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A corresponding-states approach for the calculation of the transport properties of uni-univalent molten salts

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Abstract. The extended corresponding-states principle has been applied to pure molten alkali halides for the calculation of viscosity and thermal conductivity. The model uses temperature-dependent equivalent substance reducing ratios (ESRR) to insure conformality among the various molten salts, with sodium chloride as the reference salt. The ESRR were found along the saturation boundary from saturated liquid density and vapour pressure data of the salts of interest and of the reference salt. These ESRR were then used to calculate the thermal conductivity and viscosity for the salts of interest, in the liquid state. Calculations were also made with the simple two-parameter corresponding-states principle, with melting temperature and the corresponding density as scaling factors. Agreement between calculated and experimental data is within 10% for viscosity, and within experimental accuracy for thermal conductivity, for most of the salts studied.

1 Introduction

Molten salts, alkali halides, and their mixtures in particular, are of great interest in many high-temperature engineering applications, which justifies, as pointed out by many authors, the need for accurate thermophysical property data and models for these systems. Although considerable effort has been devoted to the problem of high-temperature experimental measurement of viscosity and thermal conductivity of pure molten alkali halides and their mixtures, experimental data are still very limited. With the complexity of these experimental measurements in mind, in addition to the great number of systems of interest in existence, it becomes especially important to develop models capable of predicting these properties given a minimum amount of information as input.

The corresponding-states principle is one of the most powerful tools in this respect and has already been applied to equilibrium (Reiss et al 1961; Owens 1966; Woodcock 1976; Harada et al 1983; Tada et al 1990, 1993, 1995) and transport (White and Davies 1967; Young and O'Connell 1971; Abe and Nagashima 1981; Tada et al 1988, 1993, 1995; Harada et al 1992; Nagasaka and Nagashima 1993) property prediction of pure molten salts and their mixtures.

Here, the application of the extended corresponding-states model to the viscosity and thermal conductivity of pure molten alkali halides is discussed. The extended corresponding-states theory was originally proposed by Leland and coworkers (Leach et al 1968; Leland and Chappellear 1968; Leland et al 1968; Fisher and Leland 1970) in the early 1970s and since then it has been applied to the prediction of equilibrium and transport properties of many different systems. The basic idea of the extended corresponding-states theory consists of assuming that the intermolecular potential parameters are functions of

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the temperature and density of the system, while the potential itself is conformal to the potential of some reference fluid. This temperature and density dependence is then introduced into the equivalent substance reducing ratios (ESRR) through the use of molecular shape factors. The accuracy of this approach lies in the accuracy of the shape factors, which are used in the definition of the equivalent substance state point, and in the accuracy of the data for the properties of the reference fluid, which will be used in the prediction of the same properties for the fluids of interest. In addition this approach eliminates the need for detailed knowledge of the intermolecular potential.

In this work, saturation liquid density and vapour pressure data were used for the reference salt, chosen to be sodium chloride, and for the salts of interest, thus determining ESRR which are temperature dependent only.⁽¹⁾ These ESRR along with viscosity and thermal conductivity corresponding-states relationships were then used to predict these properties for the salts under study. In addition viscosity and thermal conductivity have been calculated at 0.1 MPa by the simple two-parameter corresponding-states theory, through the use of the melting temperature and the corresponding density as reducing parameters. Despite not being a true corresponding-states point, the melting point has been used as an approximation of the triple point, with the assumption that the melting temperature and the corresponding density are similar to the corresponding triple point values, for the alkali halides. This approach is justified by the nonexistence of triple point data for most of these salts.

2 Model description

2.1 Simple two-parameter corresponding-states principle

The corresponding-states principle for simple spherical fluids was first introduced in an empirical form by van der Waals and later demonstrated by Pitzer (1939) through dimensional analysis of the configuration integral. The basic result is that if two pure fluids, j and \circ , are conformal (obey the same reduced intermolecular potential) then it becomes possible through the use of scaling arguments to show that:

$$A_j^r(T_j, \rho_j) = f_j A_\circ^r(T_\circ, \rho_\circ) = f_j A_\circ^r\left(\frac{T_j}{f_j}, \rho_j h_j\right) \quad (1)$$

In this equation, $A^r = A(T, \rho) - A^*(T, \rho)$, where A^r is the residual Helmholtz energy (the * indicates an ideal gas value), ρ is the molar density, T is the absolute temperature, and f_j and h_j are scale factors called ESRR. The subscripts j and \circ indicate a fluid of interest and a reference fluid, respectively. The scaling arguments used in the derivation of equation (1) permit the determination of a relationship between the temperature and molar density of the fluid of interest and the corresponding values for the reference fluid, namely $T_\circ = T_j/f_j$ and $\rho_\circ = \rho_j h_j$. The scale factors f_j and h_j are related, on a microscopic scale, to the ratios of the intermolecular potential parameters, and on a macroscopic scale, to the critical parameters of the two fluids, namely, $f_j = (\varepsilon_j/\varepsilon_\circ) = (T_j^c/T_\circ^c)$, and $h_j = (\sigma_j^3/\sigma_\circ^3) = (\rho_\circ^c/\rho_j^c)$. Here ε and σ are the intermolecular potential energy and distance parameters, respectively, and the superscript c denotes a critical point value. Alternatively, the triple point can be used as the corresponding-states point, thus making $f_j = (T_j^t/T_\circ^t)$ and $h_j = (\rho_\circ^t/\rho_j^t)$, where the superscript t denotes a triple point value.

Other thermodynamic property corresponding-states relationships between the reference fluid and any fluid of interest may be found through the use of statistical thermodynamics or classical thermodynamics relationships.

⁽¹⁾There are no data on the dependence of the transport properties of these salts on pressure. Data are compared at 0.1 MPa.

2.2 Extended corresponding-states principle

The simple two-parameter corresponding-states principle, the basic result of which was discussed above, is only obeyed by spherically symmetric molecules with conformal intermolecular potentials. In an attempt to extend the principle to other molecules, Leland and coworkers (Leach et al 1968; Leland and Chappellear 1968; Leland et al 1968; Fisher and Leland 1970) proposed the use of shape factors that are introduced in the ESRR and in principle are allowed to be functions of temperature and density. As discussed earlier, the use of shape factors results from the assumption that the intermolecular potential parameters are not constant but in fact may change with temperature and density, while the potential is itself conformal to the potential of some reference fluid.

In the extended corresponding-states principle the ESRR become: $f_j = [\varepsilon_j(T, \rho)/\varepsilon_0] = (T_j^c/T_0^c)\theta_j(T, \rho)$ and $h_j = [\sigma_j(T, \rho)^3/\sigma_0^3] = (\rho_0^c/\rho_j^c)\phi_j(T, \rho)$, where θ and ϕ are called shape factors. If the two fluids are conformal, θ and ϕ are both unity and the original ESRR developed for the simple corresponding-states principle are recovered. The assumption that the potential parameters are temperature-dependent results, originally, from angle-average calculations on nonspherical potentials (Leland and Chappellear 1968), and permitted to join in the same class, in terms of corresponding-states, polar fluids and simple nonpolar fluids. In the case of molten salts, the corresponding-states approach developed by Harada et al (1983), which uses an effective diameter determined by a perturbation method which is temperature and density dependent, suggests that this temperature and density dependence of the shape factors is also correct for molten alkali halides. The shape factor approach has the advantage of not having to use any potential parameters to scale the properties.

In the extended corresponding-states principle the basic thermodynamic relationship, equation (1), found for the simple corresponding-states principle remains the same. It is found, however, that due to the density and temperature dependence of the shape factors, other thermodynamic relationships between various properties become more complex, becoming dependent on the derivatives of the ESRR with respect to density and temperature.

2.3 ESRR calculation

Ideally, the shape factors θ and ϕ could be calculated 'exactly' for each molten salt of interest through the use of high accuracy equations of state for these salts and for the reference salt, by the use of any two thermodynamic property corresponding-states relationships between the two fluids in addition to the critical temperature and density for each salt. Unfortunately these critical data have not been measured yet, nor have the experimental pressure, volume, temperature (PVT) data for these systems permitted the development of these high accuracy equations of state. In fact, most of these salts decompose before the critical point is reached. Despite this limitation in terms of shape factor calculation, at least with any experimental critical data, the properties of the salt j can be calculated once the ESRR for that salt have been determined, given the knowledge of the same properties for the reference salt.

Most of the data that are available for molten alkali halides are for the saturation boundary, viz. vapour pressures and saturated liquid densities. In this work, vapour pressure and saturation liquid density fitted equations, available in the literature, have been used to calculate the ESRR. Because the saturation boundary only depends upon temperature, density-independent ESRR are found. The vapour pressure, p^s , and saturated liquid density, ρ^s , of any salt of interest are related to the reference salt properties through the following equations:

$$p_j^s(T_j) = \frac{p_0^s(T_j/f_j)f_j}{h_j}, \quad (2)$$

and

$$\rho_j^s(T_j) = \frac{\rho_o^s(T_j/f_j)}{h_j} . \quad (3)$$

Simultaneous solution of equations (2) and (3) provides the ESRR along the saturation boundary.

The liquid-density fitted equations used in the calculation of the ESRR were taken from the NIST database (Janz 1992) for all the molten alkali halides, with the exception of sodium chloride, the density equation of which is available in the DIPPR database (Design Institute for Physical Property Data 1982 and onwards). The vapour-pressure fitted equations were taken from Janz (1967) for lithium fluoride and sodium fluoride, Topor (1976) for caesium fluoride, the DIPPR database for potassium chloride and sodium bromide, Topor (1972) for sodium iodide, and Lange (1973) for all the other molten alkali halides.

Because of the limited temperature range of the density and vapour pressure correlation equations available, these have been extrapolated in the calculation of f_j and h_j , thus increasing the uncertainty on the estimated properties.

2.4 Viscosity and thermal conductivity prediction

Ely and Hanley (1981, 1983) first employed the equations that have been used for the calculation of the viscosity and thermal conductivity for the uni-univalent salts in this work, in the early 1980s. The extended corresponding-states model then proposed permitted the calculation of density, viscosity, and thermal conductivity of nonpolar hydrocarbon mixtures. This model is often referred to as the TRAPP (TRANsport Properties Prediction) model. In this model and in the case of pure fluids the viscosity, η , of the fluid of interest is related to the viscosity of the reference fluid through the following equation:

$$\eta_j(T_j, \rho_j) = \left(\frac{M_j}{M_o} \right)^{1/2} f_j^{1/2} h_j^{-2/3} \eta_o(T_o, \rho_o) , \quad (4)$$

where M is the molecular mass.

In the case of thermal conductivity, λ , the property is separated into two contributions: λ_{tr} arising from the transfer of energy due to translations, and λ_{int} from the internal degrees of freedom. In the case of the alkali halides only λ_{tr} has been considered; it is given by:

$$\lambda_{tr,j}(T_j, \rho_j) = \left(\frac{M_o}{M_j} \right)^{1/2} f_j^{1/2} h_j^{-2/3} \lambda_{tr,o}(T_o, \rho_o) . \quad (5)$$

In the case of molten alkali halides, equations (4) and (5) were forced to be temperature dependent only because the correlation equations available in the literature for the viscosity and thermal conductivity do not take into account the density dependence of these properties. Equations (4) and (5) can be derived from the kinetic theory of gases or from the following corresponding-states relationships (Helfand and Rice 1960; Hirschfelder et al 1964; Millat et al 1996):

$$\eta^* = \frac{\eta \sigma^3}{(m\varepsilon)^{1/2}} , \quad \lambda^* = \frac{\lambda \sigma^2 m}{k_B(m\varepsilon)^{1/2}} , \quad (6)$$

where k_B is the Boltzmann constant, m is the mass of the molecule, η^* is the reduced viscosity, and λ^* is the reduced thermal conductivity. In equation (6), η^* and λ^* are universal functions of reduced temperature, $T^* = kT/\varepsilon$, and reduced volume, $V^* = V/N_0\sigma^3$, or reduced pressure, $p^* = p\sigma^3/\varepsilon$, for all conformal fluids (N_0 is Avogadro's number).

The following correlation equations have been used for the viscosity and thermal conductivity of sodium chloride, the reference fluid:

$$\eta/\text{mN s m}^{-2} = 0.109184 \exp \left[\frac{-20286.7}{(R/J \text{ K}^{-1} \text{ mol}^{-1})(T/\text{K})} \right], \quad (7)$$

$$\lambda/\text{W m}^{-1} \text{ K}^{-1} = 0.519 - 1.8 \times 10^{-4}[(T/\text{K}) - (T_m/\text{K})], \quad (8)$$

in the temperature ranges 1080–1500 and 1170–1441 K, respectively. R is the universal gas constant, T_m the melting temperature, and T the absolute temperature. Equation (7) is available in the NIST database (Janz 1992) and equation (8) is available from Nakazawa et al (1991) and Nagasaka et al (1992).

These equations, along with equations (4) and (5), have been used for the semi-theoretical estimation [see Millat et al (1996) for nomenclature] of the viscosity and thermal conductivity of the molten alkali halides, for the simple two-parameter corresponding-states theory, with the melting temperature and the corresponding density (JSTP 1990) as scale factors and the shape factors, in an attempt to force the salts to conformality. Note that the use of the melting point constants permits the prediction of density for any molten alkali halide with an absolute average deviation (AAD) smaller than 2%, while for the vapour pressure the deviations can amount to 50% and more, in particular for the molten lithium halides.

3 Results

The viscosity data calculated in this work have been compared with the data for alkali fluorides (Janz 1992), alkali chlorides (Brockner et al 1981), and alkali bromides and iodides (Sato et al 1997). In the case of thermal conductivity, the calculated data have been compared with the experimental data measured by Nagashima and coworkers (Nagasaka et al 1992; Nakazawa et al 1992a, 1992b). Because these authors did not measure the thermal conductivity of the molten alkali fluorides, nor that of lithium bromide or lithium iodide, because of the high corrosiveness of these salts, comparisons with experimental data have not been made. The thermal conductivity data (Nakazawa et al 1991; Nagasaka et al 1992) used in our model for the reference fluid show a weak negative temperature coefficient. This is in disagreement with several sets of data previously measured in other works, as discussed by Nagashima and coworkers (Nagasaka et al 1992; Nakazawa et al 1992a, 1992b). Because we believe that these data are probably the most accurate to date, the results herein presented have not been compared with any other data in the literature.

Tables 1 and 2 give the average absolute percentage deviation (AAD) and the average percentage error (BIAS) for each alkali halide, for the viscosity and thermal conductivity, respectively. The calculations were made with the simple two-parameter corresponding-states theory and the extended corresponding-states theory.

In the case of the alkali fluorides the estimated viscosities have been compared with the data calculated through the use of the correlation equations available in the NIST database (Janz 1992), with a temperature step of 1 K.

As can be seen in table 1, for most of the salts, viscosity calculation improved with the introduction of shape factors in the ESRR, in particular for the molten lithium halides. However, it is observed that for some molten salts the deviations increased with the use of shape factors. For thermal conductivity, table 2, the deviations are much larger and the introduction of shape factors increases these deviations for most of the salts. This does not necessarily mean, however, that the predictions are worse, because of the low accuracy (8%–20%) of the existing experimental data for this property. The results obtained for the viscosity of some molten salts show that the shape factors used do not force the fluids to conformality as expected, thus introducing additional errors into the predictions.

Table 1. Average absolute percentage deviation (AAD) and average percentage error (BIAS) values for viscosity of molten alkali halides calculated in the temperature range ΔT , with the simple corresponding-states theory (SCST) and the extended corresponding-states theory (ECST), together with their melting (T_m) and boiling (T_b) temperatures (n is the number of experimental data points).

| Salt ($T_m - T_b$)/K | n | ΔT /K | SCST | | ECST | |
|------------------------|-------|---------------|-------|--------|-------|--------|
| | | | AAD/% | BIAS/% | AAD/% | BIAS/% |
| LiF (1121–1954) | corr. | 1298–1317 | 27.6 | –27.6 | 1.3 | +1.3 |
| NaF (1268–1977) | corr. | 1298–1373 | 3.0 | –3.0 | 1.1 | +1.1 |
| KF (1131–1775) | corr. | 1159–1328 | 4.7 | –4.7 | 0.8 | –0.8 |
| RbF (1068–1681) | corr. | 1079–1274 | 1.9 | +0.9 | 2.2 | –1.6 |
| CsF (986–1524) | corr. | 992–1281 | 6.0 | +6.0 | 7.9 | –7.9 |
| LiCl (883–1655) | 8 | 993–1131 | 28.7 | –28.7 | 8.8 | –8.8 |
| KCl (1043–1680) | 13 | 1054–1175 | 7.2 | –7.2 | 12.2 | –12.2 |
| RbCl (990–1654) | 8 | 1062–1134 | 10.4 | –10.4 | 4.0 | +4.0 |
| CsCl (918–1573) | 12 | 948–1087 | 17.0 | –17.0 | 13.2 | –13.2 |
| LiBr (823–1583) | 10 | 941–1082 | 28.0 | –28.0 | 3.4 | –3.4 |
| NaBr (1020–1665) | 14 | 1022–1192 | 7.8 | +7.8 | 5.0 | +5.0 |
| KBr (1007–1656) | 19 | 1011–1194 | 5.1 | –5.1 | 6.9 | –6.9 |
| RbBr (953–1625) | 13 | 971–1197 | 16.3 | –16.3 | 15.0 | –15.0 |
| CsBr (909–1573) | 15 | 912–1192 | 21.2 | –21.2 | 20.4 | –20.4 |
| LiI (723–1444) | 11 | 879–1028 | 37.3 | –37.3 | 2.7 | –2.7 |
| NaI (935–1577) | 18 | 941–1117 | 7.9 | +7.9 | 8.8 | +8.8 |
| KI (958–1597) | 16 | 965–1193 | 12.7 | –12.7 | 17.8 | –17.8 |
| RbI (913–1577) | 14 | 934–1194 | 19.6 | –19.6 | 15.7 | –15.7 |
| CsI (894–1573) | 12 | 975–1198 | 19.6 | –19.6 | 1.6 | –1.3 |

Table 2. Average absolute percentage deviation (AAD) and average percentage error (BIAS) values for thermal conductivity of some molten alkali halides calculated in the temperature range ΔT , with the simple corresponding-states theory (SCST) and the extended corresponding-states theory (ECST), together with their melting (T_m) and boiling (T_b) temperatures (n is the number of experimental points).

| Salt ($T_m - T_b$)/K | n | ΔT /K | SCST | | ECST | |
|------------------------|-----|---------------|-------|--------|-------|--------|
| | | | AAD/% | BIAS/% | AAD/% | BIAS/% |
| LiCl (883–1655) | 9 | 1125–1321 | 12.9 | +12.2 | 25.9 | +25.9 |
| KCl (1043–1680) | 33 | 1056–1335 | 2.9 | +0.9 | 3.3 | –1.1 |
| RbCl (990–1654) | 26 | 1170–1363 | 11.3 | +11.2 | 14.1 | +14.1 |
| CsCl (918–1573) | 6 | 1054–1238 | 2.8 | +2.8 | 4.1 | +4.1 |
| NaBr (1020–1665) | 19 | 1107–1267 | 6.5 | +6.5 | 5.8 | +5.8 |
| KBr (1007–1656) | 13 | 1086–1245 | 19.2 | +19.2 | 19.1 | +19.1 |
| RbBr (953–1625) | 14 | 1102–1264 | 6.6 | +6.6 | 6.8 | +6.8 |
| CsBr (909–1573) | 11 | 1029–1197 | 13.6 | +13.6 | 14.1 | +14.1 |
| NaI (935–1577) | 5 | 1049–1099 | 7.4 | +7.4 | 7.8 | +7.8 |
| KI (958–1597) | 9 | 1081–1234 | 38.1 | +38.1 | 35.4 | +35.4 |
| RbI (913–1577) | 12 | 1030–1226 | 20.5 | +20.5 | 25.2 | +25.2 |
| CsI (894–1573) | 4 | 1111–1227 | 18.6 | +18.6 | 31.4 | +31.4 |

The extrapolation of vapour-pressure correlation equations is probably the major source of error in the model, which as mentioned above strongly depends on the accuracy of the shape factors.

In figure 1 the thermal conductivities calculated in this work for lithium fluoride, sodium fluoride, potassium fluoride, rubidium fluoride, and caesium fluoride, are compared with the data estimated by Nagasaka and Nagashima (1993) using a four-parameter corresponding-states principle developed by Tada et al (1988). Except for lithium fluoride

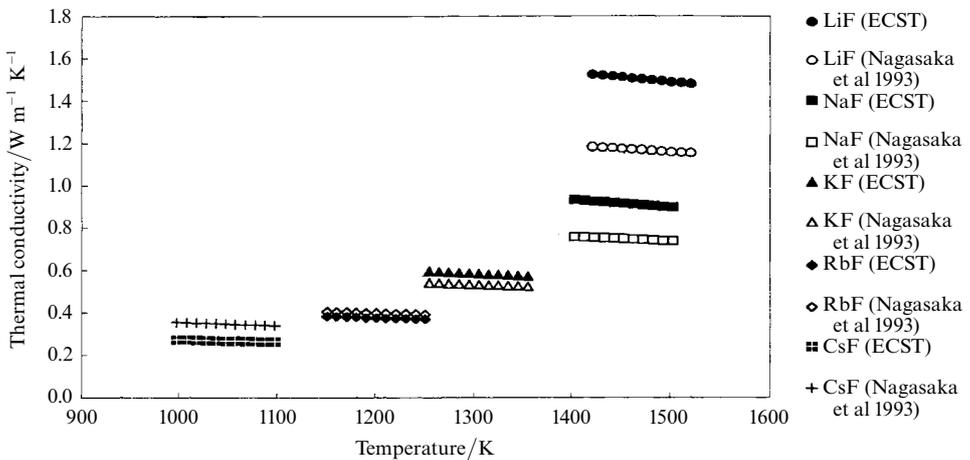


Figure 1. Comparison between the thermal conductivity data for the alkali fluorides calculated with the extended corresponding-states theory (ECST) and the corresponding-states theory developed by Tada et al (1988) and applied by Nagasaka et al (1993) to thermal conductivity of alkali halides.

and sodium fluoride, the agreement between both the estimation schemes is within the mutual uncertainty of both estimation schemes.

4 Conclusions

The simple and the extended corresponding-states methods have been applied for the first time to the semi-theoretical estimation of the viscosity and thermal conductivity of molten halide salts. The results showed that the scheme proposed works very satisfactorily, most of the time within the uncertainty of the experimental data, especially for thermal conductivity. The major uncertainty arose from the lack of vapour pressure curves covering all the temperature range used.

The shape factors used were obtained empirically. Ideally, shape-factor correlation equations in terms of characteristic molecular parameters should be developed, thus permitting the use of the corresponding-states principle in a predictive form. However, and because of the lack of experimental data for molten salts, these correlation equations are still very difficult to develop.

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