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Kinematic viscosity prediction for aqueous solutions with various solutes

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Abstract

In numerous research areas knowledge of aqueous solutions viscosity is very important to interpret the experimental data or to use it in simulation studies. When Kumar's semitheoretical equation for prediction of the dynamic viscosity of a solution of a single electrolyte is modified for prediction of kinematic viscosities, it is found that the resulting expression is valid both for salts and for certain organic solutes. The parameters characterizing individual solutes in aqueous solution at temperatures between 293.1 and 323.1 K also allow prediction of the kinematic viscosities of solutions of multiple solutes in the same temperature and concentration range, with overall errors of <2.5% in 36 of 39 multi-component systems. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Kinematic viscosity; Aqueous solutions; Electrolytes; Multi-solute solutions

1. Introduction

In numerous research areas, aqueous salt solutions are used as microbiological nutrients [1] or to control chemical properties [2], chemical reaction rates [3] or hydrodynamic characteristics [4]. The studies of gas–liquid mass transfer are frequently facilitated by using aqueous buffer solutions so as to be able to work at constant pH and hence simplify mathematical modeling of the results [5], and the main factors governing the complex mechanism of the absorption processes can be controlled by the addition of salts [6]. In most cases, the salt or salts modify the viscosity of the solvent, which must be taken into account when interpreting experimental data in terms of models involving viscosity directly or via its influence on other properties [7], or when such models are used for simulation studies of industrial processes.

To this end, and to avoid extensive viscosity measurements, and time-consuming literature searches, numerous equations have been developed for prediction of viscosities [8–10]. However, most such equations employ great number of solute-specific parameters, and are of very limited validity for multi-component solutions. One of the simplest is Kumar's expression [10] for relative dynamic viscosity as a function of mole fraction of solute. However, a parameter of more immediate interest in many situations is the kinematic viscosity, which is directly involved in many dimensionless numbers used in chemical engineering in relation to mass transfer processes.

In this work, we re-formulated Kumar's equation as an expression for relative kinematic viscosity in terms of relative density, mass fraction and temperature, and for aqueous solutions of each of 24 common saline or organic solutes determined the parameters minimizing the error in kinematic viscosity. For each solute employed, optimization was based on published data for kinematic viscosities of solutions of various concentrations and temperatures in the range 293.1–323.1 K. Finally, we investigated the accuracy with which the parameters obtained for the individual solutes allowed prediction of the published viscosities of 24 two-solute solutions and 15 three-solute solutions, with excellent results.

2. Fundamentals

Kumar's model [10] for the prediction of the dynamic viscosity μ of a solution with a single-solute is

$$\frac{\mu}{\mu_0} = \frac{1+bx}{1-hx} \tag{1}$$

where μ_0 is the dynamic viscosity of the solvent, x the mole fraction of solute, and b and h are parameters whose dependence on temperature T is given by polynomials in $(T{-}T_{\mathrm{ref}})$ with coefficients that depend only on the solute and solvent when the influence of pressure as negligible:

$$b = b_{\mathrm{ref}} + \sum_n b_n (T - T_{\mathrm{ref}})^n \tag{2}$$

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Nomenclature

b	coefficient of solute–solvent interaction
b_n	parameter defined in Eq. (2) (K^{-n})
B	parameter defined in Eq. (4)
B_n	parameter defined in Eq. (5) (K^{-n})
d_i	parameter defined in Eq. (9) (K^{1-i})
h	hydration number
h_m	parameter defined in Eq. (3) (K^{-n})
H	parameter defined in Eq. (4)
H_m	parameter defined in Eq. (6) (K^{-n})
i, j, n, m	degree of polynomial
k	number of solutes in solution
M	molecular mass ($g\,mol^{-1}$)
N	number of data evaluated
q	anion charge
T	temperature (K)
w	mass fraction of solute
x	mole fraction of solute

Greek letters

μ	dynamic viscosity ($kg\,m^{-1}\,s^{-1}$)
ν	kinematic viscosity ($m^2\,s^{-1}$)
ν_j	parameter defined in Eq. (8) ($m^2\,K^{-j}\,s^{-1}$)
ρ	density ($kg\,m^{-3}$)
ρ_i	parameter defined in Eq. (7) ($kg\,K^{-i}\,m^{-3}$)
σ	standard deviation ($m^2\,s^{-1}$)

Subscripts

cal	calculated values
exp	experimental values
o	solvent
rel	relative values
ref	values at 298.1 K
w	water

$$h = h_{\mathrm{ref}} + \sum_m h_m (T - T_{\mathrm{ref}})^m \qquad (3)$$

where b_{ref} and h_{ref} are the values of b and h at the reference temperature T_{ref}, and the degrees of the polynomials, n and m, are set in the light of the desired accuracy and the number of data available. The parameters b and h are, respectively, interpreted as a coefficient of solute–solvent interaction and as the number of solvent molecules solvating each solute molecule.

Eq. (1) may be rewritten in the form:

$$\nu_{\mathrm{rel}} = \frac{1}{\rho_{\mathrm{rel}}}\left[\frac{1 + Bw}{1 - Hw}\right] \qquad (4)$$

where w is the mass fraction of solute, ν_{rel} and ρ_{rel} are the ratios between the kinematic viscosities and densities of the solution and the pure solvent, and B and H are given by

$$B = B_{\mathrm{ref}} \sum_n B_n (T - T_{\mathrm{ref}})^n \qquad (5)$$

$$H = H_{\mathrm{ref}} \sum_m H_m (T - T_{\mathrm{ref}})^m \qquad (6)$$

(if all the above equations were exact, then B and H would be related to b and h via the expression relating mole fraction and mass fraction, i.e. for single-solute solutions, $x = wM_o/(M - wM + wM_o)$, where M and M_o are the molecular mass of the solute and solvent)

To parameterize Eq. (4) for solutions of single common solutes in water, we treated the influence of pressure as negligible under normal laboratory conditions (0.1 MPa), and used the Nelder–Mead method [11,12] to optimize the B and H of Eqs. (5) and (6) so as to minimize the deviation between the published data for the kinematic viscosities of solutions of the solute in question and the calculated values given by Eqs. (4)–(6), with the aid of the following expressions for the temperature dependence of the density, ρ_w, and kinematic viscosity, ν_w, of water

$$\rho_w = \rho_{\mathrm{ref}} + \sum_i \rho_i (T - T_{\mathrm{ref}})^i \qquad (7)$$

$$\nu_w = \nu_{\mathrm{ref}} + \sum_j \nu_i (T - T_{\mathrm{ref}})^j \qquad (8)$$

where the parameters ρ_i and ν_j of Eqs. (7) and (8) having previously been optimized by fitting these equations to published data [13] for the temperature range 293.1–323.1 K.

Independently, Eq. (7) (with the parameters optimized as above) was used together with the published density data for the same solutions as above to optimize the parameters d_1 and d_2 of the expression:

$$\rho_{\mathrm{rel}} = 1 + d_1 w + d_2 w (T - T_{\mathrm{ref}}) \qquad (9)$$

In dealing with solutions with more than one solute, the $d_1 w$, $d_2 w$, bw and hw of the individual solutes were assumed to be additive. Accordingly, the kinematic viscosities of k-solute solutions were predicted using the equation

$$\nu_{\mathrm{rel}} = \frac{1}{\rho_{\mathrm{rel}}}\left(1 + \frac{\sum_k b_k w_k}{1 - \sum_k h_k w_k}\right) \qquad (10)$$

where

$$\rho_{\mathrm{rel}} = 1 + \sum_k d_{1k} w_k + (T - T_{\mathrm{ref}}) \sum_k d_{2k} w_k \qquad (11)$$

3. Results

In all cases, the reference temperature was 298.1 K. Fitting Eqs. (7) and (8) to the published data for the density and kinematic viscosity of water [13] afforded the parameters listed in Table 1. With these parameters, none of the

Table 1
Parameters of Eqs. (7) and (8) for the density and kinematic viscosity of water at temperatures between 293.1 and 323.1 K

ρ_{ref} (kg/m^3)	ρ_1 (kg/K m^3)	$\rho_2\times10^2$ (kg/K^2 m^3)	$\nu_{ref}\times10^6$ (m^2/s)	$\nu_1\times10^8$ (m^2/K s)	$\nu_2\times10^{10}$ (m^2/K^2 s)	$\nu_3\times10^{12}$ (m^2/K^3 s)
997.07	−0.260	−4.030	0.893	−2.019	3.596	−3.822

values calculated using Eqs. (7) and (8) differed from the corresponding published value by more than 0.05%.

For 20 common salts, in Table 2 are the optimized values of the parameters of the Eqs. (5), (6) and (9), together with the number of data used, N, the ranges of mass fraction and temperature covered by these data, and the value of $\sigma=[\Sigma(\sigma_{cal}-\sigma_{exp})^2/(N-1)]^{1/2}$ for the standard deviation between the published [13–19] and the calculated values of the kinematic viscosity, which was <1% in all cases in spite of data from more than one source having been pooled for several of the salts considered. As example, Fig. 1 illustrates the fit achieved for NaCl, KNO_3 and Na_2CO_3 at 293.1 K, and Fig. 2 illustrates the validity of the assumption of linear dependence of ρ_{rel} on w, Eq. (9).

For most solutes B increases and H decreases with increasing temperature, but there are exceptions, see Figs. 3 and 4. For a given anion, the values of B_{ref} and H_{ref} for the sodium salt are in all cases greater than the corresponding value for the potassium salt; and for a given cation and anion family, B_{ref} and H_{ref} increase with the charge q of the anion (Fig. 5 shows the behavior of B_{ref} in phosphates and carbonates). These trends, like similar trends in the parameters b_{ref} and h_{ref} of Kumar's equation, appear to be mediated by the radius of the cation, the oxidation state of the anion, the number of ions that the electrolyte is capable of forming, and the adiabatic compressibility [10,20].

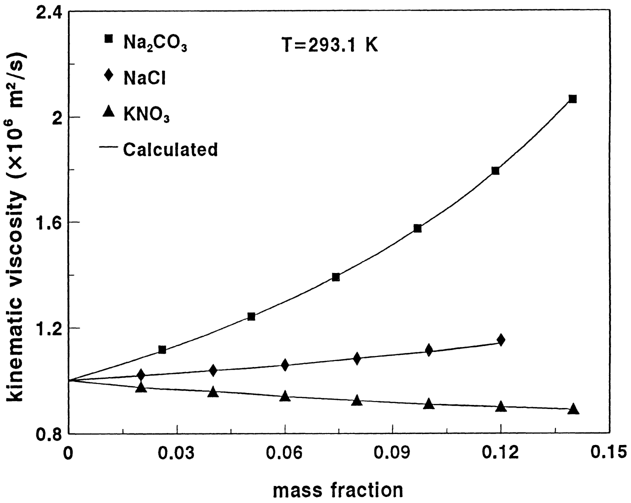

Fig. 1. Bibliographic and calculated values of the kinematic viscosity of aqueous Na_2CO_3, NaCl and KNO_3 solutions at 293.1 K.

Table 3 shows that equally good fit was obtained for the four organic solutes for which kinematic viscosity data were published [16]. It is worth noting that all four organic solutes have very similar B_{ref} values and, except for glycerin, very similar H_{ref} values. This is attributable to the structures of all

Table 2
Parameters of Eqs. (5), (6) and (9) for calculation of the densities and kinematic viscosities of aqueous salt solutions

Solute	$w\times10^2$	T (K)	d_1	$d_2\times10^3$ (1/K)	B_{ref}	$B_1\times10^2$ (1/K)	$B_2\times10^4$ (1/K^2)	H_{ref}	$H_1\times10^2$ (1/K)	$H_2\times10^4$ (1/K^2)	N	$\sigma\times10^6$ (m^2/s)
Na_2CO_3	≤14.0	293.1–323.1	1.010	1.768	4.954	1.397	1.860	3.396	−2.994	−1.762	50	0.007
K_2CO_3	≤17.9	293.1–323.1	0.908	−6.178	2.154	1.077	0.061	2.039	−0.311	−3.682	50	0.005
$NaHCO_3$	≤8.0	293.1–323.1	0.696	−2.846	2.726	−0.509	−1.087	2.028	0.423	6.445	30	0.003
$KHCO_3$	≤13.8	293.1–323.1	0.686	2.942	1.259	1.953	0.728	1.584	−3.118	1.376	50	0.003
Na_3PO_4	≤7.6	293.1–323.1	1.225	2.383	5.608	−1.459	0.955	4.306	0.712	−5.994	35	0.003
K_3PO_4	≤20.9	293.1–323.1	1.109	−5.500	2.851	0.080	−0.010	2.287	−0.253	−0.886	42	0.004
Na_2HPO_4	≤6.8	293.1–323.1	1.010	3.506	4.250	1.276	−8.321	3.319	0.564	0.071	35	0.003
K_2HPO_4	≤18.1	293.1–323.1	0.916	9.784	2.449	2.205	−2.497	1.878	−1.127	2.919	42	0.003
NaH_2PO_4	≤13.1	293.1–323.1	0.775	1.559	3.317	1.297	−3.547	2.161	−3.860	7.514	42	0.004
KH_2PO_4	≤14.7	293.1–323.1	0.757	0.337	2.164	1.429	−5.163	1.753	−2.959	11.83	42	0.002
$CuSO_4$	≤14.0	293.1–323.1	1.138	8.878	3.912	1.015	−2.027	2.756	−1.809	2.529	30	0.008
$Fe_2(SO_4)_3$	≤24.0	293.1–323.1	1.015	22.50	3.759	−0.448	1.928	2.632	−0.727	0.431	30	0.008
NaCl	≤11.0	293.1–298.1	0.741	−0.461	1.532	0.545	−11.49	1.950	−0.919	11.89	20	0.008
KCl	≤13.0	293.1–298.1	0.692	7.809	0.084	0.280	–	1.148	7.930	−14.71	10	0.006
Na_2SO_4	≤13.0	293.1–298.1	0.956	7.148	3.459	−2.462	1.682	2.065	0.984	−1.017	10	0.009
K_2SO_4	≤10.0	293.1–298.1	0.887	13.24	1.345	0.079	0.206	1.408	6.443	−13.53	10	0.008
$NaNO_3$	≤14.4	293.1–298.1	0.748	11.11	0.742	2.069	−6.185	2.004	−1.503	8.189	10	0.009
KNO_3	≤17.0	293.1–298.1	0.630	−3.817	−0.235	1.992	−0.890	0.261	−0.049	0.971	10	0.009
NaBr	≤10.0	293.1–298.1	0.827	0.381	0.467	2.710	−3.914	0.992	−1.302	3.128	10	0.005
KBr	≤11.0	293.1–298.1	0.729	−6.455	−0.215	2.397	−3.810	−0.057	−0.272	3.904	10	0.005

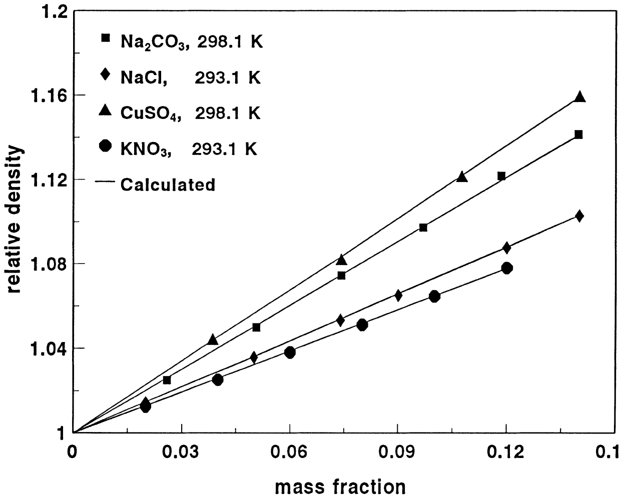

Fig. 2. Bibliographic and calculated values of the relative density of aqueous Na_2CO_3, NaCl, $CuSO_4$ and KNO_3 solutions at the indicated temperatures.

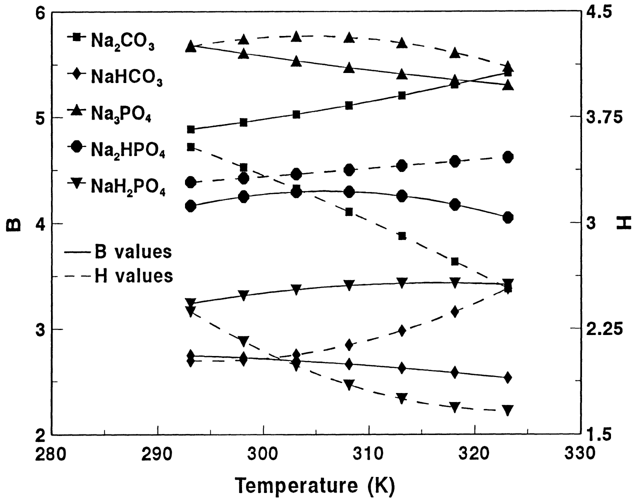

Fig. 4. Temperature dependence of B and H, Eqs. (5) and (6) for several sodium salts.

four being based on tetrahedral carbon units and containing numerous hydroxyl groups, the same features as are thought to be involved in their ability to act as gas–liquid absorption enhancers [21].

3.1. Kinematic viscosity prediction for aqueous two- and three-solute solutions

Application of Eq. (11) to the multi-solute systems listed in Table 4 using the single-solute values of d_1 and d_2 listed in Tables 2 and 3 allowed prediction of measured densities to within 1.5% in all cases.

Similarly, for concentrations and temperatures in the ranges considered for the individual solutes, the kinematic viscosities calculated from Eq. (10) agree very well with the experimental data published [15–19,22–24], with σ values <0.034 in all cases and <0.022 in all but two (see Table 4); most of this error in fact appears to be attributable to the error in the calculated relative densities.

Note that since Eq. (10) distinguishes the separate contributions of the various solutes to the kinematic viscosity, the dependence of the latter on the mass fraction of each solute can be plotted separately; this is illustrated in Fig. 6 for binary solutions of NaCl, KCl or $NaNO_3$ with a fixed concentration of $Fe_2(SO_4)_3$, and in Fig. 7 for ternary solutions of KCl, $NaNO_3$ or Na_2SO_4 with fixed concentrations of Na_2CO_3 and $NaHCO_3$.

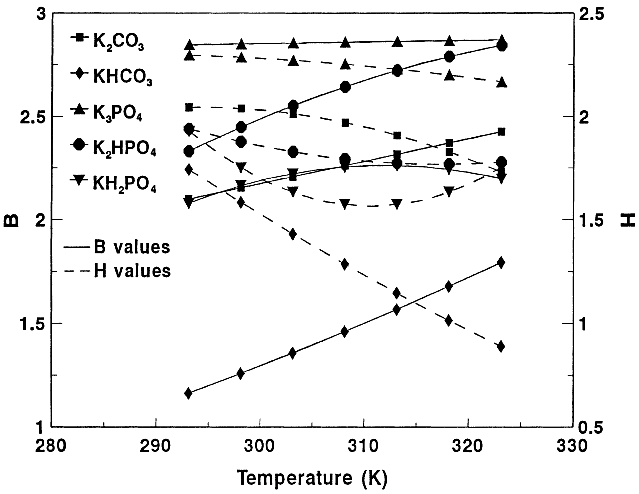

Fig. 3. Temperature dependence of B and H, Eqs. (5) and (6) for several potassium salts.

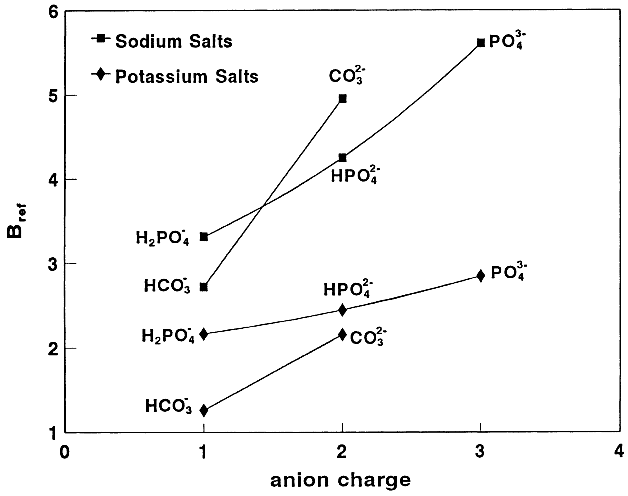

Fig. 5. Dependence of B_{ref} on the charge of the anion in homologous series of salts.

Table 3
Parameters of Eqs. (5), (6) and (9) for calculation of the densities and kinematic viscosities of aqueous solutions of organic solutes

Solute	$w\times10^2$	T (K)	d_1	$d_2\times10^3$ (1/K)	B_{ref}	$B_1\times10^2$ (1/K)	$B_2\times10^4$ (1/K^2)	H_{ref}	$H_1\times10^2$ (1/K)	$H_2\times10^4$ (1/K^2)	N	$\sigma\times10^6$ (m^2/s)
Saccharose	≤14.3	293.1–323.1	0.353	−9.918	2.654	−0.601	−0.814	2.234	−1.641	−2.215	42	0.005
Fructose	≤14.3	293.1–323.1	0.388	−3.531	2.482	−11.17	−2.373	2.128	−0.718	8.848	42	0.006
Glucose	≤14.4	293.1–323.1	0.316	−12.59	2.412	−0.432	−0.390	2.196	−2.598	5.966	42	0.008
Glycerin	≤14.9	293.1–323.1	0.227	−1.511	2.542	−0.857	1.095	1.484	−1.686	−1.720	42	0.003

Table 4
Discrepancy between experimental kinematic viscosities of multi-solute aqueous solutions and those calculated from Eq. (10)

Aqueous solutions with two-solutes			Aqueous solutions with three-solutes		
Solutes	N	$\sigma\times10^6$ (m^2/s)	Solutes	N	$\sigma\times10^6$ (m^2/s)
Na_2CO_3+$NaHCO_3$	21	0.006	Na_2CO_3+$NaHCO_3$+NaCl	28	0.009
K_2CO_3+$KHCO_3$	20	0.008	K_2CO_3+$KHCO_3$+NaCl	28	0.009
Na_3PO_4+Na_2HPO_4	14	0.010	Na_2CO_3+$NaHCO_3$+Na_2SO_4	28	0.005
Na_3PO_4+NaH_2PO_4	14	0.020	K_2CO_3+$KHCO_3$+Na_2SO_4	28	0.011
Na_3PO_4+K_2HPO_4	14	0.009	Na_2CO_3+$NaHCO_3$+$NaNO_3$	28	0.016
Na_3PO_4+KH_2PO_4	14	0.015	K_2CO_3+$KHCO_3$+$NaNO_3$	28	0.014
Na_2HPO_4+NaH_2PO_4	14	0.008	Na_2CO_3+$NaHCO_3$+K_2SO_4	21	0.013
Na_2HPO_4+K_3PO_4	14	0.034	K_2CO_3+$KHCO_3$+K_2SO_4	21	0.007
Na_2HPO_4+KH_2PO_4	14	0.011	Na_2CO_3+$NaHCO_3$+KCl	28	0.020
NaH_2PO_4+K_3PO_4	14	0.012	K_2CO_3+$KHCO_3$+KCl	28	0.002
NaH_2PO_4+K_2HPO_4	14	0.008	Na_2CO_3+$NaHCO_3$+KNO_3	28	0.022
K_3PO_4+K_2HPO_4	14	0.010	Na_2CO_3+$NaHCO_3$+saccharose	74	0.012
K_3PO_4+KH_2PO_4	14	0.013	Na_2CO_3+$NaHCO_3$+fructose	42	0.013
K_2HPO_4+KH_2PO_4	14	0.011	Na_2CO_3+$NaHCO_3$+glucose	70	0.011
$Fe_2(SO_4)_3$+NaCl	84	0.014	Na_2CO_3+$NaHCO_3$+glycerin	42	0.011
$Fe_2(SO_4)_3$+KCl	91	0.017			
$Fe_2(SO_4)_3$+NaBr	112	0.010			
$Fe_2(SO_4)_3$+KBr	91	0.008			
$Fe_2(SO_4)_3$+KNO_3	112	0.010			
$Fe_2(SO_4)_3$+$NaNO_3$	112	0.025			
Na_2CO_3+saccharose	32	0.009			
Na_2CO_3+glucose	28	0.010			
$NaHCO_3$+saccharose	32	0.010			
$NaHCO_3$+glucose	28	0.011			

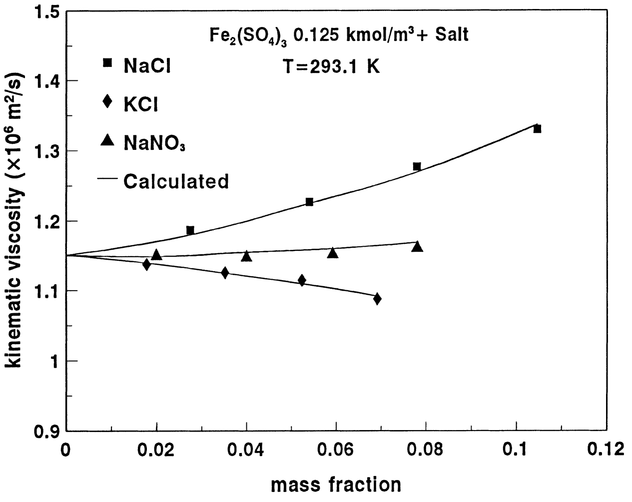

Fig. 6. Bibliographic and calculated values of the kinematic viscosity of binary aqueous solutions of $Fe_2(SO_4)_3$ 0.125 kmol/m^3 and various concentrations of $NaNO_3$, NaCl or KCl at 293.1 K.

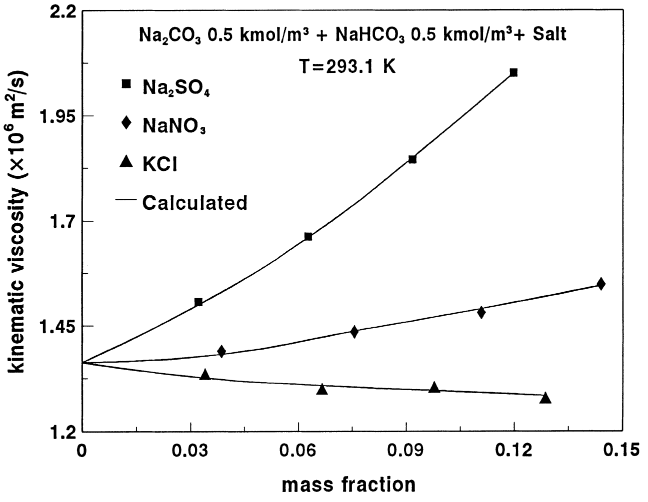

Fig. 7. Bibliographic and calculated values of the kinematic viscosity of ternary aqueous solutions of Na_2CO_3 and $NaHCO_3$, 0.5 kmol/m^3 each, and various concentrations of $NaNO_3$, Na_2SO_4 or KCl at 293.1 K.

4. Conclusions

At temperatures between 293.1 and 323.1 K, the method proposed in this work allows the kinematic viscosities of aqueous solutions of salts and certain organic solutes to be calculated over a wide range of concentrations from their mass fractions and temperatures, by means of parameters obtained in the same way. The same parameters can be used to additive manner to calculate the kinematic viscosities of multi-solute solutions. These results should facilitate both the processing of data obtained in studies of gas–liquid mass transfer and the simulation of gas–liquid mass transfer processes, because all the solutes considered in this work are commonly employed in such studies.

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