Fundamentals of Synthesis and Thermal Processes

Selection, Design of Separation

3(4)-day course at the University of Oldenburg
(Industrial Chemistry (faculty 5), Carl-von-Ossietzky Str. 9-11, Oldenburg-Wechloy (Oldb.), Germany)

Dates: October 25. – 27. (28.) 2016   Instructors: Prof. h.c. Dr. J. Rarey, Dr. Christian Möllmann

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 in four parts:

- Basic pure component 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 Aspen Plus simulator by Dr. Christian Möllmann

Practical tutorials are included to deepen the understanding of the various topics. The course will be held in the English language.
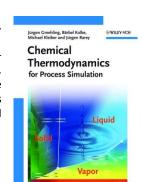
Registration

Space is limited and early registration is recommended. The number of participants is limited to 20. Up to 7 students of the University of Oldenburg will be given the possibility to participate.

Registration fee is € 1240 (€ 1530 for 4 days). Registration before 9/15/2016 is honored by an early-bird reduction of € 100. Participants from member companies of GVT receive a discount of € 50.-. The course fee is tax free according to German law (§ 4 Ziffer 22 UStG-MwSt.). The registration fee includes a copy of the course material, the textbook "Chemical Thermodynamics for Process Simulation", morning and afternoon refreshments, snacks and a get-together party at a local restaurant.

Contact

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Universität Oldenburg
26111 Oldenburg

(Most current information can be found at http://courses.rarey.net.)

University course in co-operation with

GVT Forschungs-Gesellschaft Verfahrens-Technik e.V.

Timetable

Tuesday	10.00	-	10.30	**Welcome, Introduction**

Welcome, Introduction
- Introduction of lecturer and participants
- Course introduction
- Technical information

10.30 - 12.15 **Pure Component Properties I**
- PvT-behavior of pure components
- Equations of state VdW, SRK, PR, corresponding state principle, critical data

12.15 - 13.15 Lunch Break

13.15 - 15.15 **Pure Component Properties II**
- Special equations of state, chemical theory, high precision, PC-SAFT
- Residual functions, enthalpy calculation options in a simulator
- Vapor pressure, enthalpy of vaporization

15.15 - 15.30 Coffee Break

15.30 - 16.15 **Pure Component Properties III**
- Viscosity, thermal conductivity
- Molecular structures and property estimation, Joback and new methods

16.15 - 17.30 **Importance of Phase Equilibria**
Thermodynamic Fundamentals I
- Auxiliary functions γ_i, φ_i
- Activity coefficient models (g^E-Models)

19.00 **Dinner**

Wednesday 9.00 - 10.30 **Thermodynamic Fundamentals II**
- Calculation of vapor-liquid equilibria
- Parameter fitting, consistency tests, ...
- 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

10.30 - 10.45 Coffee Break

10.45 - 11.15 **Thermodynamic Fundamentals III**
- Equations of state for mixtures, mixing rules

11.15 - 12.15 **Tutorial "Pure Component Properties" and "Phase Equilibria"**

12.15 - 13.15 Lunch Break

13.15 - 14.45 **Special Phase Equilibria I**
Liquid-liquid equilibria, gas solubilities, solid-liquid equilibria, supercritical
extraction, osmotic pressure

14.45 - 15.00 Coffee Break

15.00 - 15.45 **Special Phase Equilibria II**
Electrolyte systems

15.45 - 16.45 **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)

16.45 - 17.30 **Application of the Dortmund Data Bank, DDBSP (demo)**

Thursday	9.00	-	11.00	**Different Applications of g^E-Models** - Residual curves, distillation lines, boundary curves/surfaces **Special Separation Processes** **-** Extractive and azeotropic distillation **Criteria for Entrainer Selection**
	11.00	-	11.15	Coffee Break
	11.15	-	12.15	**Tutorial "Thermodynamic Properties and Application"**
	12.15	-	13.15	Lunch Break
	13.15	-	14.45	**Laboratory Tour at LTP (Laboratory for Thermophysical Properties)**
	14.45	-	15.30	**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
	15.30	-	15.45	Coffee Break
	15.45	-	16.30	**Summary, Discussion**
Friday	9.00	-	10.45	**Physical Properties in Aspen Plus** Methods assistant and pure component property analysis Txy diagrams for homogeneous and heterogeneous mixtures and their interpretation Ternary maps for liquid-liquid equilibrium, residual curve maps
	10.45	-	11.00	Coffee Break
	11.00	-	12.15	Flash calculations, Chemistry object and reactive systems
	12.15	-	13.15	Lunch Break
	13.15	-	14.45	Providing physical property parameters, creating user components Property data and models in Aspen Plus (estimation & regression)
	14.45	-	15.00	Coffee Break
	15.00	-	16.30	Final Workshop

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 5.00 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), 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 with the enclosed registration form:

> Forschungs-Gesellschaft Verfahrens-Technik e.V.
> Theodor-Heuss-Allee 25, 60486 Frankfurt am Main
> **Tel.:** +49 - 69 – 7564-118
> **FAX:** +49 –69 – 7564-437
> **E-**mail: gvt-hochschulkurse@gvt.org
> **Subject:** University Course „Thermal Separation Processes"

Please transfer the course fee using the subject given above, but not before having received the final confirmation of participation and invoice by GVT. The course fee is tax free in Germany (§ 4 Ziffer 22 UStG-MWSt.).

Lecturer

Jürgen Rarey (Prof. h.c. Dr.)

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
since 2005	Honorary Professor (Kwazulu-Natal, Durban, South Africa)

Co-author of DECHEMA Chemistry Data Series (4 books), "Chemical Thermodynami
Wiley 2012, approx. 45 publications in scientific journals

Christian Möllmann (Dr.)

1992 - 1996	Scientific Coworker / Research Assistant, Carl von Ossietzky Universität Oldenburg
1997 - 2004	Customer Support Consultant, AspenTech Europe S.A. / N.V., Brussels
2004 - 2010	Senior Process Engineer, UHDE GmbH, Bad Soden/Ts.
2011 - 2012	Technical Account Manager, Process Systems Enterprise Ltd., London
2012 - 2016	Senior Process Engineer, Evonik Industries AG, Hanau
since 2016	Senior Project Manager, Evonik Resource Efficiency GmbH, Darmstadt

**GVT
Forschungs-Gesellschaft
Verfahrens-Technik e.V.**
Theodor-Heuss-Allee 25

60486 Frankfurt am Main

Registration form for the GVT University Course 70221E from 25 – 27(28) October 2016

"Fundamentals of selection, synthesis and design of thermal separation

processes" in Oldenburg

Registrations are processed in order of receipt.

Participant			4 days course	❏
Mr. ❏	Ms. ❏		3 days course	❏

Family name...

First name..

Title / Profession...

Company...Dept..

Street/No..

Postcode/City/Country..

Phone / Fax...E-mail...

Invoice address (if different from the above address)

Company..

Dept..

Street / No..

Postcode/City/Country..

The registration fee is € 1240 (€ 1530 for 4 days) and for participants from corporate members of GVT € 1190 (€ 1480 for 4 days). Early registrations received on or before 15 September 2016 are eligible for a discount of 100 €. Please do not transfer the fee before receiving confirmation of participation by GVT. For cancellations received by 25 September 2016, the participation fee will be reimbursed less a processing charge of € 50,-. After that date a reimbursement cannot be made, however it is still possible to nominate a replacement. Our fees are not liable to Value Added Tax (tax exemption in accordance with § 4.22 UstG), since GVT has nonprofit status.

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