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Solubility Modeling of Air in Aqueous Electrolyte Solutions with the e-CPA Equation of State

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Short Introduction

This Supporting Information consists of three parts: The e-CPA EoS (Section A); Verification work for H₂O+salt systems (Section B); CPA parameters of water and gases (Section C); Modeling results of gas solubility (Section D).

Section A. The e-CPA EoS¹⁻²

CPA contains two contributions, a cubic EoS (in our case the Soave–Redlich–Kwong EoS (SRK)) for physical interactions, and an association term for describing associating fluids. There are five CPA pure-compound parameters: three SRK parameters and two association parameters (only for associating components). When the CPA EoS is used for mixtures, the classical van der Waals one fluid mixing rules are used for the energy and co-volume parameters¹.

In e-CPA, the residual Helmholtz energy for the cubic Soave–Redlich–Kwong EoS³ is calculated from:

$$A^{SRK} = nRT \left[-\ln \left(1 - \frac{b}{v} \right) - \frac{a(T)}{bRT} \ln \left(1 + \frac{b}{v} \right) \right] \quad (\text{S.1})$$

where n is the total number of moles, T is the temperature, R is the gas constant, v is the molar volume, and b and $a(T)$ are the co-volume parameter and the temperature dependent energy parameter of the mixture, respectively.

$$b = \sum_i x_i b_i \quad (\text{S.2})$$

where b_i is the pure co-volume parameter and x_i is the mole fraction of component i (solvent, gas, cation, anion).

For the binary system of water and gas, the classical one-fluid mixing rule is used for $a(T)$.

$$a(T) = \sum_i \sum_j x_i x_j \sqrt{a_i(T) a_j(T)} (1 - k_{ij}) \quad (\text{S.3})$$

The temperature dependent component specific parameter $a_i(T)$ is given by:

$$a_i = a_{0i} \left(1 + c_{1i} (1 - \sqrt{T_{ri}}) \right)^2 \quad (\text{S.4})$$

where T_{ri} is the reduced temperature of component i , defined as $T_{ri} = T/T_{ci}$, T_{ci} is the critical temperature of component i .

For the binary system involving an ion, the Huron-Vidal/NRTL (HV-NRTL) infinite pressure mixing rule is used, due to its additional flexibility for electrolyte systems²:

$$\frac{a}{b} = \sum_i x_i \frac{a_i}{b_i} - \frac{g^{E,\infty}}{\ln 2} \quad (\text{S.5})$$

$$\frac{g^{E,\infty}}{RT} = \sum_i x_i \frac{\sum_j x_j b_j \exp\left(-\alpha_{ji} \frac{\Delta U_{ji}}{RT}\right) \frac{\Delta U_{ji}}{RT}}{\sum_j x_j b_j \exp\left(-\alpha_{ji} \frac{\Delta U_{ji}}{RT}\right)} \quad (\text{S.6})$$

where $g^{E,\infty}$ is the excess Gibbs energy at infinite pressure calculated with the NRTL equation, α_{ji} is the NRTL non-randomness parameter, ΔU_{ji} is the change in interaction energy between like and unlike interactions ($\Delta U_{ji} = \Delta U_{ij} - \Delta U_{jj}$).

It is worth pointing out that the HV-NRTL infinite pressure mixing rule has the flexibility to reduce to the classical one-fluid mixing rule if α_{ji} is set to zero and ΔU_{ji} is appropriately chosen.

In order to apply e-CPA over a wide range of temperature, a quadratic temperature dependence for the interaction parameter was proposed²:

$$\frac{\Delta U_{ij}}{R} = \frac{\Delta U_{ij}^{ref}}{R} + \omega_{\Delta U_{ij}} \left[\left(1 - \frac{T}{T_{\Delta U_{ij}}}\right)^2 - \left(1 - \frac{T_{ref}}{T_{\Delta U_{ij}}}\right)^2 \right] \quad (\text{S.7})$$

where ΔU_{ij}^{ref} is a binary interaction parameter between cation/anion and solvent/gas at the reference temperature, $\omega_{\Delta U_{ij}}$ is an adjustable parameter for the linear dependency in the interaction energy calculation, $T_{\Delta U_{ij}}$ is a parameter of the temperature dependency. T_{ref} is the reference temperature at which ΔU_{ij}^{ref} is valid, T_{ref} is set to 298.15 K in this work.

The residual Helmholtz energy for association A^{Assoc} is based on the formulation of Wertheim's association theory⁴⁻⁵ and can be found from the solution of the constrained optimization problem⁶ given by:

$$A^{Assoc} = RT \left[\sum_i n_i \sum_{A_i} \left(\ln X_{A_i} - \frac{1}{2} X_{A_i} + \frac{1}{2} \right) \right] \quad (\text{S.8})$$

$$\frac{1}{X_{A_i}} = 1 + \sum_j \rho_j \sum_{B_i} X_{B_j} \Delta_{A_i B_j} \quad (\text{S.9})$$

where n_i is the number of moles of component i , X_{A_i} is the fraction of site A on component i that is not bonded to any other site, ρ_j is the density of component j , and $\Delta_{A_i B_j}$ is the association strength, which is calculated from:

$$\Delta_{A_i B_j} = g(\rho) \left[\exp\left(\frac{\varepsilon^{A_i B_j}}{k_B T}\right) - 1 \right] b_{ij} \beta^{A_i B_j} \quad (\text{S.10})$$

where the two association parameters are the association volume, $\beta^{A_i B_j}$, and the association energy, $\varepsilon^{A_i B_j}$, while b_{ij} is given by $b_{ij} = (b_i + b_j)/2$, corresponding to Eq. (A.2). The simplified radial distribution function is expressed as: $g(\rho) = (1 - 1.9\eta)^{-1}$, and the packing fraction η is equal to $b/4v$.

The contribution to the Helmholtz energy from the long-range interaction of the ions is calculated from the DH theory⁷, as shown in the following equation:

$$A^{DH} = -\frac{k_B T V}{4\pi N_A \sum_i n_i Z_i^2} \sum_i n_i Z_i^2 \chi_i \quad (\text{S.11})$$

And the function χ_i is given by:

$$\chi_i = \frac{1}{d_i^3} \left[\ln(1 + \kappa d_i) - \kappa d_i + \frac{1}{2} (\kappa d_i)^2 \right] \quad (\text{S.12})$$

where κ is the inverse Debye screening length, and d_i is the hard-sphere diameter of the ion.

Finally, the contribution of ion solvation comes from the Born equation²¹:

$$A^{Born} = \frac{N_A e^2}{8\pi \varepsilon_0} \sum_i \frac{n_i Z_i^2}{r_{Born,i}} \left(\frac{1}{\varepsilon_r} - 1 \right) \quad (\text{S.13})$$

where $r_{Born,i}$ is the radius of the Born cavity caused by the transfer from vacuum to the fluid phase, and e is the elementary charge.

The relative static permittivity ε_r is of central importance in the thermodynamics of electrolyte solutions. In e-CPA, the model developed by Maribo-Mogensen et al.⁸ for the relative static permittivity is used in both the DH and Born terms.

Section B. Verification Work for H2O+Salt Systems

Table S1. e-CPA performance of mean ionic activity coefficients γ_{\pm}^m and osmotic coefficients Φ for some H₂O-salt binary systems.

Salt ²	$\Delta U_{ij}^{ref} / R$ [K]	$T_{\Delta U_{ij}}$ [K]	$\omega_{\Delta U_{ij}}$ [K]	T [K]	m_{max}	RAD ^b [%]	
						γ_{\pm}^m	Φ
NaCl	-223.5	340	1573	273.15-473.15	7.973 ⁹⁻¹⁰	2.3	1.6
KCl	-130.0	340	1361	273.15-373.15	6.0 ¹¹⁻¹²	0.86	0.65
CaCl ₂	-380.8	340	2778	298.15	3.0 ¹³⁻¹⁴	5.3	3.3
MgCl ₂	-459.6	340	2439	298.15	3.0 ^{14,15}	5.9	4.0
BaCl ₂	-166.7	300	1226	298.15	2.0 ¹⁶⁻¹⁸	6.7	1.1
RbCl	-136.2	340	1087	298.15	6.0 ¹⁷	1.0	1.3
LiCl	-440.6	340	1853	298.15	6.0 ¹⁶⁻¹⁸	5.5	3.4
SrCl ₂	-315.3	340	2260	298.15	3.5 ¹⁹	5.9	4.0
NaBr	-280.3	350	1322	298.15	5.0 ^{17,20}	5.6	2.8
KBr	-162.8	350	1047	298.15	5.0 ¹⁷	1.4	0.8
CsBr	-133.3	350	673.1	298.15	5.0 ^{12,17}	4.5	1.8
NaI	-308.6	360	849.7	298.15	3.5 ¹⁷	5.7	3.3
KI	-197.8	360	1224	298.15	4.5 ¹⁷	2.6	1.3
Na ₂ SO ₄	123.8	300	1163	298.15-323.15	3.7 ²¹⁻²²	2.0	1.3
K ₂ SO ₄	77.38	300	891.5	298.15	2.0 ^{9,17-18,20}	1.2	0.7
MgSO ₄	118.9	300	2470	298.15	3.0 ¹⁷	7.5	7.9
NaNO ₃	-40.88	340	846.0	298.15	6.0 ^{17,21}	4.3	
Ca(NO ₃) ₂	-187.8	340	1624	298.15	2.0 ¹⁷	8.6	1.4
NaOH	-299.7	273	1209	298.15	6.0 ^{17,21}	3.9	4.3
KOH	-382.3	273	1145	298.15	6.0 ¹⁷	2.4	2.5

Section C. CPA Parameters of Water and Gases

Table S2. CPA parameters for pure components.

Compound	T_c [K]	b [L/mol]	Γ [K]	c_1	$\varepsilon^{A_i B_j}/R$ [K]	$\beta^{A_i B_j} \cdot 10^3$	Association scheme
H ₂ O [1]	647.13	0.014.515	1017.34	0.6736	2003.25	69.2	4C
CO ₂ [23]	304.21	0.0272	1551.222	0.7602	0	0	n.a.
CH ₄ [23]	190.56	0.02910	959.028	0.44718	0	0	n.a.
N ₂ [24]	126.20	0.02605	634.070	0.49855	0	0	n.a.
O ₂ [23]	154.58	0.0216	773.974	0.47540	0	0	n.a.
argon	150.8 ²⁵	0.02039	776.313	0.30615	0	0	n.a.

In Table A1, ‘n.a.’ means Non-association, T_c is the critical temperature, b is the CPA co-volume parameter (in Eq. (A.1)), Γ is the CPA reduced energy parameter ($\Gamma = a_0/(Rb)$), c_1 is the CPA alpha-function temperature-dependence (in Eq. (A.4)); CPA parameters of argon are obtained in this work (temperature range is 83.9K-150.4K (number of data points is 134). RAD of saturation pressure is 4.7% , RAD of liquid density is 5.6%).

Table S3. Modelling performance of gas solubilities in pure water with CPA.

Gas	Binary interaction parameters k_{ij} *	Performance of gas solubilities		
		RAD [%]/Np	T [K]	P [MPa]
CO ₂ ²⁶	-0.15508+0.000877T	8.3 / 328	273.75-473.15	0.095-82.880
CH ₄ ²⁶	0.8243-245.33/T	4.5 / 206	274.19-444.26	0.101-100.000
N ₂ ²⁷	1.0741-368.3066/T	5.4 / 176	274.10-628.00	0.534-101.325
O ₂	1.3502-377.6474/T	3.2 / 458 ²⁸⁻⁴⁶	273.15-560.93	0.026-20.684
Argon	1.5881-421.0919/ T	1.1 / 115 ^{33-34, 47-59}	273.35- 453.70	0.101-12.670

* in Eq. (S.3) of Supporting Information.

Section D. Modeling Results of Gas Solubility

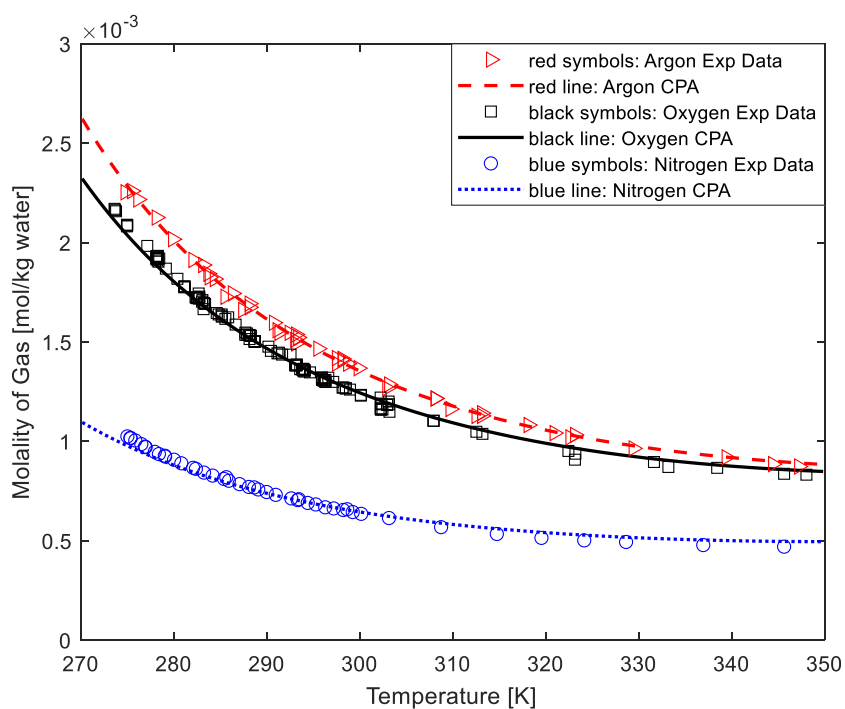


Figure S1. Solubilities of N_2 , O_2 and argon in pure water at atmospheric pressure (N_2 ^{31, 33}, O_2 ^{31-32, 34-36, 39} and argon^{33, 47-48, 52}).

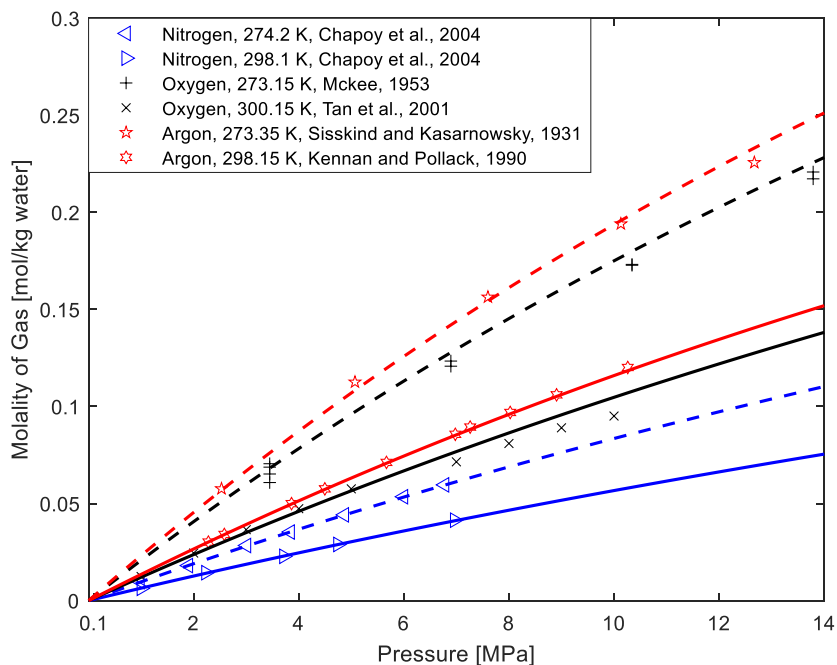


Figure S2. Solubilities of N_2 , O_2 and argon in pure water at different temperatures and pressures^{42, 45, 57, 59-60}.

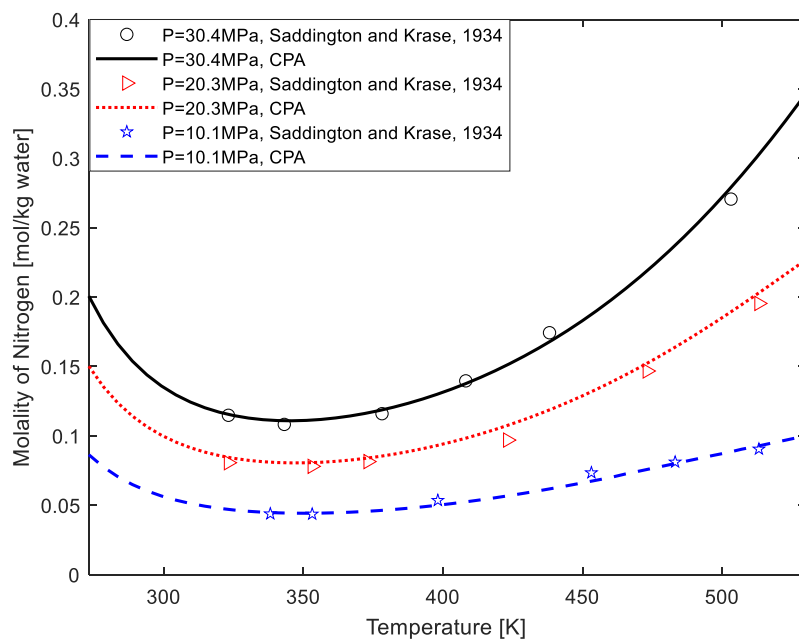


Figure S3. Solubilities of N_2 in pure water⁶¹ at different temperatures and high pressures.

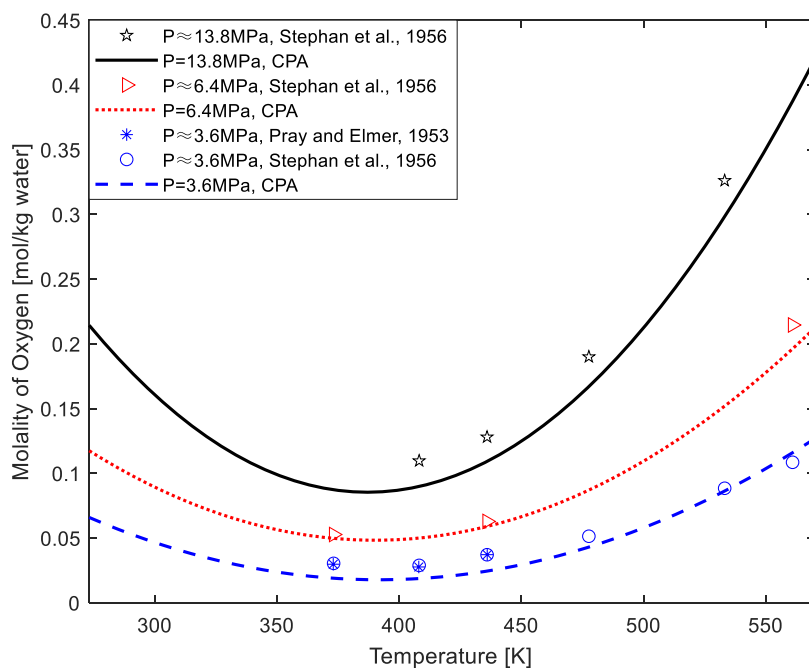


Figure S4. Solubilities of O_2 in pure water^{41, 43} at different temperatures and high pressures.

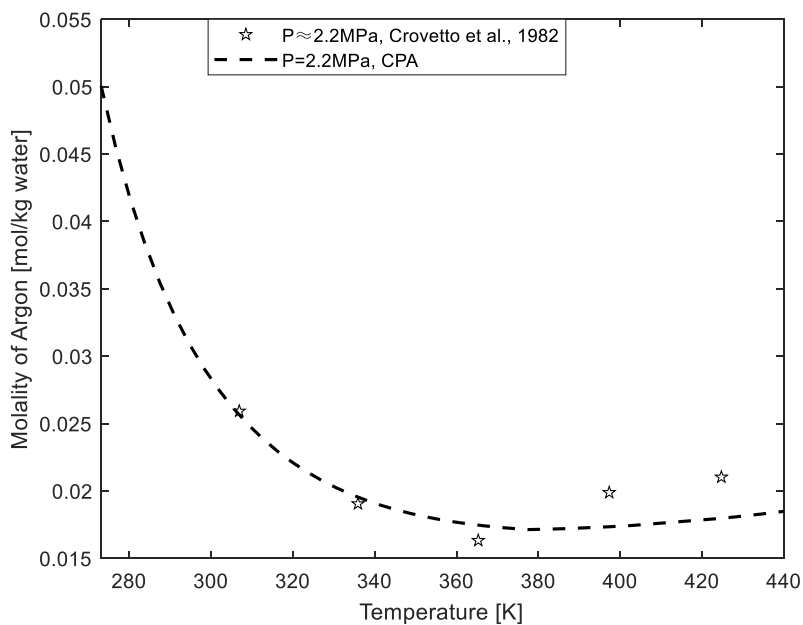


Figure S5. Solubilities of argon in pure water⁵⁸ at different temperatures and at 2.2 MPa.

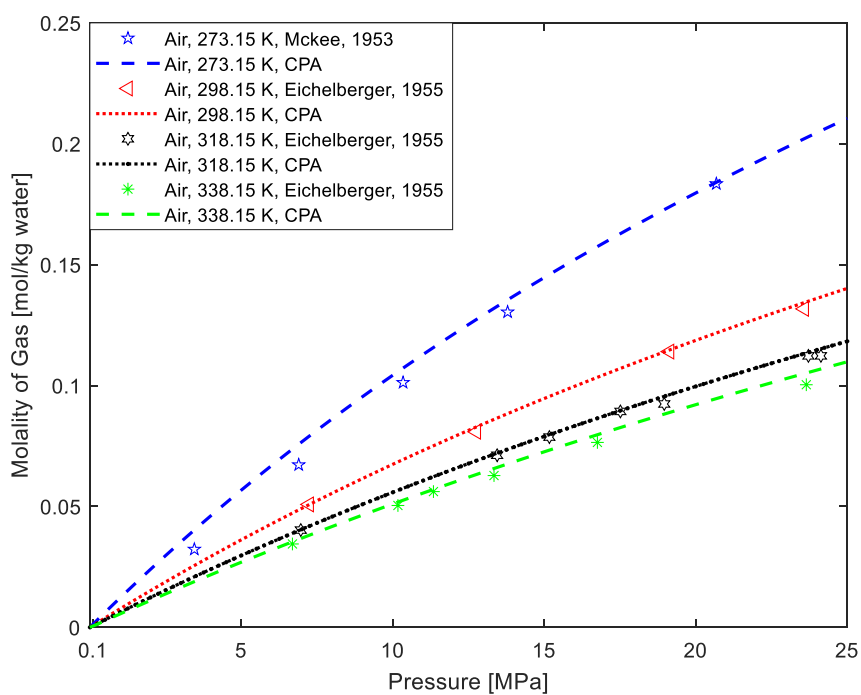
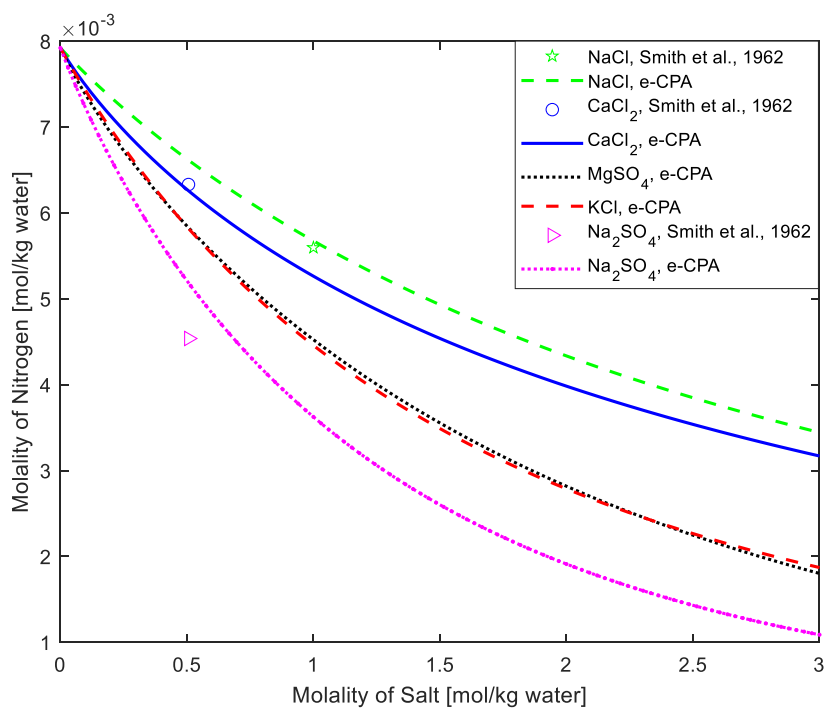
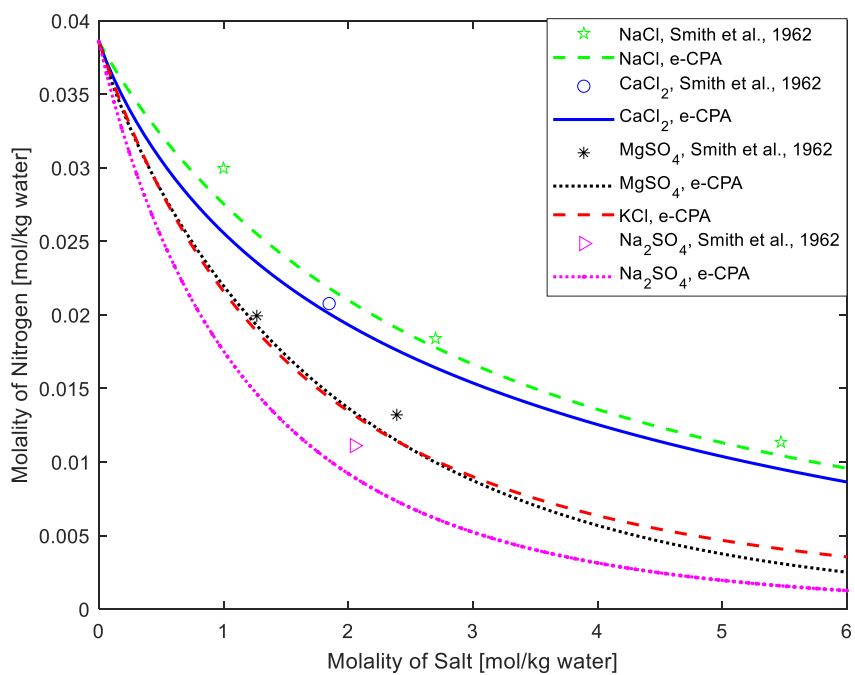


Figure S6. Solubilities of air in pure water at different temperatures and pressures^{42, 62}.



(a) P=1.25 MPa



(b) P=6.50 MPa

Figure S7. Solubilities of N₂ in different aqueous solutions at different pressures at 303.15 K⁶³.

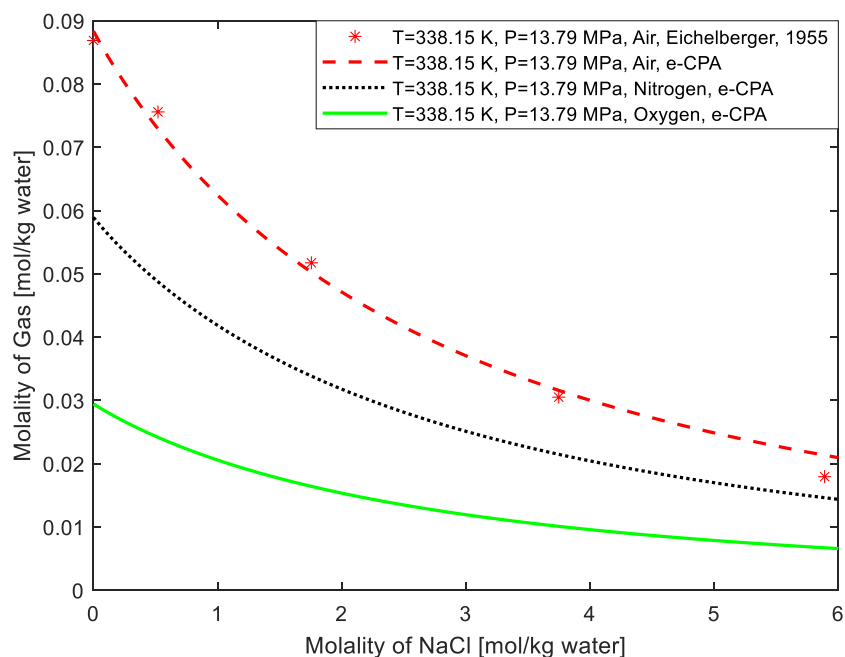


Figure S8. Solubilities of air in aqueous NaCl solution at 338.15 K⁶².

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