Chemical Thermodynamics for Process Simulation

3(4)-day Offline-course at Berlin, Germany (Art'otel, Wallstrasse 70-73, Berlin, D-10179)

Dates: April 27 to 29, 2026 Instructors: Juergen Rarey (PhD), Pascal Böwer (PhD)

Optional Aspen Plus or CHEMCAD day depending on booking (April 30)

Course Description

With the ever-increasing application of process simulation software tools like Aspen Plus®, ProSimPlus®, Hysys®, CHEMCAD®, Pro/II®, UNISIM® etc., engineers are confronted with the vast complexity of the underlying models and thermodynamic relationships. A sound knowledge and intuitive understanding of these process engineering fundamentals is vital for the development (synthesis), design and optimization of chemical processes. It is generally accepted that any flaw in the underlying models and parameters usually leads to unrealistic simulation results.

Within this very popular course (approx. 1000 participants in the last 15 years) professionals from industry and academics will become familiar with the possibilities and limitations of currently used methods and models. The course focuses on those aspects which I consider to be of primary importance for the successful modeling of single separation units or whole chemical plants.

Besides the thermodynamic properties of pure components, especially the behavior of multicomponent mixtures will be covered with special attention to phase equilibria, also those of electrolyte systems.

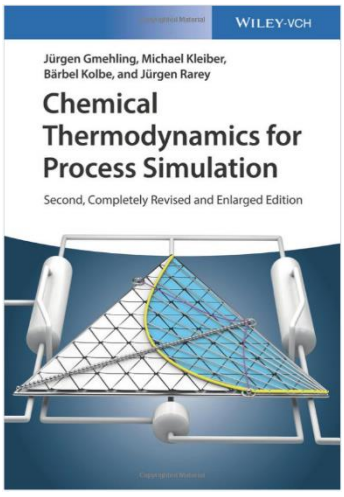
The presentation is organized into four parts:

- Basic pure components and mixture behaviors are presented together with the models that are typically employed in process simulation (equations of state, g^E-models, and special correlations for pure component properties like e.g. vapor pressure). This includes discussion of VLE (separation factor, azeotropic behavior, …) and miscibility gaps, gas solubility, solid solubility, ... and covers the different ways to obtain especially the binary interaction parameters (BIP).
- Estimation methods for pure component properties (mainly group contribution) and mixture behavior (UNIFAC, mod. UNIFAC, PSRK; …) are vital in cases no experimental data are available. Their basis and range of applicability will be discussed in detail.
- Following the basics of thermodynamics, models and property estimation, various approaches to process engineering problems using modern thermodynamic methods will be presented. These include, for example hybrid or pressure swing processes, the selection of suitable entrainers for special separation processes like azeotropic and extractive distillation and extraction. In this part, participants should gain an improved understanding of the various graphical representations of the real behavior of mixtures such as plots on solvent-free basis, contour lines, residual curves incl. boundary lines or surfaces, azeotropic points …).
- Following the first 3 days an optional fourth day offers a workshop on thermophysical properties in the AspenPlus® and/or CHEMCAD® simulator (depending on booking).

The course will be held in the English language.

Registration – Offline-course Berlin

As space is limited, early registration is recommended. Registration fee is Euro 1700 (2090 for 4 days). Registration before 02/15/2026 is honored by an early-bird reduction of Euro 100. The registration fee includes the textbook "Chemical Thermodynamics for Process Simulation" and printed course material.



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Registration

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Timetable (Central European time zone)

Day 1	9.00	-	10.00	**Welcome, Introduction** - Introduction of lecturer and participants - Course introduction, topic introduction - Technical information
	10.00	-	10.30	**Pure Component Properties I** - Physical properties, types, sources, … - PvT-behavior of pure components
	10.30	-	10.45	Coffee Break
	10.45	-	12.15	**Pure Component Properties II** - Equations of state VdW, SRK, PR, corresponding state principle, critical data
	12.15	-	13.15	Lunch Break
	13.15	-	14.45	**Pure Component Properties III** - Special equations of state, chemical theory, high precision, PC-SAFT - Residual functions, enthalpy calculation options in a simulator
	14.45	-	15.00	Coffee Break
	15.00	-	16.30	**Pure Component Properties IV** - Vapor pressure, enthalpy of vaporization - Viscosity, thermal conductivity - Molecular structures and property estimation, Joback and new methods
	16.30	-	17.00	**Importance of Phase Equilibria** **Thermodynamic Fundamentals I** - Phenomenology
Day 2	9.00	-	10.30	**Thermodynamic Fundamentals II** - Auxiliary functions γ_i, φ_i - Activity coefficient models (g^E-Models Wilson, NRTL, UNIQUAC) - Calculation of vapor-liquid equilibria - Parameter fitting, consistency tests, ...
	10.30	-	10.45	Coffee Break
	10.45	-	12.15	**Thermodynamic Fundamentals III** - Activity coefficients at infinite dilution, excess enthalpies - Simultaneous description of phase equilibria and properties (Recommended Values) - Separation factors and azeotropic points as function of temperature
	12.15	-	13.15	Lunch Break
	13.15	-	14.00	**Thermodynamic Fundamentals IV** - Equations of state for mixtures, mixing rules
	14.00	-	14.45	**Special Phase Equilibria I** Liquid-liquid equilibria, gas solubilities
	14.45	-	15.00	Coffee Break
	15.00	-	15.45	**Special Phase Equilibria II** solid-liquid equilibria, supercritical extraction, osmotic pressure

	15.45	-	16.30	**Group Contribution Methods for the Estimation of Phase Equilibria** - UNIFAC, mod. UNIFAC - Equations of state, mixing rules, modern group-contribution equations of state (e.g. PSRK, VTPR)
	16.30	-	17.00	**Application of the Dortmund Data Bank, DDBSP (demo)**
Day 3	9.00	-	10.00	**Special Phase Equilibria II** Electrolyte systems
	10.00	-	10.45	**Quantum Chemical Methods (COSMO-RS, COSMO-SAC)**
	10.45	-	11.00	Coffee Break
	11.00	-	12.15	**Different Applications of g^E-Models** - Residual curves, distillation lines, boundary curves/surfaces
	12.15	-	13.15	Lunch Break
	13.15	-	14.15	**Special Separation Processes** **-** Extractive and azeotropic distillation **Criteria for Entrainer Selection**
	14.15	-	14.45	**Further Applications of g^E-Models and Equations of State** - Chemical equilibria in gas and liquid phase, solvent effects on reaction kinetic and equilibrium, pressure effects on vapor phase equilibria - Environmental distribution coefficients - Flash point of flammable liquid mixtures
	14.45	-	15.00	Coffee Break
	15.00	-	15.45	**Further Applications of g^E-Models and Equations of State (cont.)**
	15.45	-	16.30	**Summary, Discussion**
Day 4 (A+)	9.00	-	10.45	**Session I** Introduction to Aspen Properties, Example Property Method Ideal
	11.00	-	12.15	**Session II** - Routes, Models, Methods - Selecting a Property Method - Thermodynamic Model Parameters - Property Analysis, g^E-Model BIPs
	13.15	-	14.45	Data Regression Solid Solubility
	15.00	-	16.30	Property Estimation Electrolyte Mixtures
Day 4 (CC)	9.00	-	16.30	Physical Properties in CHEMCAD - Components, physical property parameters, analysis - Adding a new component, pure component data estimation and regression - Thermodynamic wizard, settings - Binary analysis - Binary interaction parameters (BIPs), sources, regression, estimation - Ternary diagrams, residual curve plots - Electrolytes, apparent and true components, reactions and data regression - Solid-Liquid equilibria - Special models (amine, sour water, …)

Lecturers

Jürgen Rarey (Dipl.-Chem, Dr.-Ing.)

1979 - 1985	Study of Chemistry, University of Dortmund
1985 - 1989	Scientific co-worker in the group of Prof. Gmehling (Institute for Chemical Engineering, Univ. of Dortmund
1991	PhD at University of Dortmund (Institute for Chemical Engineering)
since 1989	Scientific co-worker with Prof. Gmehling (Prof. Wark) at University of Oldenburg
1989-2017	Director of DDBST GmbH, Oldenburg
2004	Honorary Research Fellow at the School of Chemical Engineering, University of Kwazulu-Natal, Durban, South Africa
2005-2018	Honorary Professor (Kwazulu-Natal, Durban, South Africa)
since 2016	Faculty member ChEPS-KMUTT, Thonburi, Thailand
since 2021	Scientfic director at Rareytec Co., Ltd.

Co-author of DECHEMA Chemistry Data Series (4 books), "Chemical Thermodynamics for Process Simulation", Wiley 2012, 2019 approx. 60 publications in scientific journals

Pascal Böwer (Dr., MSc.)

2011 - 2016	Study of Chemistry, University of Oldenburg
since 2016	Scientific co-worker in the group of Prof. Wark (Chemical Technology 1), Teaching
since 2017	Teaching Chemical Thermodynamics in industry courses
2020	PhD at University of Oldenburg