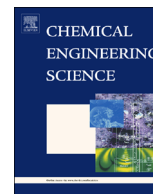




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On estimating self-diffusivities by the extended corresponding states principle

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HIGHLIGHTS

- The extended corresponding states principle is used to predict self-diffusivities.
- Corrections by the modified Enskog theory are examined.
- Correlation with a new parameter reduces the errors of the model.
- Hydrogen-bonding substances present some peculiarities.

ARTICLE INFO

Article history:

Received 23 September 2013

Received in revised form

16 December 2013

Accepted 28 December 2013

Available online 6 January 2014

Keywords:

Corresponding states principle

Helmholtz residual energy

Equation of state

Self-diffusion

Shape factor

Modified Enskog theory

ABSTRACT

The ability of the extended corresponding states principle (ECSP) to predict the self-diffusion coefficients of several types of fluids has been studied. Two versions of the model were compared with the traditional two-parameter corresponding states principle (where the equilibrium shape factors are set to unity): one using the equilibrium shape factors and another one that additionally introduces a correction based on the modified Enskog theory (MET). Ethane was chosen as a reference fluid and the experimental database comprises 3163 points from 37 substances (polar, non-polar and hydrogen-bonding ones). Results show that a third complementary parameter, generated from diffusion data, is necessary to accurately correlate this transport property.

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1. Introduction

Transport properties are the “proportionality constants” between the momentum flux and the velocity gradient (viscosity), the mass flux and the concentration gradient (diffusivity) and the heat flux and the temperature gradient (thermal conductivity). Therefore, knowledge of these properties is necessary to design industrial facilities where processes involving transfer of momentum, energy and/or mass are carried out. On the other hand, the corresponding states principle (CSP) – that states the similarity of thermodynamic properties or their departures from those properties adopted by a reference substance or predicted by a state model (EOS) in a generalized scenario – is a practical tool derived from a unitary description of the matter and its transformations.

In the late 1970s and early 1980s, Hanley (1976) and Ely and Hanley (1981, 1983) proposed the use of the extended

corresponding states principle (ECSP) for evaluating the viscosity and thermal conductivity of any fluid with respect to those of a reference fluid. This ECSP had been developed by Leach et al. (1968) and by Rowlinson and Watson (1969) for predicting thermodynamic properties, and was based on the introduction of shape factors in the temperature and density of the fluid under study, in such a way that its compressibility factor Z , and its dimensionless residual Helmholtz energy at these temperature and density were the same as those calculated from the compressibility and the dimensionless residual Helmholtz energy of the reference fluid at the modified temperature and density, as follows (Estela-Urbe and Trusler, 2003):

$$Z(T, \rho) = Z_0 \left(\frac{T}{T^*}, h\rho \right) \quad (1)$$

$$\Phi^{res}(T, \rho) = \Phi_0^{res} \left(\frac{T}{T^*}, h\rho \right) \quad (2)$$

$$f = \vartheta \frac{T_c}{T_{c0}} \quad (3)$$

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Table 1
Substances studied and available self-diffusion coefficients for them.

Substance	Formula	NDP	Experimental conditions	Literature sources
Methane	CH ₄	375	90.92–454 K 0.12–2215 bar	Greiner-Schmid et al. (1991), Harris and Trappeniers (1980), Harris (1978), Naghizadeh and Rice (1962), Dawson et al. (1970), Oosting and Trappeniers (1971) and Helbaek et al. (1996)
Ethane ^a	C ₂ H ₆	137	91.4–454 K 1.5 × 10 ⁻⁵ –2000 bar	Greiner-Schmid et al. (1991), Helbaek et al. (1996), Noble (1965), Gaven et al. (1962), Harmon and Muller (1969) and Mueller and Cahill (1964)
Propane	C ₃ H ₈	103	112–453 K 4 × 10 ⁻⁴ –2000 bar	Greiner-Schmid et al. (1991) and Robinson and Stewart (1968)
<i>n</i> -Butane	C ₄ H ₁₀	34	150–451 K 50–2000 bar	Vardag et al. (1990)
<i>n</i> -Pentane	C ₅ H ₁₂	68	174–451 K 10 ⁻³ –2000 bar	Dullien (1972), Douglass and McCall (1958), McCall et al. (1959a) and Bachi and Lüdemann (1986)
<i>n</i> -Hexane	C ₆ H ₁₄	134	181.82–443 K 1.5 × 10 ⁻⁵ –3938 bar	Harris (1982), Douglass and McCall (1958), McCall et al. (1959a), Bachi and Lüdemann (1986), Helbaek et al. (1996) and Hawlicka and Reimschuessel (1981)
<i>n</i> -Heptane	C ₇ H ₁₆	74	185.56–373 K 1.01–547.72 bar	Dullien (1972), Ertl and Dullien (1973), Moore and Wellek (1974), Douglass and McCall (1958) and McCall et al. (1959a)
<i>n</i> -Octane	C ₈ H ₁₈	81	232.11–348.16 K 1.3 × 10 ⁻⁴ –3608 bar	Harris et al. (1993), Douglass and McCall (1958), McCall et al. (1959a) and Helbaek et al. (1996)
Neopentane	C ₅ H ₁₂	43	256.41–307.69 K 0.35–689 bar	Douglass et al. (1961) and Kessler et al. (1967)
Isopentane	C ₅ H ₁₂	27	194.66–328 K 1.00–2000 bar	Enninghorst et al. (1996) and Fishman and Vassiliades (1959)
Isohexane	C ₆ H ₁₄	27	200–287.5 K 4.2 × 10 ⁻⁴ – 547.72 bar	McCall et al. (1959a)
Ethylene	C ₂ H ₄	189	123.15–398.16 K 6.36–2721 bar	Arends et al. (1981), Takahashi (1977), Peereboom et al. (1986) and Baker et al. (1984)
Cyclohexane ^b	C ₆ H ₁₂	100	281.7–358 K 8.9 × 10 ⁻² –1600 bar	Jonas et al. (1980), Polzin and Weiss (1990), O'Reilly et al., (1972a); McCool and Woolf (1972a), Freer and Sherwood (1980), Kessler et al. (1969), McCall et al. (1959b) and Fischer and Weiss (1986)
Benzene	C ₆ H ₆	167	279.06–561.7 K 7.8 × 10 ⁻² –4544 bar	Rathbun and Babb (1961), Collings and Mills (1970), Dullien (1972), Falcone et al. (1967), McCool et al., (1972), Ertl and Dullien (1973), Polzin and Weiss (1990), Fischer and Weiss (1986), Parkhurst and Jonas (1975), Holz et al. (1996), Freer and Sherwood (1980) and Hawlicka and Reimschuessel (1981)
Toluene	C ₇ H ₈	72	178.16–380 K 4.1 × 10 ⁻⁷ –3691 bar	Harris et al. (1993), Krueger and Weiss (1970) and O'Reilly and Peterson (1972)
Acetone	C ₂ H ₆ O	52	180–331.16 K 1.00–500 bar	Ertl and Dullien (1973), Krueger and Weiss (1970), McCall et al. (1959b), Holz et al. (1996) and O'Reilly and Peterson (1971)
Pyridine	C ₅ H ₅ N	76	253.16–423.16 K 1.4 × 10 ⁻³ –5000 bar	Fury et al. (1979), O'Reilly et al. (1972b) and Holz et al. (1996)
Acetonitrile	C ₂ H ₃ N	68	238.2–343.2 K 1.00–3036 bar	Holz et al. (1996) and Hurler and Woolf (1982)
Fluoromethane (R-41)	CH ₃ F	57	153–440 K 4.8 × 10 ⁻² –2000 bar	Lang et al. (1987a)
Fluoroform (R-23)	CHF ₃	114	142–433 K 1.8 × 10 ⁻² –2550 bar	Lang et al. (1987b) and Prielmeier et al. (1984)
Chloroform (R-20)	CHCl ₃	84	217–398 K 1.5 × 10 ⁻³ –3900 bar	Prielmeier and Lüdemann (1986) and Harris et al. (1990)
Carbon tetrachloride (R-10)	CCl ₄	50	283.20–350 K 1.01–1475 bar	McCool and Woolf (1972b), Rathbun and Babb (1961), Collings and Mills (1970), Fischer and Weiss (1986) and Watts et al. (1955)
Chlorodifluoromethane (R-22)	CHClF ₂	58	147.5–385.5 K 1.00–2000 bar	Vardag and Lüdemann (1988)
Trichlorofluoromethane (R-11)	CCl ₃ F	13	379–460 K 107–1594 bar	DeZwaan and Jonas (1975a)
1,2-Dichloroethane (R-150)	C ₂ H ₄ Cl ₂	23	278.15–313.15 K 1.00–2830 bar	Malhotra et al. (1990)
Fluorobenzene	C ₆ H ₅ F	18	234.96–356.16 K 1.00 bar	Ertl and Dullien (1973)
Argon	Ar	61	84.2–322.56 K 0.87–243.18 bar	Mifflin and Bennett (1958), McLaughlin (1959), Corbett and Wang (1956), De Paz (1968), De Paz et al. (1967), Naghizadeh and Rice (1962) and Cini-Castagnoli and Ricci (1960)
Krypton	Kr	133	115.76–308.16 K 5.53–230.92 bar	Carelli et al. (1973, 1976), Durbin and Kobayashi (1962), Naghizadeh and Rice (1962), Trappeniers and Michaels (1973), Cowgill and Norberg (1976) and Codastefano et al. (1978)
Xenon	Xe	94	175–343 K 1.91–1346.36 bar	Peereboom et al. (1989), Naghizadeh and Rice (1962), Amdur and Schatzki (1957) and Ehrlich and Carr (1970)
Nitrogen	N ₂	15	77.3–353.2 K 1.00–4.60 bar	Krynicky et al. (1974) and Winn (1950)
Carbon monoxide	CO	8	68.97–373.0 K 0.933–1.00 bar	Cini-Castagnoli (1964) and Amdur and Shuler (1963)
Carbon dioxide	CO ₂	238	223–450 K 2.95–2000 bar	Robinson and Stewart (1968), Etesse et al. (1992), O'Hern and Martin (1955), Groß et al. (1998) and Takahashi and Iwasaki (1966)

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