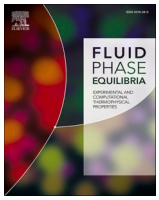
Fluid Phase Equilibria 580 (2024) 114037

Contents lists available at ScienceDirect

Fluid Phase Equilibria

journal homepage: www.journals.elsevier.com/fluid-phase-equilibria



Thermodynamic modeling using extended UNIQUAC and COSMO-RS-ES models: Case study of the cesium nitrate-water system over a large range of temperatures

Mouad Arrad [a], Kaj Thomsen [b,*], Simon Müller [c], Irina Smirnova [c]

[a] Department of Process Engineering, Equipe Énergie et Procédés Propres, National School of Mines of Rabat, BP 753 Agdal, Rabat, Morocco
[b] Center for Energy Resources Engineering, (CERE), Department of Chemical and Biochemical Engineering, Technical University of Denmark, Kongens Lyngby 2800, Denmark
[c] Institute of Thermal Separation Processes, Hamburg University of Technology, Hamburg, Germany

ARTICLE INFO

Keywords:
Cesium nitrate
Electrolyte solution
Extended UNIQUAC
COSMO-RS-ES
Application of model

ABSTRACT

A comparison of two thermodynamic models is presented using the water-cesium nitrate system as case study. Both models were able to model the thermodynamic properties such as the osmotic coefficient, vapor pressure, mean activity coefficient and solubility with good accuracy. We show that it is possible to reproduce the temperature dependency of the properties using a simple set of parameters in the case of Extended UNIQUAC. Furthermore, COSMO-RS-ES is a completely predictive model adjusted to data at 298.15 K, which is applied for the first time to other temperatures.

1. Introduction

Cesium nitrate is a highly water-soluble crystalline cesium source for uses compatible with nitrates and lower (acidic) pH. Nitrate compounds are generally soluble in water. Nitrate materials are also oxidizing agents. When mixed with hydrocarbons, nitrate compounds can form a flammable mixture. Nitrates are excellent precursors for production of ultra-high purity compounds. Certain catalysts and nanoscale products (nanoparticles and nano-powders) are based on cesium nitrate salts [1, 2]. It is used in pyrotechnic compositions, as a colorant and an oxidizer, e.g. in decoys and illumination flares. Cesium nitrate prisms are used in infrared spectroscopy, in x-ray phosphor and in scintillation counters. [3,4] It is also used in making optical glasses and lenses.

As a rare essential metal, cesium and its compounds are widely used in aerospace, electronic devices, biomedicine, and other modern technical fields [4]. The reserves of nonradioactive cesium resources in Salt Lake brine, geothermal water, and underground brines are abundant [5–7].

The study of the thermodynamic properties for this system is very important regarding the wide area of use and the valuable information that modeling can bring to the scientific community.

Previously, the ternary $CsNO_3$–NH_4NO_3–H_2O system was modeled [8] using the Pitzer model extended with Harvie-Weare equations. The focus was to reproduce the $CsNO_3$–NH_4NO_3–H_2O phase diagram at 298.15 K and 348.15 K measured by Li et al. [9]. This modeling required a total of 20 parameters [8].

In this work a comparison of two different categories of thermodynamic models was carried out. The Extended UNIQUAC and the COSMO-RS-ES models are widely different but are here applied to the same problem. The main outcome of this work is to see how easily it is to widen the applicability of Extended UNIQUAC to the binary system $CsNO_3$ and test how well the predictive model COSMO-RS-ES can be applied to systems at temperatures different from 298.15 K.

2. Analysis of available experimental data

The experimental data of the water-cesium nitrate system are relatively scarce. The work of Robinson [10] is the first set of osmotic coefficient and activity coefficient to be reported at concentrations up to 1.5 molal at 298.15 K. Fanghänel et al. [11] measured the osmotic coefficient at 373.25 K from 2.05 to 7.21 molal. Frolov et al., [12] reported water activities at 298.15 K. Ryabov et al. [13], measured the water activity at 298.15 K of one $CsNO_3$ solution. Kirgintsev et al. [14] reported the water activity of two $CsNO_3$ solutions at 298.15 K. Harned and Owen [15] measured the mean activity coefficient at very low concentration at 298.15 K using the emf method.

* Corresponding author.
E-mail address: kth@kt.dtu.dk (K. Thomsen).

https://doi.org/10.1016/j.fluid.2024.114037
Received 12 November 2023; Received in revised form 2 January 2024; Accepted 18 January 2024
Available online 19 January 2024

Table 1
Available data from the literature used for determining model parameters for the cesium nitrate-water system.

Data type	Temperature (K)	Molality	Data points	Reference
Osmotic coefficient	298.15	0.01-1.41	60	Robinson [10]
Activity coefficient	298.15	0.0005-0.01	5	Harned and Owen [15]
Vapor pressure	298.15	0.435-1.570	8	Frolov et al. [12]
	298.15	3.1	1	Ryabov et al. [13]
	298.15	1.087-1.241	2	Kirgintsev and Luk'yanov [14]
	373.45	1.115-7.212	13	Fanghänel et al. [11]
	280.95 - 323.55	0.709-3.302	28	Apelblat and Korin [20]
Freezing – SLE	271.89 - 273.08	0.018-0.437	11	Washburn and Macinnes [18]
Salt solubility	278.15 - 393.15	0.608-13.942	15	Cherkasov et al. [24,25]

Table 2
Volume and surface area parameters used in the Extended UNIQUAC model.

Species Parameter	H_2O	H^+	OH^-	$NO3^-$	Cs^+
Volume parameter	0.92[a]	0.13779[b]	9.3973[b]	5.404[b]	**5.938**
Surface area parameter	1.4[a]	$0.1{\cdot}10^{-15}$[b]	8.8171[b]	6.2074[b]	**1.485**

[a] Parameter from Abrams and Prausnitz [26].
[b] parameter from Thomsen et al., 1996 [27].

Richards and Rowe [16], reported a few heat of dilution data and heat capacity data at 293.15 K. Jauch [17] reported heat capacity data at 291.15 K. The amount of thermal property data available was considered insufficient for parameter estimation. These data points were therefore not included in this modeling project.

Freezing point data were reported by Washburn and Macinnes [18] and Roth-Greifswald [19]. Apelblat and Korin [20] measured vapor pressure data at several temperatures from 280.95 K to 323.55 K.

Solubility values were determined by Berkeley [21], Yakimov et al. [22], Arkhipov et al. [23], Cherkasov et al. [24,25], and recently by Li et al. [9].

The available experimental data are relatively limited but a good agreement between data from different sources and different types of data creates a consistent view of the thermodynamic behavior.

The experimental data used for modeling in this project are listed in Table 1.

3. Modeling approach

3.1. Extended UNIQUAC model

The Extended UNIQUAC model is a thermodynamic model for electrolyte solutions. It consists of a UNIQUAC term [26] and an Extended Debye-Hückel term. The model was developed over several years and is used in its current form here as it was presented by Thomsen et al. [27]

The Extended UNIQUAC model is mole fraction based and uses UNIQUAC interaction parameters with linear temperature dependence [27]. It therefore offers the possibility to model electrolyte solutions in the entire concentration range and over wide temperature ranges. The Extended UNIQUAC model is a good option for modeling solid-liquid equilibrium, vapor-liquid equilibrium, and various properties of aqueous salt solutions.

A significant advantage of the Extended UNIQUAC model compared to some other models is that temperature dependence is built into the model. This enables the model to also describe thermodynamic properties that are temperature derivatives of the excess Gibbs energy, such as heat of mixing and heat capacity.

For modeling the binary $CsNO_3$–H_2O system, the nitrate parameters reported by Thomsen et al. [27] were used unchanged. UNIQUAC volume and surface area parameters r, and q for the cesium ion were determined in this work. The volume and surface area parameters for ions in aqueous solutions are considered adjustable parameters in this model. Ideally, the volume and surface area parameters are determined from data for several binary and ternary aqueous solutions with several different ions. In this case, some solid-liquid equilibrium data [23, 28-31] for the Cs_2CO_3–H_2O system were included together with data for the CsNO3–H2O system to determine these parameters. The volume parameter for Cs^+ was determined to be 5.938 and the surface area parameter for Cs^+ was determined to be 1.485.

In addition to the volume and surface area parameters, the interaction parameter for the interaction of Cs^+ with NO_3^- was determined. This temperature dependent interaction parameter consists of a basis value and a temperature gradient. The basis value was determined to be 554.828 and the temperature gradient was determined to be 1.9137. The interaction parameter can therefore be written: $u_{Cs^+-NO_3^-} = 554.828 + 1.9137 * (T - 298.15)$. Finally, the interaction parameter for the interaction of Cs^+ with H_2O was determined. This parameter was determined to be $u_{Cs^+-H_2O} = -694.376 - 4.0344 * (T - 298.15)$.

A complete list of volume and surface area parameters used in the Extended UNIQUAC model is given in Table 2. The interaction parameters are listed in Table 3. The parameters determined in this work are the volume and surface area parameters for Cs^+, and the interaction parameters for the H_2O—Cs^+ interaction and the NO_3^--Cs^+ interaction. The numbers determined in this work are written in bold.

Table 3
Interaction parameters used in the Extended UNIQUAC model.

Species pair Parameter	H_2O—H_2O	H_2O—H^+	H_2O—OH^-	H_2O—NO_3^-	H_2O—Cs^+
Interaction parameter	0[b]	10,000[b]	600.4952[b]	998.9202[b]	**-694.376**
Interaction parameter, temperature gradient	0[b]	0[b]	8.5455[b]	9.3251[b]	**−4.0344**
Species pair	H^+ - H^+	H^+ - OH^-	H^+ - NO_3^-	H^+ - Cs^+	
Parameter					
Interaction parameter	0[b]	$0.1{\cdot}10^{-10}$[b]	$0.1{\cdot}10^{-10}$[b]	$0.1{\cdot}10^{-10}$[b]	
Interaction parameter, temperature gradient	0[b]	0[b]	0[b]	0[b]	
Species pair	OH^- - OH^-	OH^- - NO_3^-	OH^- - Cs^+		
Parameter					
Interaction parameter	1562.881[b]	1379.954[b]	−27.503		
Interaction parameter, temperature gradient	5.6169[b]	6.6369[b]	−3.9428		
Species pair	NO_3^- - NO_3^-	NO_3^- - Cs^+	Cs^+ - Cs^+		
Parameter					
Interaction parameter	2753.714[b]	**554.828**	0		
Interaction parameter, temperature gradient	2.2866[b]	**1.9137**	0		

[b] parameter from Thomsen et al., 1996 [27].

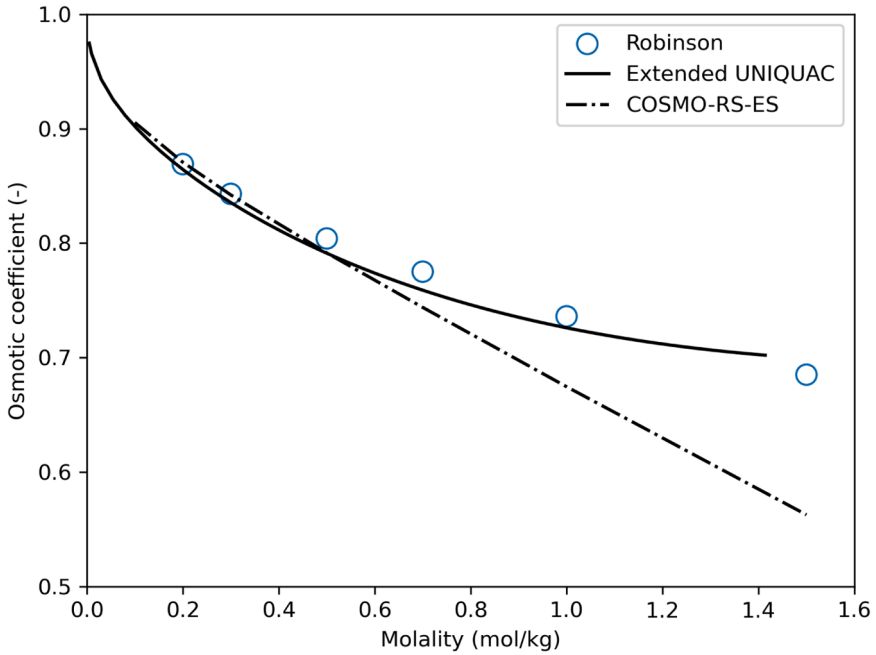


Fig. 1. Osmotic coefficient from Robinson [10] and values calculated using both models at 298.15 K.

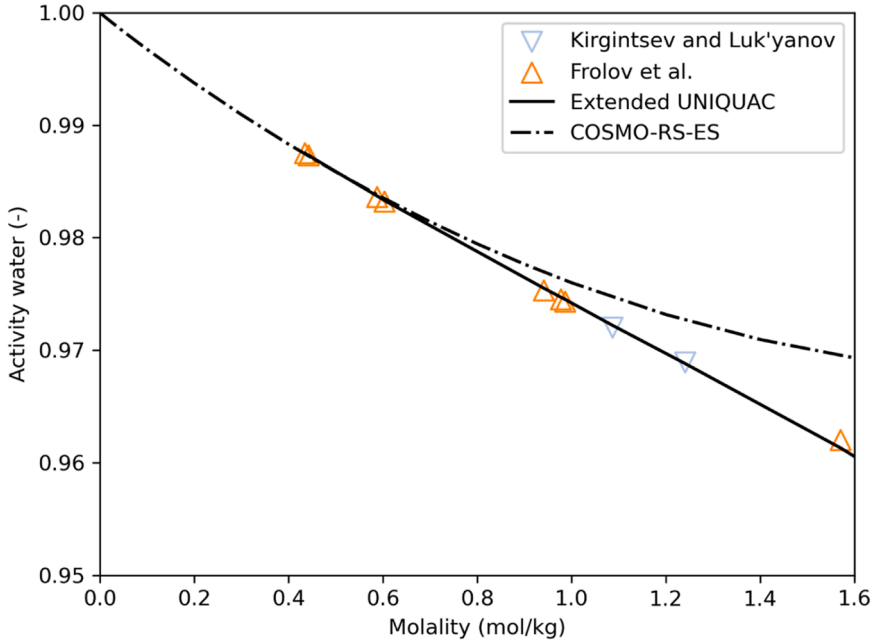


Fig. 2. Experimental water activity plotted with values calculated using COSMO-RS-ES and Extended UNIQUAC models at 298.15 K.

The model parameters were determined by minimization of the weighted difference between calculated and experimental data using a modified Marquardt subroutine for non-linear least squares from the Harwell subroutine library [33].

The Extended UNIQUAC parameters determined in this work can be extended to other systems by determining interaction parameters for Cs^+ with the ions found in the other systems. This requires experimental data for solutions containing a cesium salt and a salt containing the other ion. These experimental data can be solid-liquid equilibrium, activity coefficient data or similar. To extend the parameters to solutions containing $NaNO_3$, solid-liquid equilibrium data for the ternary $CsNO_3$–$NaNO_3$–H_2O system could be used. Assuming parameters already exist for the sodium ion, the Cs^+ - Na^+ interaction parameter can be determined from these data.

3.2. COSMO-RS-ES

COSMO-RS-ES [34,35] is a predictive model which, like Extended UNIQUAC, consists of a short-range and a long-range term. It combines a tailored version of open COSMO-RS [36] and an especially improved long-range term ME-PDH [37]. The model has seen several improvements over the years [38,39] leading to a model of broad predictive applicability for electrolyte solutions in mixed solvents up to very high salt concentrations. Even for completely non-aqueous systems and for low permittivity systems, the model is able to capture trends semi quantitatively without the need of any type of binary interaction

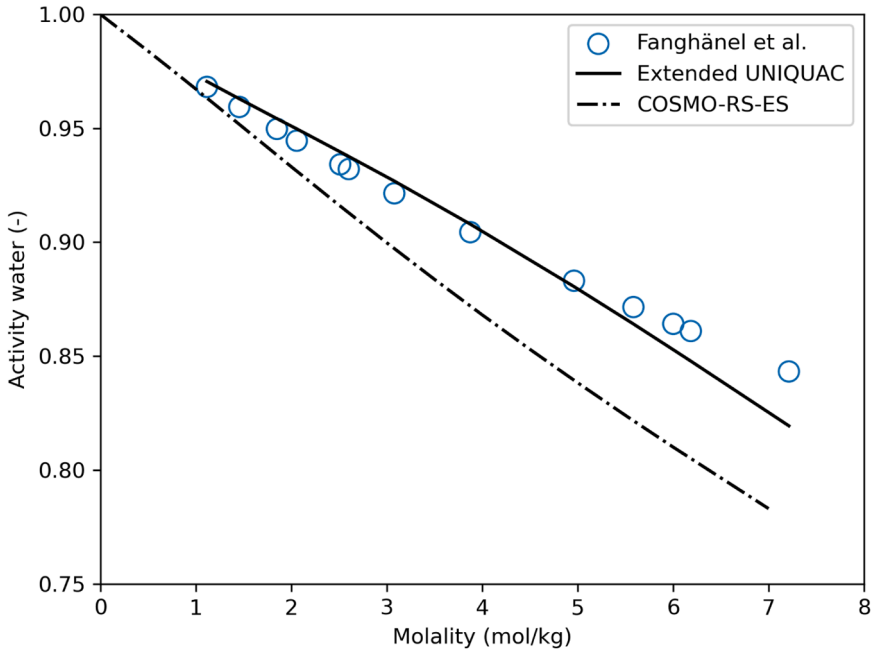


Fig. 3. Experimental water activity calculated using COSMO-RS-ES and Extended UNIQUAC models at 373.45 K.

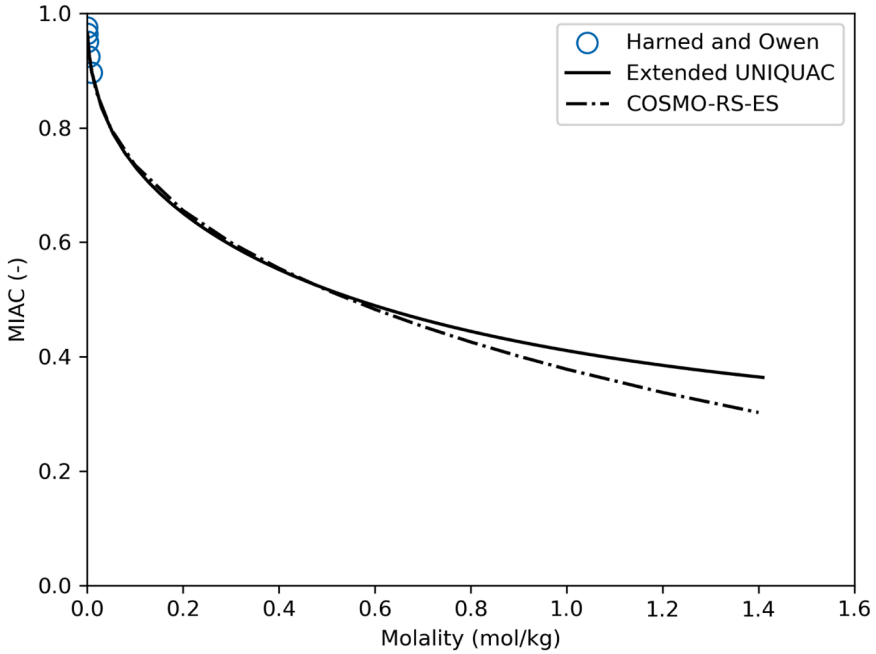


Fig. 4. Mean activity coefficient calculated using both models and low concentration data from Harned and Owen [15].

parameter. The improved long-range model has been shown to be able to describe systems including ILs better than conventional terms [40]. So far, the model has been only applied to electrolyte systems at 298.15 K which is why the application in this work is considered purely predictive. Ongoing work will include a temperature dependency to improve the model further.

No parameter adjustment was done for COSMO-RS-ES. Parameters are used as published by Castilla et al. [37]. COSMO-RS-ES is inherently predictive and can be applied to all systems for which the radii of the cations have been determined [37].

4. Results and discussion

Results of the modeling are shown in the following figures comparing calculated and experimental data. All calculations were performed with the same set of parameters for each of the two models.

The modeling results show a good agreement between the calculated osmotic coefficient from the Extended UNIQUAC model and the COSMO-RS-ES model at 298.15 K. Water activity data shows a deviation for the COSMO-RS-ES starting from 1 molal.

Water activity at around 373.15 K is correctly calculated by Extended UNIQUAC, while COSMO-RS-ES predicts the correct trend with some deviations as the salt concentration increases.

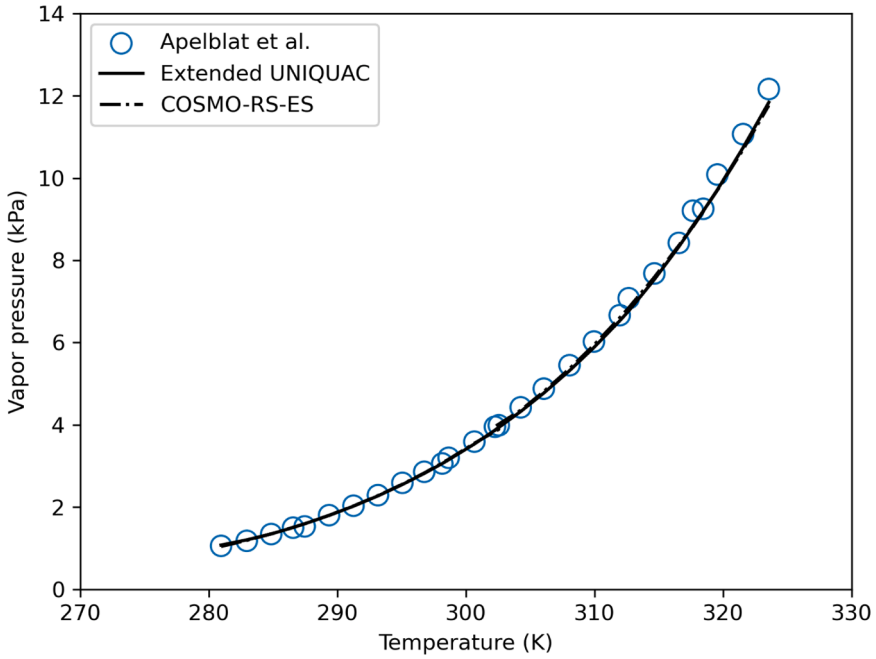


Fig. 5. Experimental vapor pressure data at saturation and calculated vapor pressures at saturation using both models in the range 280–323.15 K. The lines from the two models overlap, so only one line can be seen.

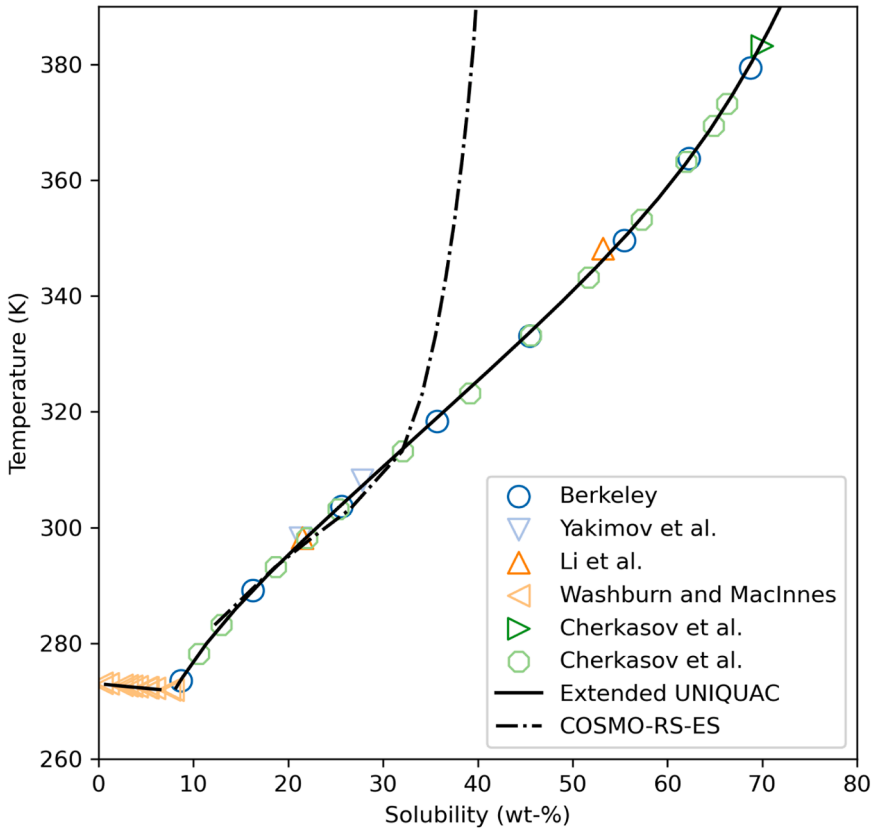


Fig. 6. Solubility calculated with both models and available experimental solubility data plotted on the graph.

Figs. 1–3 show calculated and experimental values of osmotic coefficient and water activity.

The prediction of the mean activity coefficient follow the same trend in both models at 298.15 K. Fig. 4 shows the mean activity coefficient predicted by the models.

Both models are in excellent agreement with vapor pressure data for saturated solutions measured by Apelblat and Korin [20]. This is shown in Fig. 5. The good agreement of both models is expected, as the vapor pressure is not that sensitive towards the salt concentration.

Concerning the solubility, Extended UNIQUAC was able to reproduce

the solubility phase diagram with high precision including the ice curve and the branch for anhydrous cesium nitrate using the solubility product calculated from standard state properties from the NBS tables [41–43]. In the Extended UNIQUAC model, the Gibbs-Helmholtz equation is used for determining the solubility product at temperatures different from 298.15 K as explained by Thomsen [32]. Fig. 6 shows the calculated diagram along with the experimental data from the literature. For COSMO-RS-ES the solubility calculation did not converge using the solubility product calculated from the NBS tables. This is also expected as the osmotic coefficient predicted by the model at 298.15 K deviates from the experimental value (Fig. 1). For this reason, the solubility product for COSMO-RS-ES was calculated from the activity at the experimental concentration at 298.15 K and then used to predict the solubility at other temperatures. Even though the model has no temperature dependency for electrolyte systems and was only adjusted to experimental data at 298.15 K, it reproduces relatively well the temperature dependence of the solubility in a range of 283.15 to 318.15 K.

5. Conclusions

To apply the Extended UNIQUAC model, experimental data need to be available for determining the parameters. This is a disadvantage of this model. After the parameters have been determined, the model is able to reproduce the experimental data quite accurately in a wide temperature range which is an advantage of this model. COSMO-RS-ES is a predictive model. It requires a parameterization of the relevant ions (Cs^+ and NO_3^-) without necessarily using experimental data for $CsNO_3$, which is a great advantage. The disadvantage of the COSMO-RS-ES model is that the calculated results are less accurate.

The goal of this work was to widen the applicability of Extended UNIQUAC to the system of water + $CsNO_3$ and apply COSMO-RS-ES to temperature dependent data for the first time. The models were able to predict/reproduce data for osmotic coefficients, vapor pressures, and activity coefficients quite well. The Extended UNIQUAC model was able to reproduce the solubility of the water-cesium nitrate system very accurately. COSMO-RS-ES shows its predictive capabilities, being a model without any binary interaction parameters calculating the thermodynamics purely based on ab-initio information. In current works on COSMO-RS-ES, improvements for the temperature dependence in electrolyte systems are being explored.

CRediT authorship contribution statement

Mouad Arrad: Conceptualization, Project administration, Writing – original draft. **Kaj Thomsen:** Investigation, Methodology, Resources, Software, Validation, Writing – original draft, Writing – review & editing. **Simon Müller:** Investigation, Methodology, Project administration, Resources, Software, Validation, Visualization, Writing – original draft. **Irina Smirnova:** Resources, Software, Supervision, Validation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

All data used can be found in the papers listed under references.

References

[1] W.M. Haynes (Ed.), CRC Handbook of Chemistry and Physics, 62nd ed., CRC Press, Boca Raton, FL, 2014 https://doi.org/10.1201/b17118, 9780429170195.

[2] S. Budavari, The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals, 13th ed., Merck, 2001, p. 345. ISBN 0911910131.

[3] B.M. Jones, The spontaneous crystallization of solutions of some alkali nitrates, J. Chem. Soc. Trans. 93 (1908) 1739–1747, https://doi.org/10.1039/CT9089301739.

[4] J.K. Nam, S.U. Chai, W. Cha, Y.J. Choi, W. Kim, M.S. Jung, J. Kwon, D. Kim, J. H. Park, Potassium incorporation for enhanced performance and stability of fully inorganic cesium lead halide perovskite solar cells, Nano Lett. 17 (2017) 2028–2033, https://doi.org/10.1021/acs.nanolett.7b00050.

[5] H.H. Liao, L.M. Chen, Z. Xu, G. Li, Y. Yang, Highly efficient inverted polymer solar cell by low temperature annealing of Cs2CO3 interlayer, Appl. Phys. Lett. 92 (2008) 173303, https://doi.org/10.1063/1.2918983.

[6] Z. Tang, S. Uchida, T. Bessho, T. Kinoshita, H. Segawa, Modulations of various alkali metal cations on organometal halide perovskites and their influence on photovoltaic performance, Nano Energy 45 (2017) 184–192, https://doi.org/10.1016/j.nanoen.2017.12.047.

[7] S.X. Yang, The origin and distribution of salt lakes in Qinghai-Xizang Plateau, J. Lake Sci. 1 (1989) 28–36.

[8] J. Song, Y. Meng, F. Yuan, Y. Guo, Y. Xie, T. Deng, Phase diagrams for the ternary system (NH4NO3+ CsNO3+ H2O) at 298.15 and 348.15K and its application to cesium nitrate recovery from the eluent aqueous solution of ammonium nitrate, J. Mol. Liq. 338 (2021) 117079, https://doi.org/10.1016/j.molliq.2021.117079.

[9] P. Li, K. Sun, J. Hu, Y. Guo, M. Li, J. Duo, T. Deng, Solid-liquid phase equilibria of the ternary system (CsNO3 + NH4NO3 + H2O) at (298.15 and 348.15) K and 101.325 kPa, J. Solution. Chem. 49 (2020) 1373–1381, https://doi.org/10.1007/s10953-020-00999-9.

[10] R.A. Robinson, The osmotic and activity coefficient data of some aqueous salt solutions from vapor pressure measurements, J. Am. Chem. Soc. 59 (1937) 84–90, https://doi.org/10.1021/ja01280a019.

[11] T. Fanghänel, K. Grjotheim, W. Voigt, V. Brendler, Thermodynamics of aqueous reciprocal salt systems .6. isopiestic determination of osmotic coefficients in mixtures of chlorides, bromides and nitrates of lithium, sodium, potassium and cesium at 100.3°C, Acta Chem. Scand. 46 (5) (1992) 423–431.

[12] Yu.G. Frolov, G.I. Nasonova, O.I. Shmel'kova, N.I. Martynova, Study of mixed solutions of heterovalent electrolytes without common ions by the isopiestic method, Tr. Inst. — Mosk. Khim.-Tekhnol. Inst. 136 (1985) 6–11.

[13] V.P. Ryabov, A.A. Ageev, V.P. Nikolaev, Yu.G. Frolov, Use of an isopiestic method to study mixed nickel nitrate-alkali metal nitrate solutions, Trudy Instituta — Moskovskii Khimiko-Tekhnologicheskii Institut imeni D. I. Mendeleeva 71 (1972) 307–309.

[14] A.N. Kirgintsev, A. Vluk'yanov, Ternary solutions by the isopiestic method. VI. Solutions of NaNO3-LiNO3-H2O, NaNO3-KNO3-H2O, NaNO3-NH4NO3-H2O, NaNO3-RbNO3-H2O, and NaNO3-CsNO3-H2O, Zhurnal Fizicheskoi Khimii 39 (5) (1965) 1236–1239.

[15] H.S. Harned, B.B. Owen, The Physical Chemistry of Electrolytic Solutions, 3rd ed., Reinhold Publishing Corp., New York, 1958. American Chemical Society Monograph Series No. 137.

[16] T.W. Richards, A.W. Rowe, The heats of dilution and the specific heats of dilute solutions of nitric acid and of hydroxides and chlorides and nitrates of lithium, sodium, potassium, and cesium, J. Am. Chem. Soc. 43 (1921) 770–796, https://doi.org/10.1021/ja01437a009.

[17] K. Jauch, Die specifische Wärme wässeriger Salzlösungen, Z. Phys. 4 (1921) 441–447, https://doi.org/10.1007/BF01332509.

[18] E. W.Washburn, D.A. MacInnes, The laws of "concentrated" solutions. III. 1 The ionization and hydration relations of electrolytes in aqueous solution at zero degrees: a. cesium nitrate, potassium chloride and lithium chloride, J. Am. Chem. Soc. 33 (11) (1911) 1686–1713, https://doi.org/10.1021/ja02224a005.

[19] W.A. Roth-Greifswald, Kryoskopische Präzisionsmessungen. I: nitrate einwertiger Metalle", Zeitschrift f physic. Chemie—Stochiometrie Und Verwandtschaftslehre 79 (5) (1912) 599–620, https://doi.org/10.1515/zpch-1912-7938.

[20] A. Apelblat, E. Korin, The molar enthalpies of solution and vapour pressures of saturated aqueous solutions of some cesium salts, J. Chem. Thermodyn. 38 (2) (2006) 152–157, https://doi.org/10.1016/j.jct.2005.04.016.

[21] E. Berkeley, On some Physical Constants of Saturated Solutions, Phil. Trans. Roy. Soc. (London) 203A (1904) 189–215. https://www.jstor.org/stable/90862.

[22] M.A. Yakimov, E.V. Zalkind, E.P. Vlasova, Alkali metal nitrate — strontium nitrate—water systems, Russian Journal of Inorganic Chemistry 15 (1) (1970) 103–105.

[23] S.M. Arkhipov, N.I. Kashina, The CsNO3-Cs2CO3-H2O system at 25°C, Zhurnal Neorganicheskoi Khimii 26 (8) (1981) 2272–2273.

[24] D.G. Cherkasov, V.F. Kurskii, S.I. Sinegubova, K.K. Il'in, Topological transformation of the cesium nitrate-water-isopropanol ternary phase diagram, Russian J. Inorg. Chem. 54 (6) (2009) 969–973, https://doi.org/10.1134/S0036023609060217.

[25] D.G. Cherkasov, Z.V. Chepurina, K.K. Il, Phase equilibria and critical phenomena in the cesium nitrate-water-butyric acid ternary system at 5-100°C, Russian J. Phys. Chem. A 89 (8) (2015) 1396–1401, https://doi.org/10.1134/S0036024415080063.

[26] D.S. Abrams, J.M. Prausnitz, Statistical thermodynamics of liquid mixtures: a new expression for the excess Gibbs energy of partly or completely miscible systems, AIChE J. 21 (1) (1975) 116–128, https://doi.org/10.1002/aic.690210115.

[27] K. Thomsen, P. Rasmussen, R. Gani, Correlation and prediction of thermal properties and phase behaviour for a class of electrolyte systems, Chem. Eng. Sci. 51 (1996) 1787–1802, https://doi.org/10.1016/0009-2509(95)00418-1.

[28] Forcrand de, Sur les carbonates neutres de rubidium et de coesium, Comptes rendus hebdomadaires des seances de l academie des sciences 149 (1909) 97–100.

[29] L. Carbonnel and A.P. Rollet, Le système eau-carbonate de cesium », Comptes rendus hebdomadaires des séances de l'Académie des sciences, 256(1963) : 2178–2181(10).
[30] T.A. Dobrynina, B.S. Dzyatkevich, Investigation of peroxyhydrates and hydrates of rubidium and cesium carbonates, Bull. Acad. Sci. USSR Div. Chem. Sci. 16 (4) (1967) 703–706.
[31] M. Hu, L. Jin, Q. Zhai, S. Li, Z. Liu, Liquid-liquid equilibria for some aliphatic alcohols+cesium carbonate+water systems, Fluid. Phase Equilib. 232 (1–2) (2005) 57–61.
[32] K. Thomsen, "Electrolyte solutions: thermodynamics, crystallization, separation methods", Technical University of Denmark, (2009), https://doi.org/10.11581/dtu:00000073.
[33] Harwell Subroutine Library, https://www.hsl.rl.ac.uk/.
[34] T. Gerlach, S. Müller, I. Smirnova, Development of a COSMO-RS based model for the calculation of phase equilibria in electrolyte systems, AIChE J. 64 (1) (2018) 272–285, https://doi.org/10.1002/aic.15875.
[35] T. Gerlach, S. Müller, A.G. de Castilla, I. Smirnova, An open source COSMO-RS implementation and parameterization supporting the efficient implementation of multiple segment descriptors, Fluid. Phase Equilib. 560 (2022) 113472, https://doi.org/10.1016/j.fluid.2022.113472.
[36] A.G. de Castilla, S. Müller, I. Smirnova, On the analogy between the restricted primitive model and capacitor circuits: semi-empirical alternatives for over- and underscreening in the calculation of mean ionic activity coefficients, J. Mol. Liq. 326 (2021) 115204, https://doi.org/10.1016/j.molliq.2020.115204.
[37] A.G. de Castilla, S. Müller, I. Smirnova, On the analogy between the restricted primitive model and capacitor circuits. Part II: a generalized Gibbs-Duhem consistent extension ft he Pitzer-Debye-Hückel term with corrections for low and variable relative permittivity, J. Mol. Liq. 360 (2022) 119398, https://doi.org/10.1016/j.molliq.2022.119398.
[38] S. Müller, A.G. de Castilla, C. Taeschler, A. Klein, I. Smirnova, Evaluation and refinement of the novel predictive electrolyte model COSMO-RS-ES based on solid-liquid equilibria of salts and Gibbs free energies of transfer of ions, Fluid. Phase Equilib. 483 (2019) 165–174, https://doi.org/10.1016/j.fluid.2018.10.023.
[39] S. Müller, A.G. de Castilla, C. Taeschler, A. Klein, I. Smirnova, Calculation of thermodynamic equilibria with the predictive electrolyte model COSMO-RS-ES: improvements for low permittivity systems, Fluid. Phase Equilib. 506 (2020) 112368, 10/gf98vf.
[40] H. Marques, A.G. de Castilla, S. Müller, I. Smirnova, Impact of extended long-range electrostatics on the correlation of liquid-liquid equilibria in aqueous ionic liquid systems, Fluid. Phase Equilib. 569 (2023) 113765, https://doi.org/10.1016/j.fluid.2023.113765.
[41] D.D. Wagman, W.H. Evans, V.B. Parker, R.H. Schumm, I. Halow. The NBS tables of chemical thermodynamic properties. Selected values for inorganic and C1 and C2 organic substances in SI units", DTIC Document, 1982.
[42] D.D. Wagman, W.H. Evans, V.B. Parker, R.H. Schumm, I. Halow, S.M. Bailey, K. L. Churney, R.L. Nuttall, Erratum: the NBS tables of chemical thermodynamic properties. selected values for inorganic and C1 and C2 organic substances in SI units [J. Phys. Chem. Ref. Data 11, Suppl. 2 (1982)], J. Phys. Chem. Ref. Data 18 (Nr. 4) (1989) 1807–1812, https://doi.org/10.1063/1.555845.
[43] J.J. Reed, Digitizing the NBS tables of chemical thermodynamic properties: selected values for inorganic and C1 and C2 organic substances in SI units, NIST 125 (2020). https://www.nist.gov/publications/digitizing-nbs-tables-chemical-thermodynamic-properties-selected-values-inorganic-and.