Curriculum vitae – Kaj Thomsen

Personal data:

- Name: Kaj Thomsen, born Nov. 16th, 1953
- Work address: Department of Chemical Engineering, DTU, Building 229, DK-2800 Kongens Lyngby, Denmark, Tel. 4525 2860, kth@kt.dtu.dk

Education:

- 1994-1997: Ph.D. in Chemical Engineering, Technical University of Denmark. The ph.d. thesis was titled "Aqueous Electrolytes: model parameters and process simulation". As a part of the ph.d. study, I spent six month at FMC Chemical Research and Development Center in Princeton, New Jersey, USA.
- 1989-1994: M.Sc. in Chemical Engineering, the Technical University of Denmark. The M.Sc. project was titled: "Simulation and design of processes with electrolyte mixtures".

Work:

- 2002- Associate professor at the department of Chemical Engineering, Technical University of Denmark.
- 2002 Founded the consultancy company Aqueous Solutions Aps with expertise in electrolyte solution thermodynamics
- 1999-2002: Assistant professor at the department of Chemical Engineering, Technical University of Denmark.
- 1997-1999: Assistant research professor at the department of Chemical Engineering, Technical University of Denmark.

Research area:

- Thermodynamic modeling of solutions containing electrolytes and non-electrolytes.
- Measurement of the properties of solutions containing electrolytes and non-electrolytes
- Modelling of CO_2 capture processes
- Corrosion
- Ionic liquids
- Development of alternative separation processes
- Crystallization

Patent:

SE 522434: Gudmundson Claes, Kockum Henrik, Joergensen Lars Bo, Andersen Torben Boech, Thomsen Kaj, Rasmussen Peter, "Preparation of sugar from sugar beet or sugarcane, by treating molasses with carbon dioxide at high pressure and separating gas hydrate crystals" (2004)

Evaluator of Research Proposals: Research Councils of Norway, Portugal, Chech Republic

Referee for the following international scientific journals within the last year:
Chemical Engineering Science, Environmental Science & Technology, Fluid Phase Equilibria, Molecular Liquids, AIChE Journal, Industrial and Engineering Chemistry Research, Energy & Fuels, Journal of Chemical and Engineering Data, International Journal of Greenhouse Gas Control.

Project Management:

Attended an AMU course on Project Management at the Business School, Copenhagen North, in September-October 2009

Supervision of Research Projects:

- 2009-2011: "Ionic liquids for CO_2 capture", (Funding: The strategic research council of Denmark)
- 2008-2010: "Liquefaction of Unprocessed WellStreams", LUWS, (Funding: The Norwegian Research Council and Statoil)
- 2008: "Modelling of molten salt mixtures" (Funding: SQM CL)
- 2007: "Chilled ammonia process for CO2 capture" (Funding: DONG energy and Vattenfall)
- 2007: "Comparison of Electrolyte Models", (Funding: Shell Global Solutions NL, Akzo-Nobel NL, and SQM CL)
- 2004-2005: "Recycling of Alkali in bio fly ash", (Funding: PSO)
- 1998-2000: "Extension of thermodynamic model to systems with mixed solvents" (Funding: IVC-SEP)

Supervision of Ph.D. students:

- Krishna Hara Chakravarty, Modeling of Salt Solubility/Dissolution in Water flooding of Petroleum Reservoirs(2012-2015, main supervisor)
- Jozsef Gaspar (2012-2015, main supervisor)
- Xiaodong Liang, Thermodynamic modeling of oil-sea water mixtures (2011-2014, co-supervisor)
- Bjørn Maribo-Mogensen, Development of an Electrolyte Equation of State for Applications in the Petroleum and Chemical Industries, (2010-2013, co-supervisor)
- Muhammad Waseem Arshad, Thermodynamic Modeling for CO2 Capture Systems (2010-2013, main supervisor)
- Peter Jørgensen Herslund, Thermodynamic and Process Modelling of Gas Hydrate Systems in CO2 Capture Processes (2010-2013) (co-supervisor)
- Negar Sadegh, Thermodynamic modelling of acid gases – alkanolamine systems (2009-2012, main supervisor)
- Benedicte Mai Lerche, CO_2 capture from flue gas using amino acid salt solutions (2008-2011) (main supervisor)
- Ferdinand Hingerl, Geochemical Evolution of Enhanced Geothermal Systems: Coupling Chemistry to Heat and Fluid Transport (ETH, 2008-2012) (External supervisor)
- Victor Darde, CO_2 capture with aqueous ammonia (2008-2011) (Industrial Ph.D. , main supervisor)
- Lars Jensen, Kinetics of Gas Hydrate formation (2007-2010) (co-supervisor)
- Leila Faramarzi, Design of CO_2 capture units using aqueous alkanolamines (2007-2010) (co-supervisor)
- Rudi Pankratz Nielsen, Optimization and Physical Chemistry of the CatLiq^{TM} Process (2006-2009) (External supervisor)
- Philip Loldrup Fosbøl, Corrosion in Wet Gas Pipelines (2005-2008, main supervisor)

- Yi Lin, Development of an Equation of State for Electrolytes (2004-2007, main supervisor)
- Ada Villafáfila Garcia, Measurement and Modeling of Scaling Minerals (2003-2006, main supervisor)
- Søren Gregers Christensen, Thermodynamics of Aqueous Electrolyte Solutions – Application to ion exchange systems (2002-2005, main supervisor)

Teaching Portfolio:

Attended the following courses on teaching:

- 2007: Course on "Peer Coaching and Supervision" at Learning Lab, DTU
- 2005: Short course on "PhD Supervision" at DTU
- 2005: Short course on "Mentoring of Experts" at DTU
- 2001-2002: Education in Didactics and Teaching Methodology for Teachers at DTU
- 2000: Basic course on Teaching and Learning, DTU

Currently teaching:

- Course 28020, Introduction to Chemical and Biochemical Engineering
- Course 28322, Technical Thermodynamics
- Course 28231, Laboratory in Chemical and Biochemical Engineering
- Course 28423, Phase Equilibria for Separation Processes
- Course 28928, Electrolyte Solution Thermodynamics and Separation Processes

In addition, I supervise 10 - 15 students per year in their MSc and BSc projects.

International teaching experience:

- 2008, April 4-11: Gave workshop on Thermodynamic modeling of properties of salt solutions at University of Cape Town, South Africa
- 2006, August to December: Visiting Professor at Department of Chemical and Biological Engineering, University of Wisconsin-Madison, USA

List of publications in peer reviewed journals

1. Muhammad Waseem Arshad; Philip Loldrup Fosbøl, Nicolas von Solms; Hallvard Fjøsne Svendsen; Kaj Thomsen, Heat of Absorption of CO2 in Phase Change Solvents, J. Chem. Eng. Data, 58(2013)1974-1988, DOI: 10.1021/je400289v
2. Muhammad Waseem Arshad, Philip Loldrup Fosbøl, Nicolas von Solms, and Kaj Thomsen, Freezing Point Depressions of Phase Change CO_2 Solvents, J. Chem. Eng. Data, 58(2013)1918-1926, DOI: 10.1021/je3013167,
3. Maribo-Mogensen, Bjørn • Kontogeorgis, Georgios M. • Thomsen, Kaj, Modeling of dielectric properties of complex fluids with an equation of state, Journal of Physical Chemistry B, 117(2013)3389-3397
4. Liang, Xiaodong; Maribo-Mogensen, Bjorn; Thomsen, Kaj; et al., Approach to Improve Speed of Sound Calculation within PC-SAFT Framework, Industrial & Engineering Chemistry Research 51(2012)14903-14914(45)
5. Linnenberg, Sebastian; Darde, Victor; Oexmann, Jochen • Kather, Alfons; van Well, Willy J.M.; Thomsen, Kaj, Evaluating the impact of an ammonia-based post-combustion

CO2 capture process on a steam power plant with different cooling water temperatures, International Journal of Greenhouse Gas Control, 10(2012)1-14

6. Victor Darde; Bjørn Maribo-Mogensen; Willy JM van Well; Erling H Stenby; Kaj Thomsen, Process simulation of CO2 capture with aqueous ammonia using the Extended UNIQUAC model, International Journal of Green House Gas Control 10(2012)74-87
7. Subham Paul, Kaj Thomsen, Kinetics of Absorption of Carbon Dioxide into Aqueous Potassium Salt of Proline, International Journal of Greenhouse Gas Control, 8(2012)169-179.
8. Maribo-Mogensen, Bjørn; Kontogeorgis, Georgios M.; Thomsen, Kaj, Comparison of the Debye-Huckel and the Mean Spherical Approximation Theories for Electrolyte Solutions, Industrial & Engineering Chemistry Research 51(2012)5353-5363(14)
9. Jørgensen Herslund P, Thomsen K, Abildskov J, von Solms N, Phase equilibrium modeling of gas hydrate systems for CO2 capture, J. Chem. Thermodynamics, 48(2012)13–27
10. Darde V, Thomsen K, van Well W, Bonalumi D, Valenti G, Macchi E, Comparison of two electrolyte models for the carbon capture with aqueous ammonia, International Journal of Greenhouse Gas Control, 8(2012)61-72.
11. Darde, Victor; van Well, Willy J. M.; Stenby, Erling H.; Thomsen, Kaj. CO2 capture using aqueous ammonia: kinetic study and process simulation, Energy Procedia, 4(2011)1443-1450
12. Fosbøl PL, Neerup R, Arshad MW, Tecle Z, and Thomsen K, Aqueous Solubility of Piperazine and 2-Amino-2-methyl-1-propanol plus Their Mixtures Using an Improved Freezing-Point Depression Method, J. Chem. Eng. Data, 56(2011)5088-5093, DOI: 10.1021/je200959m
13. Victor Darde, Willy J.M. van Well, Philip L. Fosboel, Erling H. Stenby, Kaj Thomsen, Experimental measurement and modeling of the rate of absorption of carbon dioxide by aqueous ammonia, International Journal of Greenhouse Gas Control, 5(2011)1149–1162
14. Hingerl, F. F. ; Wagner, T. ; Kulik, D. ; Driesner, T. ; Kosakowski, G. ; Thomsen, K. Enhanced geothermal systems: Influence of thermodynamic data and activity models on predicted mineral precipitation-dissolution reactions, Geochimica et Cosmochimica Acta, 74(2010)A406-A406
15. Jensen L, Thomsen K, von Solms N, Inhibition of Structure I and II Gas Hydrates using Synthetic and Biological Kinetic Inhibitors, ENERGY & FUELS 25(2011)17-23
16. Fosbøl PL, Pedersen MG, and Thomsen K, Freezing Point Depressions of Aqueous MEA, MDEA, and MEA-MDEA Measured with a New Apparatus, J. Chem. Eng. Data 56(2011)995-1000 DOI: 10.1021/je100994v
17. D. Möhlmann and K. Thomsen, Properties of cryobrines on Mars, ICARUS, 212(2011) 123–130.
18. Victor Darde, Willy J. M. van Well, Erling H. Stenby, and Kaj Thomsen, Modeling of Carbon Dioxide Absorption by Aqueous Ammonia Solutions Using the Extended UNIQUAC Model, Ind. Eng. Chem. Res., 49(2010)12663–12674(issue 24)
19. Lewis, A.E.; Nathoo, J.; Thomsen, K.; Kramer, H.J.; Witkamp, G.J.; Reddy, S.T.; Randall, D.G., Design of a Eutectic Freeze Crystallization process for multicomponent waste water stream, Chemical Engineering Research and Design, 88(2010)1290-1296(9)

20. L Faramarzi; GM Kontogeorgis; ML Michelsen; K Thomsen; EH Stenby, Absorber Model for CO2 Capture by Monoethanolamine, Industrial & Engineering Chemistry Research, 49(2010)3751-3759(issue 8)
21. Yi Lin, Antoon ten Kate, Miranda Mooijer, Javier Delgado, Philip Loldrup Fosbøl, Kaj Thomsen, Comparison of activity coefficient models for electrolyte systems, AIChE Journal, 56(2010)1334-1351(issue 5)
22. A. Fettouhi, K. Thomsen, Solid–liquid equilibria for binary and ternary systems with the Cubic-Plus-Association (CPA) equation of state, Fluid Phase Equilibria 293(2010)121-129, DOI:10.1016/j.fluid.2010.02.017
23. Lars Jensen; Hans Ramløv; Kaj Thomsen; Nicolas von Solms, Inhibition of Methane Hydrate Formation by Ice-Structuring Proteins, Industrial & Engineering Chemistry Research 49(2010)1486-1492(issue 4)
24. Jensen L, Thomsen K, von Solms N, Wierzchowski S, Walsh MR, Koh CA, Sloan ED, Wu DT, Sum AK, Calculation of Liquid Water-Hydrate-Methane Vapor Phase Equilibria from Molecular Simulations, JOURNAL OF PHYSICAL CHEMISTRY B, 114(2010)5775-5782
25. T. Boch Andersen; K. Thomsen, Separation of water through gas hydrate formation, International Sugar Journal, 111(2009)632-636(issue 1330)
26. Victor Darde, Kaj Thomsen, Willy J.M. van Well, Erling H. Stenby, Chilled ammonia process for CO2 capture International Journal of Greenhouse Gas Control, 4(2010)131–136
27. Victor Darde; Kaj Thomsen; Willy J.M. van Well; Erling H. Stenby, Chilled ammonia process for CO_2 capture, Energy Procedia, 1(2009)1035-1042(issue 1)
28. Leila Faramarzi; Georgios M. Kontogeorgis; Kaj Thomsen; Erling H. Stenby, Thermodynamic modeling of the solubility of CO_2 in aqueous alkanolamine solutions using the extended UNIQUAC model application to monoethanolamine and methyldiethanolamine, Energy Procedia, 1(2009)861-867(issue 1)
29. Leila Faramarzi, Georgios M. Kontogeorgis, Kaj Thomsen, Erling H. Stenby, Extended UNIQUAC model for thermodynamic modeling of CO_2 absorption in aqueous alkanolamine solutions, Fluid Phase Equilibria, 282(2009)121–132
30. Philip L. Fosbøl; Kaj Thomsen; Erling H. Stenby, , Modeling of the Mixed Solvent Electrolyte System CO_2-Na_2CO_3-$NaHCO_3$-Monoethylene Glycol-Water, Industrial & Engineering Chemistry Research, 48(2009)4565-4578
31. Javeed Awan; Kaj Thomsen; Christophe Coquelet; Philip Fosbøl; Dominique Richon, VLE Measurements and Modeling of the n-Propyl Mercaptan-Methane-Water System J. Chem. Eng. Data, 55(2009)842-846
32. Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby, "A Review and Recommended Thermodynamic Properties of $FeCO_3$", Corrosion Engineering Science and Technology, 45(2010)115-135(issue 2)
33. Philip Loldrup Fosbøl, Kaj Thomsen; Erling Halfdan Stenby, "Solubility Measurements in the Mixed Solvent Electrolyte System Na_2CO_3-$NaHCO_3$-Monoethylene Glycol-Water", Industrial & Engineering Chemistry Research, vol: 48(4), p. 2218-2228 (2009).
34. Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby, "Reverse Schreinemakers method for experimental analysis of mixed-solvent electrolyte systems", J. Solution Chem. 38(2009)1–14.
35. Lars Jensen, Kaj Thomsen, and Nicolas von Solms, "Propane Hydrate Nucleation: Experimental Investigation and Correlation" (Chemical Engineering Science 63(2008)3069-3080)

36. Zheng Guo, Bena-Marie Lue, Kaj Thomsen, Anne Boye Strunge Meyer and Xuebing Xu, ”Predictions of flavonoid solubility in ionic liquids by COSMO-RS: experimental verification, structural elucidation, and solvation characterization”, (Green Chemistry, 9(2007)1362-1373)
37. Yi Lin, Kaj Thomsen, and Jean-Charles de Hemptinne, “Multi component equations of state for electrolytes”, (AIChE Journal, 53(4)(2007)989-1005)
38. Ada Villafáfila García, Kaj Thomsen, and Erling H. Stenby, “Prediction of Mineral Scale Formation in Geothermal and Oilfield operations using the Extended UNIQUAC Model. Part II: Carbonate Scaling Minerals”. (Geothermics, 35(2006)239-284)
39. Kaj Thomsen, “Modeling Electrolyte Solutions with the Extended Universal Quasichemical (UNIQUAC) Model” (Invited lecture presented at the 11th ISSP in Aveiro, Portugal, 2004) (Pure and Applied Chemistry, 77(2005)531-542, issue 3)
40. Søren Gregers Christensen and Kaj Thomsen, “Experimental measurement and modeling of the distribution of solvent and ions between an aqueous phase and an ion exchange resin” (Fluid Phase Equilibria, 228-229(2005)247-260).
41. Ada Villafáfila García, Kaj Thomsen, and Erling H. Stenby, “Prediction of Mineral Scale Formation in Geothermal and Oilfield Operations using the Extended UNIQUAC Model. Part I: Sulphate Scaling Minerals” (Geothermics 34(2005)61-97)
42. Kaj Thomsen, Maria Iliuta, and Peter Rasmussen “Extended UNIQUAC model for correlation and prediction of vapour-liquid-liquid-solid equilibria in aqueous salt systems containing non-electrolytes. Part B. Alcohol (Ethanol, Propanols, Butanols) - water - salt systems”. Chemical Engineering Science 59(2004)3631-3647.
43. Søren Gregers Christensen and Kaj Thomsen, “Modeling of Vapor-Liquid-Solid Equilibria in Acidic Aqueous Solutions” (Ind. & Eng. Chem. Res. 42(2003)4260-4268, issue 18)
44. Maria C. Iliuta, Kaj Thomsen and Peter Rasmussen "Modeling of heavy metal salt solubility using the Extended UNIQUAC model" (AIChE Journal, 48(11)(2002)2664-2689)
45. Raphaël Huyghe, Peter Rasmussen, and Kaj Thomsen, "Solid-Liquid Equilibria for the Binary Mixtures 1,4-Xylene + Ethylbenzene and 1,4-Xylene + Toluene". (Chemical Engineering Communications, 191(8)(2004)1017-1023+Erratum 193(2006)272)
46. Selva Pereda, Kaj Thomsen and Peter Rasmussen, "Vapor-Liquid-Solid Equilibria of Sulfur Dioxide in Aqueous Electrolyte Solutions", Chemical Engineering Science 55(2000)2663-2671.
47. Maria Iliuta, Kaj Thomsen and Peter Rasmussen, "Extended UNIQUAC model for correlation and prediction of vapour-liquid-solid equilibria in aqueous salt systems containing non-electrolytes . I. Methanol - water - salt systems", Chemical Engineering Science, 55(2000)2673-2686
48. Thomsen K., Rasmussen P.: "Modeling of Vapor-Liquid-Solid Equilibria in Gas - Aqueous Electrolyte Systems. Chemical Engineering Science, 54(1999) 1787-1802.
49. Thomsen K., Rasmussen P., and Gani R.: "Simulation and optimization of fractional crystallization processes". Chemical Engineering Science 53(1998)1551-1564.
50. Thomsen, K., Rasmussen, P., Gani, R.: "Correlation and prediction of thermal properties and phase behaviour for a class of aqueous electrolyte systems". Chemical Engineering Science 51(1996)3675-3683
51. Thomsen, K., Gani, R., Rasmussen, P.: "Synthesis and analysis of processes with electrolyte mixtures" Computers and Chemical Engineering 19(1995)S27-S32

Books and chapter in books

52. Kaj Thomsen, "Chemical Absorption Materials for CO_2 capture" Efficient Carbon Capture for Coal Power Plants, Edited by Stolten and Scherer, Wiley-VCH 2011, p155-174
53. Kaj Thomsen, "Electrolyte Solutions, Thermodynamics, Crystallization, and Separation Methods", 2006. Study material developed and used while being visiting professor at University of Wisconsin-Madison. (To be published)
54. Kaj Thomsen "Thermodynamics of Electrolyte Systems of Industry", (Chapter 19 in book, Thermodynamics for Industry, Edited by TM Letcher, 2004, 219-229)
55. Kemiske Enhedsoperationer 5. udgave, Karsten H. Clement, Peder Fangel, Anker Jensen, Kaj Thomsen, (2004, Chemical Unit Operations, Language: Danish).

Proceedings

1. Fosbøl, Philip Loldrup; Thomsen, Kaj; Stenby, Erling Halfdan, "Improving Mechanistic CO2 Corrosion Models", Presented at: CORROSION 2009, NACE International´s 64 Annual Conference and Exposition. Atlanta, Georgia, USA, 2009, Proceedings from CORROSION 2009 NACE International, 2009
2. Darde, Victor Camille Alfred; Thomsen, Kaj; Well, Willy van; Stenby, Erling Halfdan, "Chilled ammonia process for CO2 capture", Presented at: ICPWS XV, Berlin 2008. Conference paper published in book/proceeding.
3. Leila Faramarzi, Georgios Kontogeorgis, Kaj Thomsen, Erling Halfdan Stenby, "Thermodynamic modeling of the solubility of CO2 in aqueous alkanolamine solutions using the extended UNIQUAC model. Application to monoethanolamine and methyldiethanolamine", Energy Procedia, (2008)
4. Kaj Thomsen, Duc Thoung Vu, Mette Stenby, Jørgen Peter Jensen, Peter Simonsen and Bo Sander "Leaching of Nutrient Salts from Fly Ash from Biomass Combustion", Proceedings from 14th European Conference and Technology Exhibition on Biomass for Energy, Industry and Climate Protection, October 2005, p. 1273-1276.
5. Morten Mejlholm, Kaj Thomsen, Peter Rasmussen, Jørgen Vergod, Freddy Knudsen, Hugo Høyer: "SODIUM CHLORIDE DIHYDRATE - A POTENTIAL CAUSE OF SLIPPERY ACCIDENTS" Presented at the XIth PIARC International Winter Road Congress, Sapporo, Japan, January 28-31, 2002. Proceedings of the XIth PIARC International Winter Road Congress, Sapporo, Japan (2002))
6. Kaj Thomsen and Peter Rasmussen, "CO_2 hydrates in Aqueous electrolyte and sucrose solutions" Presentation given at 18th ESAT (18. European Seminar on Applied Thermodynamics, Kutná Hora, Czech Republic, 2000).
7. K. Thomsen and P. Rasmussen, "Thermodynamic Model for the Ammonia-Water System" ("Steam Water and Hydrothermal Systems: Physics and Chemistry Meeting the Needs of Industry" Proceedings of the 13th International Conference on the Properties of Water and Steam, Editors: P.G. Hill, P. Tremaine, D. Irish, and P.V. Balakrishnan, NRC Press, Ottawa, 2000, 118-125)

Reports

8. Victor Camille Alfred Darde, Kaj Thomsen, Erling Halfdan Stenby, "Chilled ammonia process for CO_2 capture", (2008)
9. Philip Loldrup Fosbøl, Erling Halfdan Stenby, Kaj Thomsen, "The chilled ammonia process - Evaluation of the energy requirements", (2008)
10. Kaj Thomsen, Jørgen Peter Jensen, Peter Simonsen, Bo Sander "Reuse of Alkali from Fly Ash from Biomass Combustion", Report on research project sponsored by PSO (Danish Power Plants), February 2006.

11. Thomsen K.: "Aqueous Electrolytes: Model Parameters and Process simulation". Dissertation, DTU, 1997.
12. Thomsen, Kaj, "Soda ash liquors: Phase diagrams and process simulation", Confidential report, FMC Chemical Research and Development Center, Princeton, NJ., 1996

Other publications

13. Philip Fosbøl, Kaj Thomsen, and Erling H. Stenby, "CO_2 - A greenhouse gas and a corrosion problem" (Dansk Kemi 89(2008)19-22)
14. Peter Jørgensen Herslund, Claus Maarup Rasmussen, and Kaj Thomsen, "Development of method for the removal of NH_3 from flyash" (Dansk Kemi 88(2007)14-17)
15. Helge Danneskiold-Samsøe and Kaj Thomsen, "Selective Crystallization of Potassium Salts from Biomass Fly Ash", (Dansk Kemi 87(2006)16-19)
16. Martin Feldskov and Kaj Thomsen, "Precipitation of Vanadium Salts", (Dansk Kemi, 87(2006)13-15)
17. Kaj Thomsen and Peter Rasmussen, "Salt Solubility", (Dansk Kemi, 85(8)(2004)22)
18. Søren Gregers Christensen and Kaj Thomsen, "Modelling of equilibria in ionexchange processes", (Dansk Kemi 84, 9(2003) 21-23)
19. Søren Gregers Christensen and Kaj Thomsen, "Production of fertilizer salts" (Dansk Kemi 83(2)(2002)18-19)
20. Thomsen, Kaj, Rasmussen, Peter. "Nickel sulfate - some supplementary information", (Dansk Kemi 80(1999),(5),33)
21. Kaj Thomsen, Peter Rasmussen, and Rafiqul Gani, "Simulation of fractional crystallization of electrolyte solutions" (Dansk Kemi 76(1995)(10)23-27