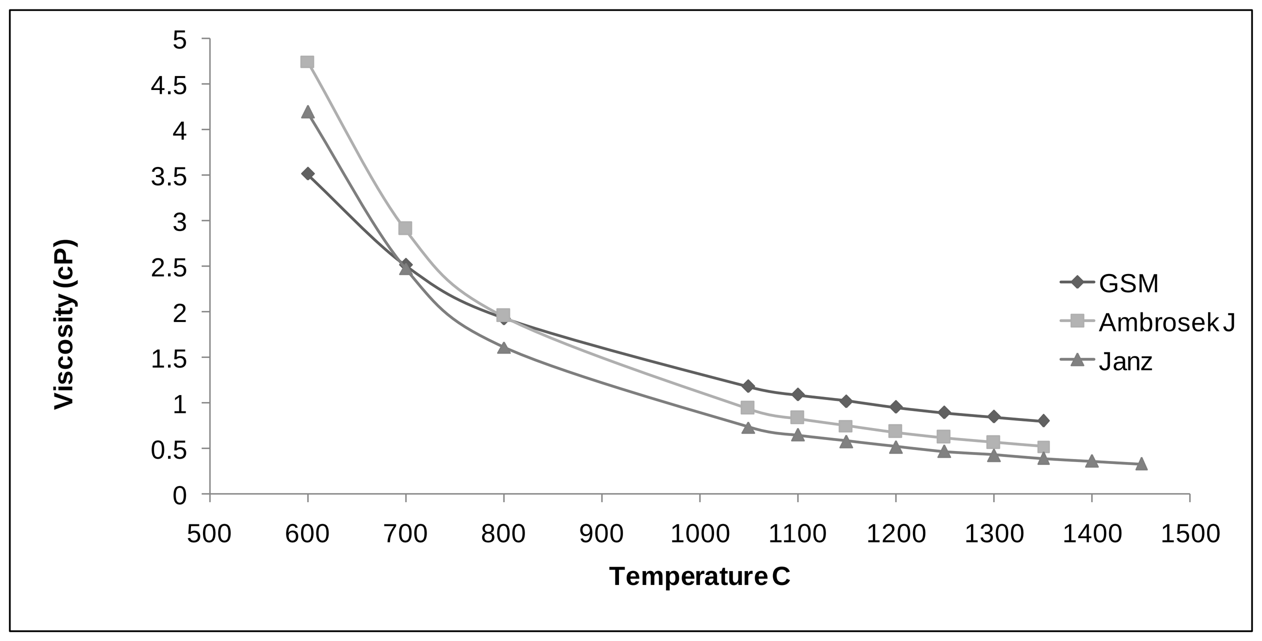

Figure. 2 Comparison of GSM with calculated viscosity of FLiNaK with literature data.

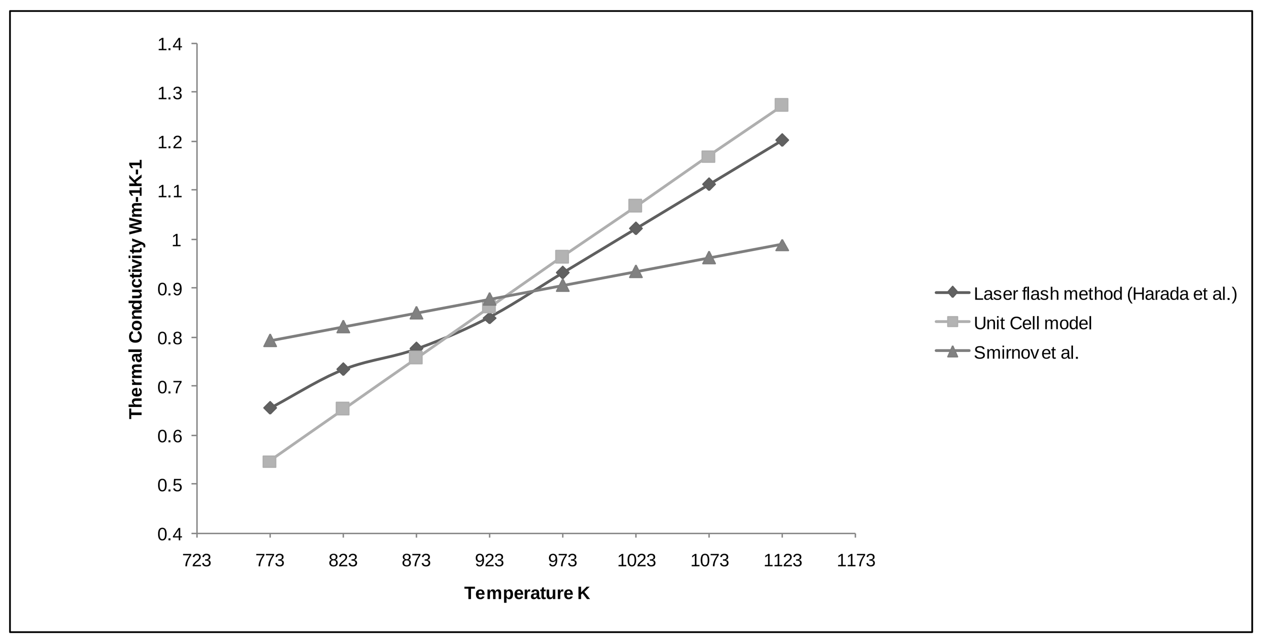

Figure. 3 Comparison of unit cell model for thermal conductivity with literature data.

Conclusions

• Maximum deviation in density was only 0.0735 g/cc which is only 4.76 %. This shows that GSM model is suitable to predict density.
• The high error in viscosity calculation could be due to the result of the compounding of errors in the measurement of unary and binary components that were used to calculate the ternary viscosity of the two salt systems.
• The model presented in this paper breaks the boundary between symmetric and asymmetric models and simplifies various kinds of models to one.
• This new model doesn't require any human interference in selecting models and arranging the three components to apexes of composition triangle.
• Unit cell model can be used to predict high temperature thermal conductivity

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