Progress in Nuclear Energy 70 (2014) 119–127

Contents lists available at ScienceDirect

Progress in Nuclear Energy

journal homepage: www.elsevier.com/locate/pnucene

Review

The thermophysical properties of binary mixtures of molten alkali fluoride salts. Part II: Correlations for the transport properties in reduced form

Cory Griffard [a, *], Steven G. Penoncello [a, b, 1], John C. Crepeau [a, c, 2]

[a] Center for Applied Thermodynamic Studies, University of Idaho, Moscow, ID 83844-0902, USA
[b] Mechanical Engineering Department, University of Idaho, Gauss-Johnson 234D, Moscow, ID 83844-0902, USA
[c] Mechanical Engineering Department, University of Idaho, Engineering Physics Building 324I, Moscow, ID 83844-0902, USA

ARTICLE INFO

Article history:
Received 25 March 2013
Received in revised form
25 August 2013
Accepted 26 August 2013

Keywords:
Molten salts
Transport properties
Fluoride mixtures

ABSTRACT

Correlations for predicting the transport properties of molten salts and their binary mixtures are presented as functions of temperature. The molten salt mixtures considered contained lithium fluoride (LiF), sodium fluoride (NaF), and potassium fluoride (KF). The properties and temperature were reduced using potential parameters. Mixing rules were used to determine these parameters for the mixtures. Certain parameters for the correlations were determined for each property by non-linear regression between experimental data and values calculated from the correlations. The correlations are valid in the liquid phase for temperatures ranging from 765 K to about 1280 K, depending on the salt. Comparison of the experimental data to values calculated from the correlations indicates that viscosities can be calculated to within ±3%, surface tensions within ±2%, and thermal conductivities within ±3%.

1. Introduction

Molten fluoride salts have been considered for use as coolants in Molten Salt Reactors (MSR) due to their good heat transfer properties, low vapor pressures, and low reactivity with air and water. One of the most common salts used as a coolant for MSRs is a ternary mixture of the alkali fluoride salts LiF, NaF, and KF (Sohal et al., 2010). To design nuclear energy systems that use this molten salt, certain thermophysical properties of the salt must be known. This work focuses on the binary mixtures LiF–NaF, LiF–KF, and NaF–KF because the thermophysical properties of a ternary mixture can be better predicted if the properties of all three of its binary mixtures are well known.

The thermodynamic properties of the alkali fluoride binary mixtures were analyzed in Part I of this series using the Soft-Sphere Equation of State. The transport properties were analyzed separately from the thermodynamic properties, since they cannot be derived from an equation of state. The transport properties that are commonly used for heat transfer analyses in nuclear reactors are the viscosity μ, the surface tension σ, and the thermal conductivity k.

A corresponding states law by Tada et al. (1988) was used to predict the transport properties for a variety of alkali halides, in reduced form. This corresponding states law was then applied to binary mixtures of these salts using methods developed by Tada et al. (1990b). However, it is not clear how accurate this model was when applied to the viscosity of the fluoride mixtures. Furthermore, Tada et al. (1990a) clearly stated that the corresponding states model for the surface tension did not work well for the fluoride salts in particular. A corresponding states model was not developed for the thermal conductivity of any of the salts. Therefore, different models were developed in this paper for predicting the transport properties of the alkali fluoride binary mixtures, by regression to experimental data of these properties. Because the properties were not measured at different pressures, and the salts are considered incompressible, these models only take into account temperature dependence.

2. Reducing parameters and related terms for the transport properties

Even though models different from that of Tada et al. (1988, 1990a,b) were developed, the same methods were used to reduce the transport properties and temperature in nondimensional form.

* Corresponding author. 8186 Westview Dr., Coeur d'Alene, ID 83815, USA. Tel.: +1 (208) 661 3141.
E-mail addresses: cgriffard@vandals.uidaho.edu (C. Griffard), stevep@uidaho.edu (S.G. Penoncello), crepeau@uidaho.edu (J.C. Crepeau).
[1] Tel.: +1 (208) 885 9048.
[2] Tel.: +1 (208) 885 5228.

0149-1970/$ – see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.pnucene.2013.08.009

Nomenclature

AAD	absolute average deviation
A	coefficient in Arrhenius relation
BIP	binary interaction parameter
d	minimum separation distance between unlike ions
e_c	electron charge
E	activation energy
F	coefficient used in transport property correlations, extended to mixtures
G	coefficient used in transport property correlations, extended to mixtures
H	coefficient used in transport property correlations, extended to mixtures
k	thermal conductivity
$\tilde{k}$	reduced thermal conductivity
k_B	Boltzmann's constant
$\tilde{K}$	reduced transport property
KF	potassium fluoride
LiF	lithium fluoride
m_a	mass of salt anion
m_c	mass of salt cation
m_s	characteristic mass
MSR	molten salt reactor
NaF	sodium fluoride
R	universal gas constant
SSR	sum of the square residuals
T	absolute temperature
$\tilde{T}$	reduced absolute temperature
x_2	molar fraction of second fluid in binary mixture
Y	coefficient used in transport property correlation
Z	coefficient used in transport property correlation
%DEV	percent deviation

Greek symbols

δ_{12}	binary interaction parameter
ζ	parameter used as a modifying factor
Λ	parameter used to reduce transport properties
μ	viscosity
$\tilde{\mu}$	reduced viscosity
ξ	parameter that incorporates effects of long-range potential
ρ	potential parameter of repulsion
σ	surface tension
$\tilde{\sigma}$	reduced surface tension
ψ	potential parameter of repulsion
ω_ξ	perturbation term dependent on ξ
ω_ρ	perturbation term dependent on ρ

Subscripts

cal	calculated from SSEOS
exp	determined from experiments
i	specific to data point i
k	specific to thermal conductivity
$\tilde{K}$	specific to thermodynamic property $\tilde{K}$
m	melting point
μ	specific to viscosity
σ	specific to surface tension

Tada et al. (1988) used several reducing parameters to non-dimensionalize these properties for the molten salts. Two of these parameters are potential parameters of repulsion unique to each salt, and are defined as ρ, in units of distance, and ψ, in units of energy. Values for both parameters were determined by Tosi and Fumi (1964a,b) for a variety of alkali halide salts. Other salt-specific parameters are ξ and ζ, which were determined by Harada et al. (1983). ξ incorporates the effects of weak long-range potential and has units of J-m/C^2, where C is the unit of electric charge, the coulomb. The parameter ζ is unitless and is used as a modifying factor. Tada et al. (1988) also used a characteristic mass to reduce the transport properties. This mass is defined by

$$m_s = \left(\frac{2\sqrt{m_A m_C}}{\sqrt{m_A}+\sqrt{m_C}}\right)^2 \tag{1}$$

where m_A and m_C are the masses, in kg, of the anion and cation of the salt. Table 1 shows the values of these parameters for the alkali fluorides, as well as m_s.

Harada et al. (1983) used some of these parameters to define the minimum separation distance d between unlike ions with the following relation:

$$\frac{d}{\rho} = \zeta\left[0.4069 + 0.9075\ln\left(\frac{\psi}{k_B T}\right) + \left(6.042\cdot 10^{-7}\right)\frac{\psi}{k_B T}\right] \tag{2}$$

where k_B is Boltzmann's constant, 1.381 $\times$ 10^{-23} J/K. Using d, another parameter Λ is calculated:

$$\Lambda = \psi\exp\left(-\frac{d}{\rho}\right) \tag{3}$$

Values of d and Λ are used to reduce the transport properties.

With all of the appropriate parameters and characteristic mass m_s, the temperature T and the transport properties in their reduced form are defined by:

$$\tilde{T} = \frac{T k_B d}{\xi e_C^2}$$

$$\tilde{\mu} = \frac{\mu d^2}{\sqrt{\Lambda m_S}}$$

$$\tilde{\sigma} = \frac{\sigma d^3}{\xi e_C^2}$$

$$\tilde{k} = \frac{k d^2}{k_B\sqrt{\Lambda/m_S}} \tag{4}$$

where e_C is the elementary charge of an electron, 1.602 $\times$ 10^{-19} C. In Eq. (4), T has units of K, μ has units of kg/m-s, σ has units of N/m, and k has units of W/m-K.

Tada et al. (1990a) developed a number of mixing rules for the reducing parameters of the binary mixtures, making them dependent on the molar fraction x_2 of the additional component. The mixing rules for ψ, ξ, and ρ are expressed as

Table 1
Parameters used to reduce transport properties.

Salt	ψ ($\times 10^{-17}$ J)	ρ ($\times 10^{-11}$ m)	ξ ($\times 10^{-10}$ J m/C^2)	ζ	m_s ($\times 10^{-26}$ kg)
LiF	2.67	2.99	8.27	0.970	1.791
NaF	4.17	3.30	8.67	0.929	3.462
KF	8.39	3.38	8.93	0.931	4.381