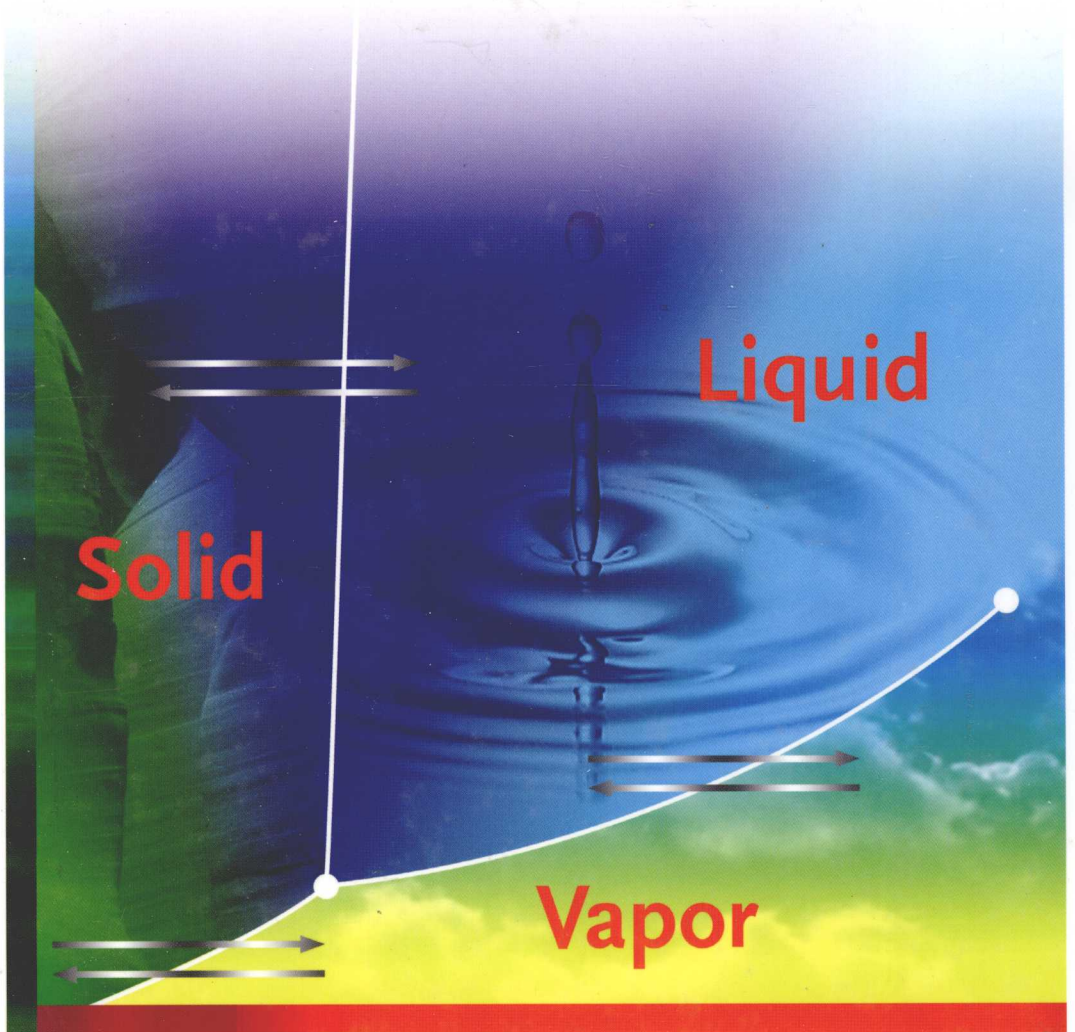


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Michael Kleiber and Jürgen Rarey

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Chemical Thermodynamics for Process Simulation



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and Jürgen Rarey*

Chemical Thermodynamics

for Process Simulation



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Authors



Jürgen Gmehling I finished an apprenticeship as a laboratory technician and studied Chemical Engineering at the Technical College in Essen before studying Chemistry leading to the degree of Diplom-Chemiker in 1970 and my doctoral degree from the University of Dortmund in Inorganic Chemistry in 1973. After graduation I worked in the research group of Prof. Ulfert Onken (Chair of Chemical Engineering) at the University of Dortmund. My research activities were directed to applied thermodynamics, in particular the development of group contribution methods

and the synthesis of separation processes. From 1977–1978 I spent 15 months with Prof. J.M. Prausnitz at the Department of Chemical Engineering in Berkeley, California.

In 1989 I joined the faculty of the University of Oldenburg as Professor of Chemical Engineering. The research activities of my group are mainly directed to the computer-aided synthesis, design and optimization of chemical processes. Our research results, in particular the software products, such as the Dortmund Data Bank, the group contribution methods for nonelectrolyte and electrolyte systems (UNIFAC, modified UNIFAC, PSRK, VTPR, LIQUAC, LIFAC, COSMO-RS(Ol)) and the sophisticated software packages for process developments are used worldwide by a large number of chemical engineers in industry during their daily work. The importance of the group contribution methods developed by us is demonstrated by the fact that the systematic further development of these methods is supported by a consortium of more than 50 companies for more than 15 years.

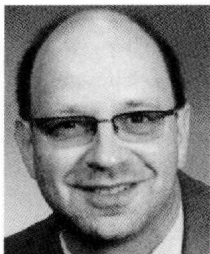
I am also president and CEO of the company “DDB Software and Separation Technology (DDBST), Oldenburg, Germany (www.ddbst.com)” founded by myself and two coworkers in 1989. This company is responsible for the Dortmund Data Bank (DDB), the largest worldwide factual data bank for thermophysical properties, and at the same time engaged in consulting and developing software for the synthesis and design of separation processes. In collaboration with Dr. K. Fischer I founded the “Laboratory for Thermophysical Properties (LTP GmbH (www.ltp-oldenburg.de))” as an “An-Institute” at the Carl von Ossietzky University of Oldenburg in 1999, a company that is engaged in the measurement of thermophysical data (pure component properties, phase equilibria, excess properties, transport properties, reaction rates, etc.) over wide temperature and pressure ranges.

For my research activities I have received various awards, e.g. the “Arnold-Eucken Prize” in 1982 from GVC (Gesellschaft für Verfahrenstechnik und Chemieingenieurwesen), the “Rossini Lecture Award 2008” from the International Association of Chemical Thermodynamics and 2010 the “Gmelin-Beilstein Denkmünze” from GDCh (Gesellschaft Deutscher Chemiker).



Bärbel Kolbe After graduating in Chemical Engineering I finished my thesis on the description and measurement of the properties of liquid mixtures at the University of Dortmund in the research group of Jürgen Gmehling in 1983. I continued to work with Jürgen Gmehling for another 3 years. During this time I participated in the publication of the Dechema Chemistry Data Series on VLE and the first edition of this book in the German language was being written.

I have been working for more than twenty years as a senior process engineer first for the Krupp Koppers GmbH and, since 1997, for ThyssenKrupp Uhde. Within the research and development department of ThyssenKrupp Uhde my main focuses are thermophysical properties, thermal separation technology and new processes.



Michael Kleiber After having graduated in mechanical engineering, I worked as a scientific assistant and finished my thesis at the Technical University of Brunswick in 1994 with a supplement to the UNIFAC method for halogenated hydrocarbons. In the following years, I worked for the former Hoechst AG and their legal successors in a wide variety of tasks in the fields of process development, process simulation and engineering calculations. Meanwhile, I moved to ThyssenKrupp Uhde as a colleague of Bärbel Kolbe as Chief Development Engineer. I am a member of the German Board of Thermodynamics and have made contributions to several process engineering standard books like VDI Heat Atlas, Winnacker-Küchler and Ullmann's Encyclopedia of Industrial Chemistry.



Jürgen Rarey I studied and graduated in Chemistry and did my PhD in Chemical Engineering. I built my first computer in the 3rd year of study and developed some interfacing to lab equipment and control software. I became fascinated by the possibilities of simulation and learned the importance of the correct description of basic phenomena to the outcome of simulations (garbage in – garbage out).

In 1989, near the end of my PhD study, I moved to Oldenburg in northern Germany. Since April 1989 I have held a permanent position at the University of Oldenburg in the group of Prof. Gmehling.

In the same year I cofounded DDBST GmbH (www.ddbst.com). This company today is the most well-known provider of thermophysical property data and estimation methods for process simulation and further applications in safety, environmental protection, etc.

Since the 1980s I have taught many courses on applied thermodynamics for chemical process simulation for external participants from industry both in Oldenburg and in-house for companies in Europe, the US, Middle East, South Africa, Japan, etc. (alone or together with Prof. Gmehling).

An additional role in my professional life is a Honorary Professor position in Durban, South Africa. Currently, my group there consists of 4 MSc students, all highly motivated. We developed and published estimation methods for a number of important properties like vapor pressure, liquid viscosity, water and alkane solubility, etc. The first of our methods on normal boiling point estimation is already generally regarded as the primary and best method available.

Preface

More than 20 years ago, the first edition of the textbook *Thermodynamics* was published in the German language.

Its target was to demonstrate the basic principles, how thermodynamics can contribute to solve manifold kinds of problems in gas, oil and chemical processing, pharmaceutical and food production, in environmental industry, in plant design by engineering companies, and also for institutions dealing with hazardous materials like the fire brigade, transport companies or the Technical Supervisory Associations. For all these purposes, it is often decisive to have a profound knowledge of the thermophysical properties, transport properties, phase equilibria, and chemical equilibria. Therefore, a large part of the first edition and also of this completely new edition is dedicated to the evaluation of these quantities. The mentioned properties are also helpful in the evaluation of nonequilibrium properties such as kinetic data and reaction rates, which are not subject of this book.

Databases filing published experimental physical properties and phase equilibrium data are a prerequisite for developing thermodynamic models and for determining reliable model parameters, which describe the problem to be solved with adequate accuracy. A long way has been covered since the beginning of the professional filing of phase equilibrium data. Starting with a few hundred compounds in 1973, pure component and mixture properties for more than 33 000 components can now be found in the Dortmund Data Bank (DDB). A great step forward in modeling was the further development of the solution of group concept, which makes the prediction of, for example, phase equilibria possible. A lot of experimental work was performed to systematically fill the gaps where no data for the determination of group interaction parameters were available. Together with the fast developing computer technology and on the basis of professional databases like the DDB, process simulators nowadays allow rapid calculation of phase equilibria, transport properties, caloric data, the various thermophysical properties, and chemical equilibria. Even the thermodynamics of large industrial processes is routinely modeled using commercial process simulators. While a large variety of models and model options can be selected by a simple mouse-click, the task of the engineer or chemist remains to choose the most appropriate model, and one should be aware of its accuracy, its possible limitations, and the quality

of the model parameters for the system of interest. A thorough understanding of thermodynamics is still obligatory; otherwise misconceptions of processes or design errors are the consequences.

The new edition of the textbook, now written in the English language, is called *Chemical Thermodynamics for Process Simulation*. It specifically targets readers working in the fields of process development, process synthesis, or process optimization and therefore presents the fundamentals of thermodynamics not only for students but also on the level required for experienced process engineers. The most important models that are applied in process industry are thoroughly explained, as well as their adjustment with the help of factual databases (data regression). Cubic equations of state with g^E mixing rules present a great step forward toward a universal model for both subcritical and supercritical systems and are therefore emphasized.

In addition, models for special substances like carboxylic acids, hydrogen fluoride, formaldehyde, electrolytes, and polymers are introduced and the capabilities of high-precision equations of state and various predictive methods are explained. Recommendations for the parameter fitting procedure and numerous hints to avoid pitfalls during process simulation are given. Because of the space limitation in the book we were not able to cover the whole range of thermodynamics, for example, adsorption has been left out completely as it cannot be presented within a short chapter.

The English language was chosen to extend the readership to students and engineers from all over the world. Although none of the authors is a native speaker, we found it even more convenient to describe the particular issues in the language generally used in scientific publications.

The team of four authors with considerably different backgrounds reflects the importance of thermodynamics in both academia and industrial application. The authors present their biography and special research interests on separate pages following this preface.

In contrast to other textbooks on thermodynamics, we assume that the readers are familiar with the fundamentals of classical thermodynamics, that means the definitions of quantities like pressure, temperature, internal energy, enthalpy, entropy, and the three laws of thermodynamics, which are very well explained in other textbooks. We therefore restricted ourselves to only a brief introduction and devoted more space to the description of the real behavior of the pure compounds and their mixtures. The ideal gas law is mainly used as a reference state; for application examples, the real behavior of gases and liquids is calculated with modern g^E models, equations of state, and group contribution methods.

Of course, by taking into account the real behavior the solution of the examples becomes much more complex, but at the same time they are closer to industrial practice. For a textbook, there is a difficulty to describe the typical iterative procedures in phase equilibrium and process calculations. In order to achieve a better understanding, we decided to provide MathCAD-sheets and DDBST programs so that the reader has the chance to reproduce the examples on his own. MathCAD was chosen because of its convenient way to write equations in

close-to-textbook form and without cryptic variable names. We prefer SI units but do not stick to them obsessively. In the examples and diagrams we used the most convenient units. We think that the parallel use of various units will remain the status quo for the time being, and engineers and chemists should be able to cope with this situation. We are aware that the current value of the gas constant is $R = 8.31447 \text{ J}/(\text{mol K})$. However, still many applications are based on the old value $R = 8.31433 \text{ J}/(\text{mol K})$. Luckily, except for the high-precision equations of state this distinction is by far beyond the accuracy scope of our calculations.

For a complete understanding, mathematical derivations can often not be avoided or are even necessary for the understanding. If they interrupt the flow of the presentation, we have moved them to a special chapter in the Appendix, so that the reader can follow the main ideas more easily. Of course, no textbook can cover all possible and interesting derivations, but we hope that the reader will gain a feeling for the methodology in thermodynamics and is able to carry out similar derivations on his own.

We hope that this book closes a gap between scientific development and its application in industry. We are grateful to all the people who gave us valuable support and advice during the compilation of the manuscript. None of the authors was capable to write an adequate chapter on polymer thermodynamics. Therefore we are especially obliged to Prof. Dr. Sabine Enders. She wrote an excellent chapter fully in line with the targets and structure of this book. Many other people gave valuable advice. We are thankful to Prof. Dr. Wolfgang Wagner, Prof. Dr. Hans Hasse, Prof. Dr. Josef Novak, Prof. Dr. Roland Span, Todd Willman, Dr. Michael Sakuth, Ingo Schillgalies, Jens Otten, Dr. André Mohs, Dr. Bastian Schmid, Dr. Jens Ahlers, Dr. Silke Nebig, Dr. Torben Laursen, Dr. Heiner Landeck, Prof. Dr. Ravi Prasad Andra, Dr. Michael Benje, the colleagues and coworkers from DDBST GmbH and the research group at the Carl-von-Ossietzky-University of Oldenburg, who provided many impressive figures of the book. Furthermore, we are deeply thankful to our families for supporting us during all the time.

*Jürgen Gmehling
Bärbel Kolbe
Michael Kleiber
Jürgen Rarey*

List of Symbols

a	attractive parameter in cubic equations of state	$\text{J m}^3 \text{mol}^{-2}$
a	specific Helmholtz energy	$\text{J mol}^{-1}, \text{J kg}^{-1}$
a_i	activity of component i	
$a_{ij}, b_{ij}, c_{ij}, d_{ij}$	binary or group interaction parameter in local composition models (Wilson, NRTL, UNIQUAC, UNIFAC ...)	
A	Helmholtz energy	J
A	area	m^2
A_m	parameter in Debye–Hückel equation	$\text{kg}^{0.5} \text{mol}^{0.5}$
a, b, c, \dots	constants in pure component property correlations	
A, B, C, \dots	constants in pure component property correlations	
A_n, B_n	parameters for the description of association reactions of degree n	
A_ϕ	parameter in Pitzer–Debye–Hückel term	
b	repulsive parameter in equations of state	$\text{m}^3 \text{mol}^{-1}$
B	second virial coefficient	$\text{m}^3 \text{mol}^{-1}$
B_{ij}	parameter in Pitzer equation	
B_{ij}	cross second virial coefficient	$\text{m}^3 \text{mol}^{-1}$
c	volume concentration	mol m^{-3}
c_p	specific isobaric heat capacity	$\text{J mol}^{-1} \text{K}^{-1},$ $\text{J kg}^{-1} \text{K}^{-1}$
c_v	specific isochoric heat capacity	$\text{J mol}^{-1} \text{K}^{-1},$ $\text{J kg}^{-1} \text{K}^{-1}$
c_σ	specific liquid heat of vaporization along the saturation line	$\text{J mol}^{-1} \text{K}^{-1},$ $\text{J kg}^{-1} \text{K}^{-1}$
C	third virial coefficient	$(\text{m}^3)^2 \text{mol}^{-2}$
d	droplet diameter	m
d_i	segment diameter (PC-SAFT)	m
D_{ij}	diffusion coefficient of component i in component j	$\text{m}^2 \text{s}^{-1}$
e	elementary charge; $e = 1.602189 \cdot 10^{-19} \text{ C}$	C
E	Ackermann correction factor	
f_i	fugacity of component i	Pa
F	objective function	
F	Faraday's constant; $F = 96484.56 \text{ C/mol}$	C mol^{-1}
F_i	surface area/mole fraction of component i (UNIQUAC, UNIFAC)	–
$F(x)$	integral distribution function	

F_{ij}	force between two ions i and j	N
g	specific Gibbs energy	J mol ⁻¹
Δg	Gibbs energy of mixing	J mol ⁻¹
Δg_{ij}	interaction parameter of the NRTL equation	K
Δg_R^0	standard Gibbs energy of reaction	J mol ⁻¹
G	Gibbs energy	J
h	Planck's constant; $h = 6.6242 \cdot 10^{-34}$ Js	Js
h	specific enthalpy	J mol ⁻¹ , J kg ⁻¹
Δh_f^0	standard enthalpy of formation	J mol ⁻¹
Δg_f^0	standard Gibbs energy of formation	J mol ⁻¹
Δh_R^0	standard enthalpy of reaction	J mol ⁻¹
Δh_m	specific enthalpy of fusion	J mol ⁻¹ , J kg ⁻¹
$h - h^{\text{id}}$	specific isothermal enthalpy difference between actual and ideal gas state, calculated with an EOS	J mol ⁻¹
$\Delta h_i^{\infty L}$	specific enthalpy of solution of Henry component i	J mol ⁻¹
Δh_{sol}	enthalpy of solution	J mol ⁻¹ , J kg ⁻¹
Δh_v	specific enthalpy of vaporization	J mol ⁻¹ , J kg ⁻¹
H	enthalpy	J
H_{ij}	Henry constant of component i in solvent j	Pa
I	ionic strength	mol kg ⁻¹
I_x	molar ionic strength	mol mol ⁻¹
J_i	flux through membrane of component i	kg s ⁻¹ m ⁻²
k	Boltzmann's constant; $k = 1.38048 \cdot 10^{-23}$ J/K	J/K
k_{ij}	binary interaction parameter in cubic equations of state	
K	chemical equilibrium constant	
K	liquid-liquid distribution coefficient	
K_{cry}	cryoscopic constant	K kg mol ⁻¹
K_{sp}	solubility product	
K_n	chemical equilibrium constant for association of degree n	
K_{in}	chemical equilibrium constant for association of degree n , component i	
K_{Mij}	chemical equilibrium constant for mixed association, components i and j	
K_i	K-factor for component i ($K_i = y_i/x_i$)	
l	membrane thickness	m
L	amount of liquid	mol, kg
m	arbitrary specific thermodynamic function	
m	mass	kg
m_i	molality of component i	mol kg ⁻¹
\bar{m}_i	partial molar property	
\dot{m}	mass flow	kg s ⁻¹
M	molar mass	g mol ⁻¹
\bar{M}	moment of distribution function	
$\Delta m, \Delta M$	property change of mixing	
n	number of components	
n	number of data points	
\dot{n}	mole flow	mol s ⁻¹
n_A	number of atoms in a molecule	
N_A	Avogadro's number; $N_A = 6.023 \cdot 10^{23}$	
N_{th}	number of theoretical stages	

n_f	number of degrees of freedom	
n_i	number of moles of component i	mol
n_T	total number of moles	mol
N	total number of species	mol
Nu	Nusselt number	
p_i	partial pressure of component i	Pa
P	Parachor	
P	total pressure	Pa
P_i	permeability	$\text{kg s}^{-1} \text{m}^{-1} \text{Pa}^{-1}$
P^G	vapor pressure around a droplet	Pa
P^*	apparent permeability	$\text{kg s}^{-1} \text{m}^{-2} \text{Pa}^{-1}$
P_i^s	vapor pressure of component i	Pa
Poy_i	Poynting factor of component i	
Pr	Prandtl number	
q_i	relative van der Waals surface area of component i	
q	charge	C
q	vapor fraction	
q	specific heat	$\text{J mol}^{-1}, \text{J kg}^{-1}$
\dot{q}	specific heat flux	$\text{W mol}^{-1}, \text{W kg}^{-1}$
Q	heat	J
\dot{Q}	heat flow	W
Q_k	relative van der Waals surface area of group k	
r_i	relative van der Waals volume of component i	
r_i	ionic radius	
r_i	segment number	
r_{ij}	distance between two ions i and j	m
R	universal gas constant; $R = 8.314471 \text{ J/mol K} = 1.98721 \text{ cal/mol K}$	$\text{J mol}^{-1} \text{K}^{-1}$
Re	Reynolds number	
R_k	relative van der Waals volume of group k	
s	specific entropy	$\text{J mol}^{-1} \text{K}^{-1},$ $\text{J kg}^{-1} \text{K}^{-1}$
s_{abs}	absolute specific entropy	$\text{J mol}^{-1} \text{K}^{-1},$ $\text{J kg}^{-1} \text{K}^{-1}$
Δs^{id}	specific entropy of mixing	$\text{J mol}^{-1} \text{K}^{-1},$ $\text{J kg}^{-1} \text{K}^{-1}$
Δs_R^0	standard entropy of reaction	$\text{J mol}^{-1} \text{K}^{-1},$ $\text{J kg}^{-1} \text{K}^{-1}$
S	entropy	J K^{-1}
S_{12}	selectivity	
T	absolute temperature	K
u	specific internal energy	$\text{J mol}^{-1}, \text{J kg}^{-1}$
Δu_{ij}	interaction parameter of the NRTL equation	K
u	internal energy	J
V	amount of vapor	mol, kg
v	specific volume	$\text{m}^3 \text{mol}^{-1},$ $\text{m}^3 \text{kg}^{-1}$
v^*	characteristic volume	$\text{m}^3 \text{mol}^{-1}$
V	volume	m^3
V_i	volume fraction/mole fraction of component i (UNIQUAC, UNIFAC)	

w	specific work	$\text{J mol}^{-1}, \text{J kg}^{-1}$
w	velocity	m s^{-1}
w^*	speed of sound	m s^{-1}
W_t	technical work	J
w_t	specific technical work	$\text{J mol}^{-1}, \text{J kg}^{-1}$
w	weighting factor in objective functions	
$W(r)$	distribution function	
w_i	weighting factor of data point i	
w_i	weight fraction of component i	
x_i	mole fraction of component i in the liquid phase	
x_i'	mole fraction of component i on salt-free basis	
X	group mole fraction	
X	chemical conversion	
γ	mole fraction in the vapor phase	
z	compressibility factor; $z = Pv/RT$	
z	length	m
z_i	charge of ion i	C
z_i	mole fraction	
z_n	true mole fraction of associate of degree n	
z_{in}	true mole fraction of associate of degree n , component i	
z_{Mij}	true mole fraction of mixed associate, components i and j	
\bar{z}	segment molar quantity	

Greek Symbols

α_{ij}	separation factor	
α_{ij}	nonrandomness parameter in the NRTL equation	
α	thermal expansion coefficient	K^{-1}
α	degree of dissociation	
α	heat transfer coefficient	$\text{W m}^2 \text{K}^{-1}$
α	function in cubic EOS	
α	reduced Helmholtz energy in high precision EOS	
α, β, γ	constants in pure component property correlations	
γ_i	activity coefficient of component i	
β	parameter in Bromley equation	kg mol^{-1}
β	mass transfer coefficient	m s^{-1}
Γ_k	group activity coefficient	
δ_i	solubility parameter of component i	$(\text{J m}^{-3})^{0.5}$
δ_{ij}	excess virial coefficient	$\text{m}^3 \text{mol}^{-1}$
Δ	difference value of a thermodynamic property	
Δ_b	group increment for normal boiling point	
$\Delta_A, \Delta_B, \Delta_C, \Delta_D$	group constants for c_p^{id}	
$\Delta_{\text{Born}}^{\text{E}}$	Born term for regarding the dielectricity constant of the solvent	J mol^{-1}
Δ_G	group increment for standard Gibbs energy of formation	
Δ_H	group increment for standard enthalpy of formation	
Δ_T	group increment for critical temperature	
Δ_P	group increment for critical pressure	
Δ_V	group increment for critical volume	
ε	depth of potential well (PC-SAFT)	

ε	stop criterion	
ε	performance number	
ε	relative dielectricity constant	
ε_0	vacuum dielectricity constant; $\varepsilon_0 = 8.854188 \cdot 10^{-12} \text{ C}^2 \text{ N}^{-1} \text{ m}^{-2}$	$\text{C}^2 \text{ N}^{-1} \text{ m}^{-2}$
ζ	local volume fraction	
ζ	local volume fraction	
η	dynamic viscosity	Pa s
η	efficiency	
ϑ	Celsius temperature	$^{\circ}\text{C}$
Θ_k	surface area fraction of group k (UNIFAC)	
Θ_{ij}	local concentration of species i around species j	
χ	isothermal compressibility factor	Pa^{-1}
κ	isentropic exponent; $\kappa = c_p^{\text{id}}/c_v^{\text{id}}$	
λ	reduced well width (PC-SAFT)	
λ	thermal conductivity	$\text{W K}^{-1} \text{ m}^{-1}$
λ_{ij}	parameter in Pitzer model	
$\Delta\lambda_{ij}$	interaction parameter of the Wilson equation	K
Λ_{ij}	Wilson parameter	
μ	dipole moment	Debye
μ_i	chemical potential of component i	J mol^{-1}
μ_{ijk}	parameter in Pitzer equation	
ν	kinematic viscosity	$\text{m}^2 \text{ s}^{-1}$
ν_0	frequency	s^{-1}
ν_k	number of structural groups of type k	
ν_i	stoichiometric coefficient of component i	
ξ	local volume fraction	
Π	osmotic pressure	Pa
π	number of phases	
ρ	density	$\text{mol m}^{-3}, \text{kg m}^{-3}$
σ	hard sphere segment diameter (PC-SAFT)	
σ	standard deviation	
σ	surface tension	N m^{-1}
σ	symmetry number	
τ	shear stress	N m^{-2}
τ_{ij}	binary interaction parameter in the UNIQUAC model	
Φ	osmotic coefficient	
Φ_i	volume fraction of component i	
ϕ_i	factor defined in Eq. (5.15)	
φ_{el}	electric potential	V
φ_i	fugacity coefficient of component i	
χ	Flory-Huggins parameter	
Ψ	UNIFAC parameter	
ω	acentric factor	

Special symbols

$-$	partial property
∞	value at infinite dilution

Subscripts

\pm	entire electrolyte
0	reference state
1,2,3,4 ...	process steps
<i>a</i>	anion
amb	ambient
az	value at the azeotropic point
<i>b</i>	value at the normal boiling point
<i>c</i>	critical property
<i>c</i>	cation
calc	calculated value
Comp	compressor
CWR	cooling water return
CWS	cooling water supply
<i>D</i>	value for the dimer
DH	Debye–Hückel
dil	dilution
elec	electrolyte
exp	experimental value
eut	value at the eutectic point
<i>f</i>	value for the formation reaction
<i>G</i>	gas phase
HF	hemiformal
<i>i, j, ...</i>	component
inv	inversion temperature
LC	local composition model
LR	long range
<i>m</i>	value at the melting point
max	maximum occurring value
mix	mixture
<i>M</i>	value for the monomer
MR	middle range
MSA	Mean Spherical Approximation method
<i>P</i>	at constant pressure
<i>R</i>	value for the chemical reaction
<i>r</i>	reduced property
ref	reference state
rev	for reversible processes
solv	solvent
SR	short range
tot	total
tr	value at the triple point
trans	transition point
trs	transition
true	true value in maximum likelihood method
<i>v</i>	vaporization
<i>V</i>	at constant volume

Superscripts

*	electrolyte reference state
assoc	association term

rep	caused by repulsive forces
att	caused by attractive forces
$\alpha, \beta, \varphi, \pi, ', ''$	phases
C	combinatorial part
disp	dispersion
E	excess property
hs	hard sphere
hc	hard chain
id	in the ideal gas state
L	liquid phase
m	molality scale
0	standard state
R	residual part
(r)	reference fluid
o	at zero pressure
pure	pure component
S	salt free
s	saturation state
S	solid phase
S	solvent free basis
subl	sublimation
tot	totally dissociated
V	vapor phase
(0)	simple fluid
(1)	deviation from the behavior of simple fluids (corresponding state principle)
∞	at infinite dilution
I, II, III ...	phases

Mathematics

ln logarithm basis e

log logarithm basis 10

Conversion factors

1 kPa = 0.009869 atm = 0.01 bar = 7.50062 Torr = 10^3 N/m² = 1000 Pa

1 J = 1 kg m²/s² = 1 Nm = 0.238846 cal

1 Debye = $3.336 \cdot 10^{-30}$ C m