



3(4)-day course at the Chair of Industrial Chemistry, University of Oldenburg

Course Director: Prof. Dr. J. Gmehling

Location: University of Oldenburg, Industrial Chemistry, Carl-von-Ossietzky Str. 9-11, Oldenburg - Wechloy (Oldb.), Germany

Dates: February 22<sup>nd</sup> – 24<sup>th</sup> (25<sup>th</sup>), 2005

Instructors: Prof. Dr. J. Gmehling, Dr. J. Rarey

## Course Description

A sound knowledge of process engineering fundamentals becomes increasingly important due to the broader application of process simulation software for the development (synthesis), design and optimization of chemical processes. Within this course participants from academia and industry should become familiar with the possibilities and limitations of currently used methods and models. The course will focus on those aspects, which we 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.

Following a detailed discussion of the basics of thermodynamics, various approaches to process engineering problems using modern thermodynamic methods will be presented.

These include for example the selection of suitable entrainers for special separation processes like azeotropic and extractive distillation, extraction as well as hybrid or pressure swing processes and a discussion of reactive distillation.

Participants should gain an improved understanding of the various graphical representations of the real behavior of mixtures such as solvent-free plots, contour lines, residual curves incl. boundary lines or surfaces, ...).

Practical tutorials are included to deepen the understanding of the various topics.

The course will be held in English.

Following the first 3 days an optional fourth day offers an introduction to the process simulation package Aspen Plus. On the last day, the number of participants is limited to 10.

## Registration

Space is limited and early registration is recommended. The number of participants is limited to 25. Up to 5 students of the University of Oldenburg will be given the possibility to participate.

Registration fee is €900.- (€1120.- for 4 days). Participants from member companies of GVT receive a discount of € 50.-. VAT cannot be specified in the invoice. The registration fee includes a copy of the course material, morning and afternoon refreshments and a get-together party at a local restaurant.

## Contact

Most current information can be found at <http://www.uni-oldenburg.de/tchemie/main.html>. Concerning further information please contact

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Lehrstuhl Technische Chemie (F V)  
Universität Oldenburg  
26111 Oldenburg

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Fax: ++49 441 798 3330  
E-Mail: [gmehling@tech.chem.uni-oldenburg.de](mailto:gmehling@tech.chem.uni-oldenburg.de)

## Timetable

Tuesday, 02/22/2005	10.00 -	10.30	<b>Welcome, Introduction</b> <ul style="list-style-type: none"><li>- Introduction of the Participants</li><li>- Importance of Physical Properties for the Synthesis, Design and Optimization of Chemical Processes</li><li>- Research Activities incl. History and Development of the Dortmund Data Bank (DDB) and the Integrated Software Package</li><li>- History and Development of Thermodynamic Models</li><li>- Technical Information</li></ul>	Prof. Dr. J. Gmehling
	10.30 -	12.15	<b>Pure Component Properties I</b> <ul style="list-style-type: none"><li>- PvT-Behavior of Pure Components</li><li>- Equations of State, Corresponding State Principle</li><li>- Critical Data</li><li>- Residual Functions</li></ul>	Dr. J. Rarey
	12.15 -	13.15	Lunch Break	
	13.15 -	14.30	<b>Pure Component Properties II</b> <ul style="list-style-type: none"><li>- Vapor Pressure, Enthalpy of Vaporization</li><li>- Melting Temperature as f(T), Viscosity, Thermal Conductivity</li><li>- PURE Data Bank, Molecular Structures and Property Estimation</li></ul>	Dr. J. Rarey
	14.30 -	15.15	<b>Importance of Phase Equilibria Thermodynamic Fundamentals I</b> <ul style="list-style-type: none"><li>- Auxiliary Functions <math>\gamma_i</math>, <math>\phi_i</math></li><li>- Activity Coefficient Models (<math>g^E</math>-Models)</li><li>- Calculation of Vapor-Liquid Equilibria</li></ul>	Prof. Dr. J. Gmehling
	15.15 -	15.30	Coffee Break	
	15.30 -	17.00	<b>Thermodynamic Fundamentals II</b> <ul style="list-style-type: none"><li>- Parameter Fitting, Consistency Tests, ...</li><li>- Activity Coefficients at Infinite Dilution</li><li>- Excess Enthalpies</li><li>- Separation Factors and Azeotropic Points as Function of Temperature</li><li>- Simultaneous Description of Phase Equilibria and Excess Properties (Recommended Values)</li></ul>	Prof. Dr. J. Gmehling
	19.00		<b>Dinner</b>	
Wednesday, 02/23/2005	9.00 -	10.40	<b>Introduction to MathCAD, Tutorial "Pure Component Properties", Tutorial "Phase Equilibria"</b>	Dr. J. Rarey
	10.40 -	10.55	Coffee Break	
	10.55 -	11.15	<b>Thermodynamic Fundamentals III</b> <ul style="list-style-type: none"><li>- Equations of State, Mixing Rules</li></ul>	Prof. Dr. J. Gmehling
	11.15 -	12.15	<b>Special Phase Equilibria I</b> Liquid-Liquid Equilibria, Gas Solubilities, Solid-Liquid Equilibria, Supercritical Extraction, Osmotic Pressure	Dr. J. Rarey
	12.15 -	13.15	Lunch Break	
	13.15 -	14.00	<b>Special Phase Equilibria II</b>	Dr. J. Rarey

Electrolyte Systems

	14.00 -	15.30	<b>Group Contribution Methods for the Estimation of Phase Equilibria</b> - UNIFAC, mod. UNIFAC - Equations of State, Mixing Rules, Modern Group-Contribution Equations of State (e.g. PSRK, VTPR)	Prof. Dr. J. Gmehling
	15.30 -	15.45	Coffee Break	
	15.45 -	17.00	<b>Application of the Dortmund Data Bank, DDBSP</b>	Dr. J. Rarey
	17.00 -	19.00	<b>Laboratory Tour and Discussion (for Interested Participants)</b>	
Thursday, 02/24/2005	9.00 -	10.30	<b>Different Applications of <math>g^E</math>-Models and Equations of State</b> - Residual Curves, Distillation Lines, Boundary Curves/Surfaces <b>Special Separation Processes</b> - Extractive and Azeotropic Distillation <b>Criteria for Entrainer Selection</b> - Using Thermodynamic Models - Using The DDB - Extractive and Adductive Crystallization - Reactive Distillation - Demonstration of the Program Package SYNTHESE	Prof. Dr. J. Gmehling
	10.30 -	10.45	Coffee Break	
	10.45 -	12.15	<b>Tutorial "Thermodynamic Properties and Application"</b>	Dr. J. Rarey
	12.15 -	13.15	Lunch Break	
	13.15 -	14.45	<b>Discontinuous Distillation, Absorption, Extraction, Supercritical Extraction, Crystallization, Adsorption, Membrane Processes</b>  <b>Further Applications of <math>g^E</math>-Models and Equations of State (e.g. Chemical Equilibria)</b>	Dr. J. Rarey
	14.45 -	15.00	Coffee Break	
	15.00 -	16.30	<b>Tutorial Separation Technology (partly with Computer)</b>	Dr. J. Rarey
	16.30 -	17.30	<b>Summary</b> <b>ASPEN Plus (I)</b>	
Friday, 02/25/2005	9.00 -	10.30	- Graphical User Interface, Data Browser - Forms: Functionality, Input, Setup, Components, Properties, Streams, Blocks	Dr. J. Rarey
	10.30 -	10.45	Coffee Break	
	10.45 -	12.15	<b>ASPEN Plus (II)</b> - Unit Operations: Mixer, Splitter, Columns - RadFrac: Configuration, Variables, Specifications, Convergence	Dr. J. Rarey
	12.15 -	13.15	Lunch Break	
	13.15 -	16.00	<b>ASPEN Plus (III)</b> - Reactors: Types, Equilibrium, Kinetics - ...	Dr. J. Rarey

## O R G A N I S A T I O N

The course starts on Tuesday morning at 10 am and ends on Thursday at 5.30 pm (resp. Friday at 4.30 pm). Oldenburg (Oldb.) is situated approx. 45 km west of Bremen (the nearest international airport), and can be conveniently reached by train. For participants arriving by plane, a transfer from Bremen airport can be reserved in advance ([www.luftibus.de](http://www.luftibus.de)), which should be booked one week in advance. Oldenburg can also be reached by car via highways from all directions. Details on the contents of the course can be found in the timetable above. A get-together party at a local restaurant is included.

For registration please contact:

Forschungs-Gesellschaft Verfahrens-Technik e.V.  
 Theodor-Heuss-Allee 25, 60486 Frankfurt am Main  
**Tel.:** +49 - 69 - 7564-118  
**FAX:** +49 -69 - 7564-414  
**E-mail:** GVT-Hochschulkurse@Dechema.de  
**Subject:** University Course „Thermal Separation Processes“

Please transfer the course fee using the subject given above to the account 930 945 00, BLZ 500 800 00, Dresdner Bank AG, Frankfurt but not before having received the final confirmation of participation by GVT. The course fee is tax free in Germany (§ 4 Ziffer 22 UStG-MWSt.).

### Referees

#### **Prof. Dr. Jürgen Gmehling**

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1962 - 1965 Education as Laboratory Technician at Duisburger Kupferhütte / Duisburg  
 1965 - 1968 Study of Chemical Engineering at School of Engineering, Essen  
 1968 - 1970 Study of Chemistry at University of Clausthal and University of Dortmund  
 1973 PhD at University of Dortmund ( Inorganic Chemistry )  
 1977 – 1978 Research stay in Berkeley, USA ( Prof. Dr. J. M. Prausnitz )  
 1982 Habilitation at Institute for Chemical Engineering, University of Dortmund (Venia Legendi for Industrial Chemistry)  
 1970 - 1989 Scientific co-worker, Privatdozent and associated Professor at University of Dortmund  
 since 1989 Professor (C4) Technical Chemistry, University of Oldenburg  
 President/CEO of DDBST GmbH, Oldenburg  
 since 1999 Director of LTP GmbH, Oldenburg  
 Author of DECHEMA Chemistry Data Series (VLE,  $h^f$ ,  $\gamma^c$ ) and "Azeotropic Data" (Wiley-VCH Weinheim)(>40 parts), Author of "Vapor-Liquid Equilibria Using UNIFAC" and the textbooks "Thermodynamik", "Lehrbuch der Technischen Chemie II – Grundoperationen" and " Thermodynamik der Phasengleichgewichte", "Thermische Verfahrenstechnik" in Winnacker-Küchler (2004), Arnold-Eucken-Preis of GVC 1982, more than 300 publications in scientific journals  
 Elected member of different boards of GVC and DECHEMA and member in various editorial boards.

#### **Dr. Jürgen Rarey**

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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 at University of Oldenburg  
 Director of DDBST GmbH, Oldenburg  
 Since 2004 Honorary Research Fellow at the School of Chemical Engineering, University of Kwazulu -Natal, Durban, South Africa  
 Co-author of DECHEMA Chemistry Data Series (4 books), more than 25 publications in scientific journals