

Celebrating 50 Years

# Distillation & Absorption 2010

12-15 September 2010  
Eindhoven, the Netherlands



# Distillation Absorption 2010

12-15 September 2010  
Eindhoven University of Technology  
Eindhoven, The Netherlands  
[www.da2010.nl](http://www.da2010.nl)

# Final Programme & Abstracts



# DSTI a career opportunity

## *for you?*



**DSTI** is a Technology Development and Implementation Platform for the Process Industry. Industry and knowledge institutes work closely together under the motto: "Together we can take bigger steps, have more impact, and share the risks".

So far, 50 companies from the Food, Pharmaceutical, Oil and Gas, Chemical and Process Water Industries, and 10 knowledge institutes, have joined DSTI. The total size of the program is almost 100 million Euro and over 300 (ca. 100fte) people are involved in the project execution.

### **Developing what really matters**

Seventy percent energy savings, medicines with reduced side effects, compact and waste-free manufacturing processes, high value feed supplements from milk, process water of the required quality, a doubling of the amount of recoverable oil per field, and technologists with R&D and business skills. These are some of the targets our partners have defined.

DSTI offers the best of the scientific and industrial world. You will be working in a project team with top level researchers from universities, industry and contract research organisations on the cutting edge of Process Technology. Joining the DSTI means exploring the multi-disciplinary network of the Food, (Bio)Chemical, Pharmaceutical and Oil & Gas industries. The R&D program covers all aspects from (fundamental) knowledge generation to technology implementation.

### **DSTI a career opportunity for you?**

DSTI is continuously looking for enthusiastic junior and experienced researchers. Are you interested in a challenging position at DSTI than please visit [www.dsti.nl](http://www.dsti.nl) for our vacancies.

## **DUTCH SEPARATION TECHNOLOGY INSTITUTE**

Postbus 247  
3800 AE Amersfoort  
T 033 467 6241  
E [recruiting@dsti.nl](mailto:recruiting@dsti.nl)  
[www.dsti.nl](http://www.dsti.nl)





INTRODUCTION

On behalf of the organizing committee, it gives us great pleasure to invite you to the 9th Distillation & Absorption Conference in Eindhoven, The Netherlands on **12-15 September 2010**. Leading the organization has been the Dutch separation technology community, working in close collaboration with the European Federation of Chemical Engineers' Working Party on Fluid Separations. Delegates from all corners of the world are making the journey to London and we look forward to meeting all of you during the course of your stay.

The conference will showcase the newest and best in Distillation and Absorption technology while celebrating the **50th anniversary** of this well-known series of conferences that began in Brighton, UK, in 1960. The latest conferences took place in 1992 Birmingham (UK), 1997 Maastricht (Netherlands), 2002 Baden-Baden (Germany) and last 2006 in London (UK).

**Distillation & Absorption 2010** will cover a broad range of contributions on fundamental and applied aspects of distillation and absorption technology from all over the world, presented in 5 plenary lectures, 52 scientific lectures and 60 posters. Special theme is **Carbon Dioxide Mitigation by Energy Efficiency and Capture**. Outside the session lecture theatres, you will also find numerous sponsors and exhibitors are presenting their contributions.

We wish you all an exciting and productive conference in Eindhoven.

André de Haan  
Chair

Harry Kooijman  
Vice Chair

Andrzej Górak  
Scientific Chair

Eva Sorensen  
Chair EFCE-WP  
Fluid Separations



## A Global Force in Heat and Mass Transfer Products

RASCHIG JAEGER offers a diverse array of products to meet the mass transfer needs of the industries. While specialising in high performance products, the comprehensive product line includes traditional packing types in metal, plastic, ceramic and fibreglass best fitting the application.

### Markets

- Refineries
- Petrochemical plants
- Chemical plants
- Environmental applications
- Natural gas plants



Raschig test stand - 12 m diameter and liquid loading to 2400 m<sup>3</sup>/h



RASCHIG GmbH • Mundenheimer Strasse 100 • 67061 Ludwigshafen • Germany  
Tel. + 49 621 5618 648 • Fax. + 49 621 5618 627 • [www.raschig.de](http://www.raschig.de) • email. [MSchultes@raschig.de](mailto:MSchultes@raschig.de)

## Powering Your Performance



INNOVATION



ENGINEERING



OPTIMIZATION

Creating value and providing a distinctive competitive edge for our customers – that is the mission of Bayer Technology Services as a fully integrated technology partner. 2,600 employees worldwide work on this aim – at 13 locations on 3 continents. As a Bayer company, we combine longtime experience and close ties to operators with supreme innovative capabilities. Along the entire lifecycle – from developing processes and products through engineering and building plants to automating and optimizing processes – our know-how delivers high-performance technology solutions. With the objective of sustainably increasing our customers efficiency – **Powering Your Performance.**

Bayer Technology Services GmbH • 51368 Leverkusen, Germany  
E-mail: [info@bayertechnology.com](mailto:info@bayertechnology.com) • [www.bayertechnology.com](http://www.bayertechnology.com)



Bayer Technology Services

**National Organizing Committee**

<b>André de Haan</b>	Eindhoven University of Technology ( <b>chair</b> )
<b>Harry Kooijman</b>	Shell Global Solutions International BV ( <b>vice chair</b> )
<b>Andrzej Górak</b>	Technische Universität Dortmund ( <b>scientific chair</b> )
<b>Zarko Olujic</b>	Delft University of Technology
<b>Menno Plantenga</b>	Dutch Separation Technology Institute
<b>Jeffrey Felix</b>	Sulzer Chemtech Ltd.
<b>Peter Alderliesten</b>	Energy Research Centre of the Netherlands (ECN)
<b>Caroline van Os</b>	Eindhoven University of Technology (conference secretariat)
<b>Pleunie Smits</b>	Eindhoven University of Technology (conference secretariat)
<b>Joan Houtsmuller</b>	Eindhoven University of Technology (congress office)
<b>Karine vd Wildenberg</b>	Eindhoven University of Technology (congress office)

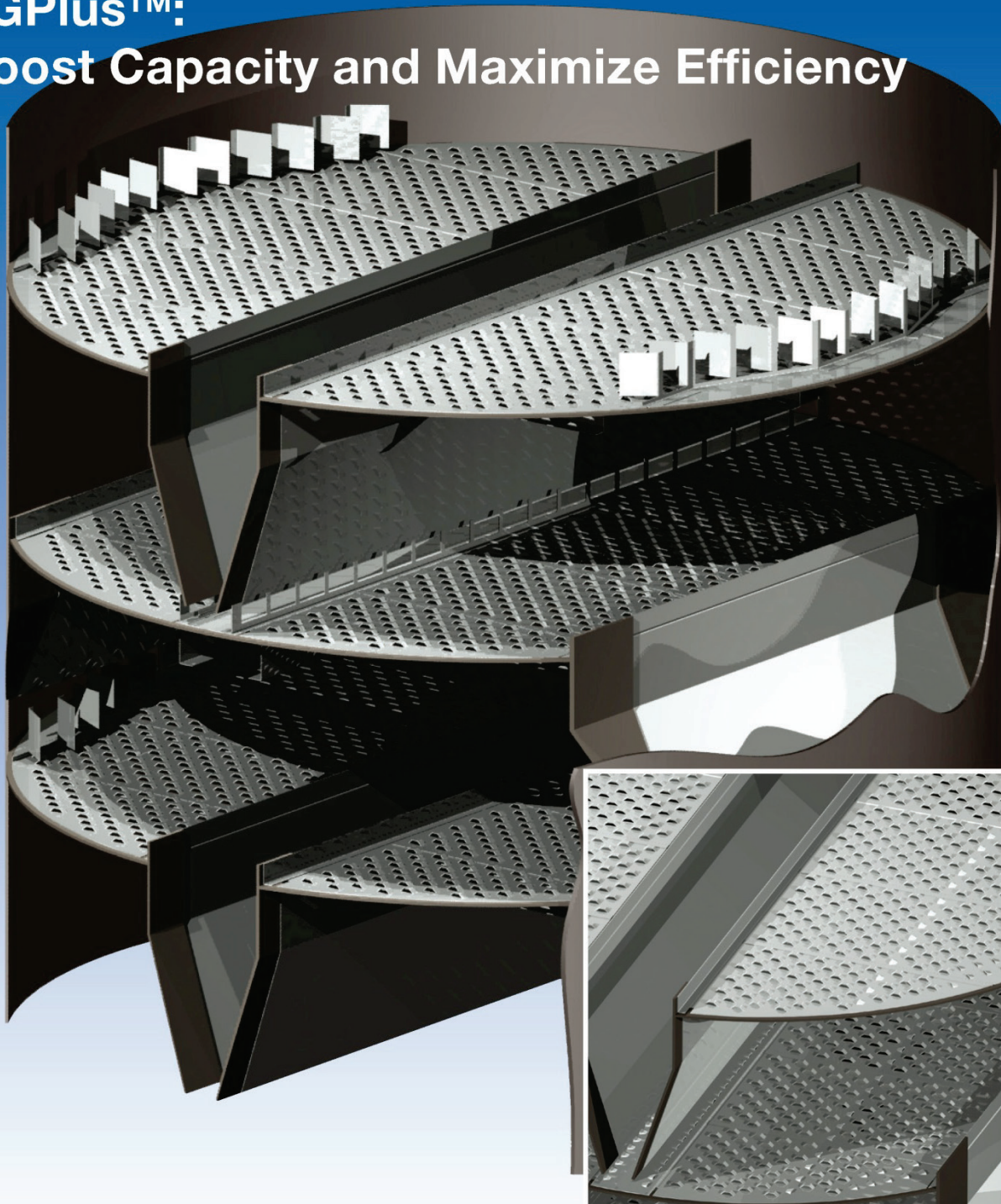
**Topic Coordinators**

Energy Efficiency	<b>Megan Jobson</b>
Carbon Dioxide Capture	<b>Lothar Spiegel</b>
Integrated, Hybrid and Novel Processes	<b>Andrzej Górak</b>
Basic Data	<b>André de Haan</b>
Modelling and Simulation	<b>Harry Kooijman</b>
Control and Operation	<b>Eva Sorensen</b>
Equipment Design and Operation	<b>Zarko Olujic</b>
Process Troubleshooting and Handling Operational Problems	<b>Izak Nieuwoudt</b>

**Scientific committee**

Rakesh Agrawal	USA	Wolfgang Marquardt	Germany
Juhani Aittamaa	Finland	Michel Meyer	France
Wolfgang Arlt	Germany	Masaru Nakaiwa	Japan
Santanu Bandyopadhyay	India	Izak Nieuwoudt	USA
Magdalena Bendova	Czech Republic	Knut Nordstad	Norway
Jose Bravo	USA	Ralf Proplesch	Switzerland
Elisabetta Brunazzi	Italy	Gary Rochelle	USA
I-Lung Chien	Taiwan	Sigurd Skogestad	Norway
Richard Darton	UK	Eva Sorensen	UK
Paul Feron	Australia	Lothar Spiegel	Switzerland
David Glasser	South Africa	Ross Taylor	USA
Kejin Huang	China	Robin Thiele	Germany
Megan Jobson	UK	Alexander Toikka	Russia
Henry Kister	USA	Johan de Wet	South Africa
Peter Lang	Hungary	Maria Regina Wolf Maciel	Brasil
Sanjay Mahajani	India	Gunter Wozny	Germany

# VGPlus™: Boost Capacity and Maximize Efficiency



MOVING AHEAD

CT.19e

**SULZER**

Sulzer Chemtech offers the best ever tested and industry proven, high performance chordal downcomer tray, VGPlus. The VGPlus tray enables you to push towers to their capacity limits. With years of experience in developing, designing and operating trays, application know-how, and successful FRI testing, you can be assured that Sulzer Chemtech has the optimal solution to your high performance needs. The combination of patented and proven technologies increases capacity

without compromising efficiency. VGPlus tray technology is the key to economically unlocking revamp barriers and exceeding target capacity. Optimized MVGTM valve layout, high performance downcomers, redirecting devices and froth promotion are applied individually to meet the demanding requirements of each service. From Superfractionators to fouling services: VGPlus can do it all!

For more information, visit our pages at [www.sulzerchemtech.com](http://www.sulzerchemtech.com)

**Sulzer Chemtech**

Europe, Middle East and Africa  
Sulzer Chemtech Ltd, 8404 Winterthur, Switzerland  
Phone +41 52 262 50 28, Fax +41 52 262 01 82  
[chemtech@sulzer.com](mailto:chemtech@sulzer.com)

North and South America  
Sulzer Chemtech USA, Inc., Humble, TX 77396, USA  
Phone +1 281 441 5800, Fax +1 281 291 0207  
[chemtech@sulzer.com](mailto:chemtech@sulzer.com)

Asia Pacific  
Sulzer Chemtech Pte. Ltd., Singapore 629845  
Phone +65 6515 5500, Fax +65 6862 7563  
[chemtech@sulzer.com](mailto:chemtech@sulzer.com)

(This technical programme may be subject to change)

**Sunday 12 September 2010**

17.00 – 19.00 Registration and Welcome Reception

Sponsored by: **SULZER**

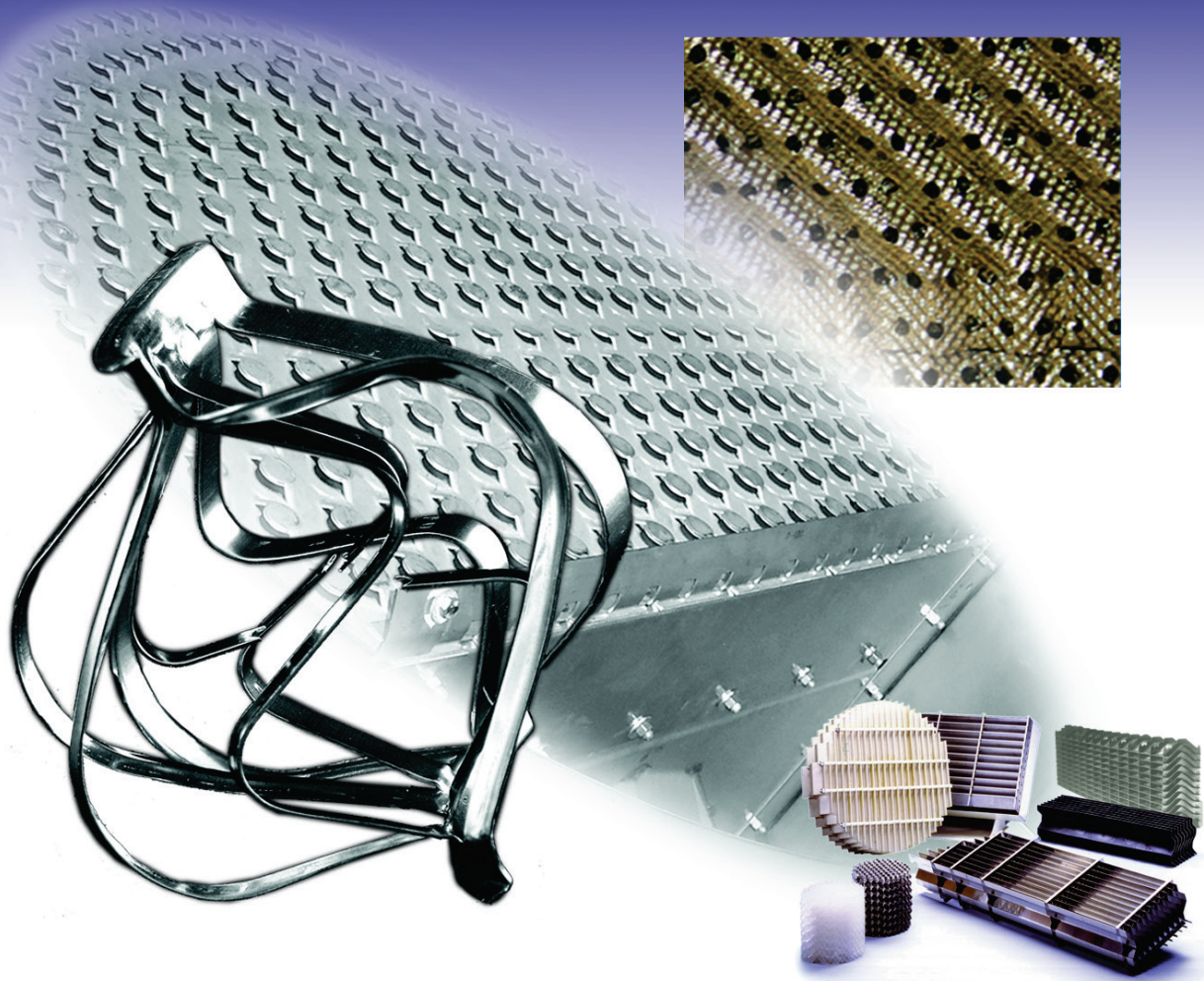
**Monday 13 September 2010**

08.00 Registration  
 09.00 Opening Ceremony  
 09.05 **Celebrating 50 years of Distillation Absorption Conferences**  
*Richard Darton, EFCE President, University of Oxford, UK*  
 09.25 Plenary Lecture: **Shell's Response to Climate Change and the Challenges in Innovation**  
*Frigyes Lestak, Annet Stones, Jose Bravo*  
*General Manager Existing Assets, Group CO<sub>2</sub>, Shell International Petroleum Company Limited, UK*  
 Session Chairs: André de Haan, TU-Eindhoven, The Netherlands & Harry Kooijman, Shell Global Solutions, The Netherlands

**Parallel Sessions**

	Theme: <b>Energy Efficiency</b> Session Chair: Megan Jobson, University of Manchester, UK		Theme: <b>Modeling and Simulation</b> Session Chair: Jens-Uwe Repke, TU Bergakademie Freiberg, Germany
10.15	<b>A Design Simplification of the Ideal Heat-Integrated Distillation Column</b> <i>K. Huang, H. Chen, S. Wang, China</i>	10.15	<b>A Memetic Algorithm for the Design Optimization of Reactive Distillation Columns</b> <i>M. Urselman, S. Engell, Germany</i>
10.40	<b>Identifying Optimal Mixture Properties for HiDiC Application</b> <i>A. Harwardt, K. Kraemer, W. Marquardt, Germany</i>	10.40	<b>Optimal Design Methodology for Divided Wall Columns</b> <i>C. Gutiérrez-Antonio, A. Briones-Ramírez, Mexico</i>
11.05	Coffee Break		
11.30	<b>Multicomponent Distillation Configurations with Large Energy Savings</b> <i>V.H. Shah, R. Agrawal, USA</i>	11.30	<b>Extended Channel Model for Prediction of Hydraulics and Mass Transfer of Random Packing Columns for Gas-Liquid Systems</b> <i>J. Maćkowiak, Germany</i>
11.55	<b>Multi Objective Optimization for an Economical Dividing Wall Column Design</b> <i>C. Hiller, S. Storm, M. Leipold, G. Fieg, Germany</i>	11.55	<b>Rate Based Modeling of Two Commercial Scale H<sub>2</sub>S Stripping Columns</b> <i>R. Taylor, P. Wilkinson, H.A. Kooijman, USA</i>

Imagine the possibilities.  
Discover the difference.



## **SUPERFRAC® tray**

highest combined capacity and efficiency crossflow tray tested at FRI

## **FLEXIPAC® HC® structured packing**

highest efficiency, high capacity structured packing

## **INTALOX® ULTRA™ PACKING**

## **BRIDGING THE GAP BETWEEN**

## **CAPACITY & EFFICIENCY**

## **FLEXICHEVRON® mist eliminators**

highest capacity and best for fouling applications.

Biofuels **MINING**  
ENVIRONMENTAL  
Food Processing  
CHEMICAL **POWER**  
Petrochemical  
GAS PROCESSING  
INDUSTRIAL GAS  
PHARMACEUTICAL  
Pulp & Paper  
PETROLEUM REFINING

**KOCH-GLITSCH**

[koch-glitsch.com](http://koch-glitsch.com)



12.20 **Designing Four-Product Dividing Wall Columns for Separation of a Multicomponent Aromatics Mixture**  
*I. Halvorsen, I. Dejanović, Z. Olujić, L. Matijašević, S. Skogestad, H. Jansen, B. Kaibel The Netherlands*

12.20 **A Computational Fluid Dynamics and Experimental Approach to the Effects of Push Valves on Sieve Trays**  
*R. Rahimi, T. Zarej, A. Zarei, N. Naziri, Iran*

12.45 – 13.30 Lunch Break

13.30 Plenary Lecture: **New solvent systems for distillation and absorption intensification**  
*Matthias Seiler, Evonik, Germany*  
Session Chair: Peter Alderliesten, ECN, The Netherlands

## Parallel Sessions

Theme: **Carbon Dioxide Capture**  
Session Chair: Lothar Spiegel, Sulzer Chemtech, Switzerland

14.20 **Energy Efficient Synthesis and Design for Carbon Capture**  
*A. Lucia, A. Roy, M. Sorin, USA*

14.45 **Pilot Plant Experiments with MEA and New Solvents for Post Combustion CO<sub>2</sub> Capture by Reactive Absorption**  
*H.P. Mangalapally, H. Hasse, Germany*

15.10 **Optimized Absorber Design for Post Combustion CCS**  
*M. Duss, A. Menon, Switzerland*

15.35 **Update on Aqueous Ammonia Based Post Combustion Capture Pilot Plant at Munmorah**  
*H. Yu, S. Morgan, A. Allport, T. Do, A. Cottrell, J. McGregor, P. Feron, Australia*

16.00 **Use of Multi-Scale Simulations for Lowering the Cost of Carbon Dioxide Capture**  
*L. Raynal, P. Font, T. Janeiro, Y. Haroun, P.-A. Bouillon, France*

Theme: **Modeling and Simulation**  
Session Chair: Ross Taylor, Clarkson University, USA

14.20 **Design of Complex Distillation Columns Separating Ternary Heterogeneous Azeotropic Mixtures**  
*P. Prayoonyoung, M. Jobson, UK*

14.45 **A Generalized Methodology for Optimal Configurations of Hybrid Distillation-Pervaporation Processes**  
*Y. Naidu, R.K. Malik, India*

15.10 **Column Profiles for Membrane Column Sections**  
*M. Peters, S. Kauchali, D. Hildebrandt, D. Glasser, South Africa*

15.35 **Thermodynamic Insight in Extractive Distillation with Entrainer Forming New Azeotropes**  
*I. Rodriguez Donis, V. Gerbaud, X. Joulia, France*

16.00 **Short-Cut Methods for the Optimal Design of Simple and Complex Distillation Columns**  
*C. Adiche, A. Vogelpohl, Germany*

16.30 – 19.00 Poster Session with light refreshments

Sponsored by:  **KOCH-GLITSCH**

# Challenge the future

What if we could reduce our carbon footprint? What if we could produce products where we need them, based on renewable resources? And what if we could efficiently capture CO<sub>2</sub> and reuse it in our processes?

At AkzoNobel, we're passionate about innovation. Which is why our 57,000 employees thrive on changing bright ideas into innovative products and processes.

That's how we became the world's largest coatings company and a leading supplier of speciality chemicals. We believe in challenging the future so that we can deliver Tomorrow's Answers Today.

Which is why AkzoNobel is proud to sponsor the 9th International Conference on Distillation & Absorption.

**Please contact Cornald van Strien, present at the conference, if you are interested in working with AkzoNobel.**



**AkzoNobel**  
Tomorrow's Answers Today

Theme: <b>Carbon Dioxide Capture</b>			
PO05	<p><b>Mass Transfer and Pressure Drop of a Novel Structured Packing for CO<sub>2</sub> Post-Combustion Capture</b>  <i>P. Alix, L. Raynal, A. Royon-Lebeaud, F. Abbe, V. Bessou, M. Meyer, M. Prevost, D. Rouzineau, France</i></p>	PO58	<p><b>Reactive Absorption of CO<sub>2</sub> in MEA: a Scale-up Study</b>  <i>C. Kale, A. Müller, I. Tönnis, H. Hasse, A Górak, Germany</i></p>
PO06	<p><b>CO<sub>2</sub> Capture Solvent Selection by Combined Absorption-Desorption Analysis</b>  <i>U.E. Aronu, H.F. Svendsen, K.A. Hoff, Norway</i></p>	PO59	<p><b>Equilibrium Behaviour of a Novel Gas Separation Process, with Application to Carbon Capture</b>  <i>M. Sweatman, UK</i></p>
PO07	<p><b>Carbon Dioxide Chemical Absorption with Glucosamine in Air-Lift Reactor</b>  <i>A. Garcia-Abuín, D. Gómez-Díaz, J.M. Navaza, I. Vidal-Tato, Spain</i></p>	PO60	<p><b>Challenges and Opportunities for Post-Combustion CO<sub>2</sub> Capture in Australia</b>  <i>P.H.M. Feron, Australia</i></p>
PO08	<p><b>Rate Based Modeling and Validation of a Carbon Dioxide Pilot Plant Absorption Column Operating on Monoethanolamine</b>  <i>L.L. Simon, Y. Elias, G. Puxty, Y. Artanto, K. Hungerbuhler, Switzerland</i></p>		
PO09	<p><b>CO<sub>2</sub> Absorption into Biphasic Amine Solvent and Reduction of Solvent Losses</b>  <i>J. Zhang, O. Nwani, D.W. Agar, Germany</i></p>		Theme: <b>Energy Efficiency</b>
PO10	<p><b>Aqueous Solutions of Pyrrolidine for Carbon Dioxide Capture</b>  <i>A. Blanco, A. Garcia-Abuín, D. Gómez-Díaz, J.M. Navaza, I. Vidal-Tato, Spain</i></p>	PO01	<p><b>Exergy Losses Relation with Driving Forces in Distillation Column</b>  <i>S.A. Ashrafizadeh, M. Amidpour, Z. Heydaricesht, Iran</i></p>
PO11	<p><b>Development of Task Specific Hyperbranched Polymers for the Separation of Carbon Dioxide: Carbon Capture and Biogas Upgrade</b>  <i>J. Völkl, J. Rolker, W. Art, Germany</i></p>	PO02	<p><b>Synthesis and Optimization of Demethanizer Flowsheets for Low Temperature Separation Processes</b>  <i>M. Nawaz, M. Jobson, UK</i></p>
PO12	<p><b>Preliminary Analysis of Process Flow Sheet Modifications for Energy Efficient CO<sub>2</sub> Capture from Flue Gases using Chemical Absorption</b>  <i>A. Cousins, L.T. Wardhough, P.H.M. Feron, Australia</i></p>	PO03	<p><b>Conceptual Design and Comparison of Four-Products Dividing Wall Columns for Separation of a Multicomponent Aromatics Mixture</b>  <i>I. Dejanović, L. Matijašević, Z. Olujić, I. Halvorsen, S. Skogestad, H. Jansen, B. Kaibel, The Netherlands</i></p>
PO13	<p><b>Capital Costs and Energy Considerations for Different Alternative Stripper Configurations for Post Combustion CO<sub>2</sub> Capture</b>  <i>M. Karimi, M. Hillestad, H.F. Svendsen, Norway</i></p>	PO04	<p><b>Establishing Internal Configuration of Dividing Wall Column for Separation of a Multicomponent Aromatics Mixture</b>  <i>I. Halvorsen, I. Dejanović, L. Matijašević, Z. Olujić, S. Skogestad, The Netherlands</i></p>



# CSIRO Coal Technology

CSIRO is Australia's national science organisation. We are researching and developing technologies to support safe, efficient and environmentally sound coal mining operations and to accelerate the deployment of low emissions coal-based power technologies.

**Contact:** Dr John Carras – Director, CSIRO Coal Technology  
ph: 61 2 9490 8644 email: [john.carras@csiro.au](mailto:john.carras@csiro.au)

[www.csiro.au/science/Coal](http://www.csiro.au/science/Coal)



Theme: <b>Integrated, Hybrid and Novel Processes</b>			
PO14	<p><b>Reactive Dividing Wall Columns: Towards Enhanced Process Integration</b>  <i>A.A. Kiss, J.J. Pragt, C.J.G. van Strien, The Netherlands</i></p>	PO61	<p><b>Optimisation Based Design of Membrane Assisted Hybrid Separation Processes using an Evolutionary Algorithm</b>  <i>K. Koch, D. Sudhoff, S.Kreiß, P. Kreis, Germany</i></p>
PO15	<p><b>Novel Graphical Design Methods for Complex Membrane Configurations</b>  <i>M. Peters, S. Kauchali, D. Hildebrandt, D. Glasser, South Africa</i></p>	PO62	<p><b>How to Separate Two Near Azeotropes. Case of the Separation of the Mixture Phenol-Hydrocarbons</b>  <i>F. Oprea, Romania</i></p>
PO16	<p><b>Synthesis of Novel Ternary Heterogeneous Azeotropic Distillation Flowsheets</b>  <i>P. Prayoonyoung, M. Jobson, UK</i></p>	PO63	<p><b>Reactive Distillation for Selectivity Improvement in the Transesterification of Dimethyl Carbonate</b>  <i>T. Keller, A. Niesbach, A. Hoffmann, A. Górak, Germany</i></p>
PO17	<p><b>An Introduction into New Higeer Device and Its Industrial Applications</b>  <i>G.Q. Wang, Z.C. Xu, X.H. Li, J.B. Ji, China</i></p>	PO64	<p><b>Modeling and Simulation of the TAAE Synthesis by Catalytic Distillation</b>  <i>C.A. González-Ruggerio, W. Salacki, J. Pilarczyk, A. Górak, Germany</i></p>
PO18	<p><b>Catalytically Activated SiC Foam for Reactive Distillation</b>  <i>J. Lévêque, D. Rouzineau, M. Prevost, M. Meyer, France</i></p>		<p>Theme: <b>Basic Data</b></p>
PO19	<p><b>Effect of Hydrodynamic Conditions on Mass and Heat Transfer in a Novel Membrane-Based Continuous Micro Distillation Device: Experimental Approach</b>  <i>C. Adiche, K. Sundmacher, Germany</i></p>	PO26	<p><b>The Simulation of Vapor-Liquid Equilibrium in Ternary Systems with Two Ternary Azeotropes</b>  <i>A.K. Frolkova, T.V. Chelyuskina Russian Federation</i></p>
PO20	<p><b>Experimental Validation of a New Double-Column for Heteroazeotropic Batch Distillation</b>  <i>F. Denes, P. Lang, X. Joulia, Hungary</i></p>	PO27	<p><b>Absorption Rates of CO<sub>2</sub> into Solutions of MEA/2-Propanol</b>  <i>L.J. du Preez, C.E. Schwarz, J.H. Knoetze, South Africa</i></p>
PO21	<p><b>Solvent Recovery from a Multicomponent Mixture by Batch Extractive Distillation and Hybrid Process</b>  <i>P. Lang, L. Hegely, G. Kovacs, J. Gaal-Szilagyi, B. Kotai, Hungary</i></p>	PO28	<p><b>Experimental Study on Contact Angle of Ethanol and n-Propanol Aqueous Solutions on Metal Surfaces</b>  <i>C.X. Zhou, X.G. Yuan, L.T. Fan, A.W. Zeng, K.T. Yu, M. Kalbassi, K.E. Porter, China</i></p>
PO22	<p><b>Reactive Packed Bubble Column for the Synthesis of Isopropyl Myristate</b>  <i>M.C. de Jong, E. Zondervan, A.B. de Haan, The Netherlands</i></p>	PO29	<p><b>Phase Equilibria of Organic Sulfur Compounds for Cleaner Fuels</b>  <i>E. Sapei, P. Uusi-Kyynty, K.I. Keskinen, J. Aittamaa, Finland</i></p>
PO23	<p><b>Biodiesel Production from Reactive Distillation Process: A Comparative Study Between Experimental Results and Simulation</b>  <i>N. de Lima da Silva, C.M. Garcia Santander, C. Benedito Batistella, R. Maciel Filho, M.R. Wolf Maciel, Brasil</i></p>	PO30	<p><b>New Methodology of Determination of Boiling Point at Very Low Pressure: Petroleum Case</b>  <i>M. Savioli Lopes, P. Sbaite, C. Benedito Batistella, M.R. Wolf Maciel, R. Maciel Filho, A. de Oliveira Gomes, L. Carmen Medina, Brasil</i></p>
PO24	<p><b>Selective Removal of Carbon Dioxide from Aqueous Ammonia Solutions</b>  <i>J.F. Maćkowiak, A. Górak, Germany</i></p>	PO31	<p><b>Modeling and Experimental Study of Carbon Dioxide Absorption into Aqueous Amine Based Solvents</b>  <i>L. Dubois, D. Thomas, Belgium</i></p>
PO25	<p><b>Cyclohexanol Production from Cyclohexane in a Reactive Divided Wall Column: a Feasibility Study</b>  <i>S. Thotla, A. Katariya, H. Freund, K. Sundmacher, Germany</i></p>	PO65	<p><b>Multi-Effect Distillation – Wettability of Polymeric Falling Film Heat Transfer Surfaces</b>  <i>J.B.P. Christmann, L.J. Krätz, H.-J. Bart, Germany</i></p>

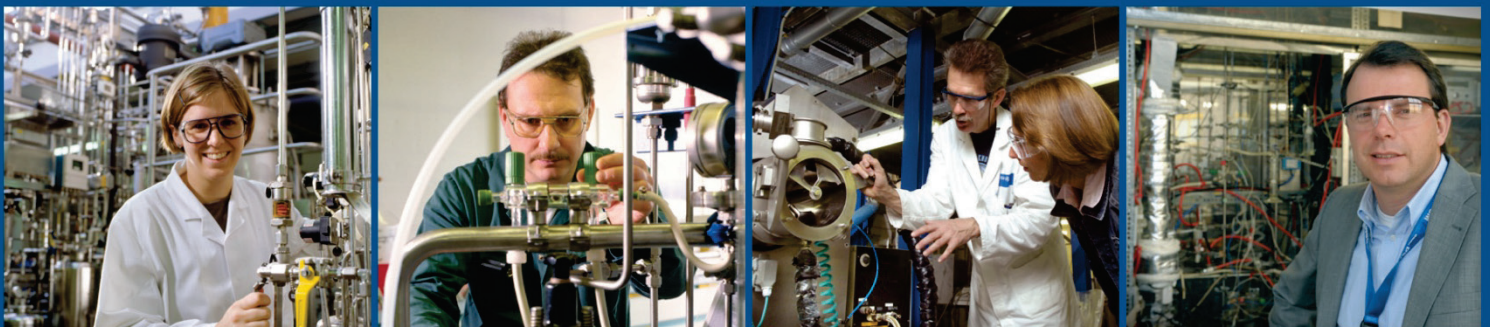


# DSM – the Life Sciences and Materials Sciences Company

We are DSM – a company of innovators. And we're always on the lookout for new talent to join our global team. One of our core competence areas is Process Technology. So if you're a high-caliber engineer in this field (MSc or PhD level), we'd like to hear from you. Chances are we can offer you an exciting career. Contact us now – let's discover each other!

If you are interested in DSM and our career opportunities, please go to our website [www.dsm.com/careers](http://www.dsm.com/careers), where you will find more information on current job openings and where you also may submit an open (speculative) application.

Contact us:  
DSM Recruitment  
DSM Expert Center  
P.O. Box 6500, 6401 JH Heerlen, The Netherlands  
Telephone: +31 (0)45-5782037



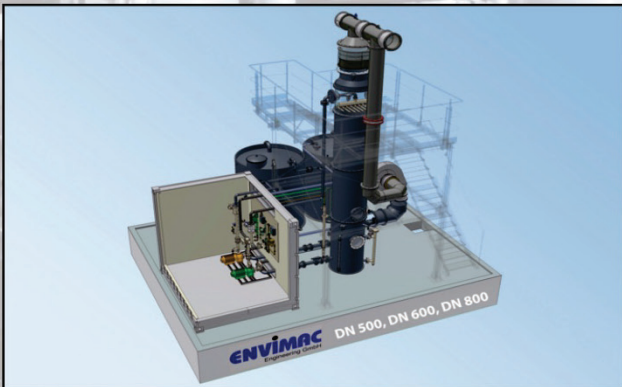
*Unlimited.* **DSM**

Theme: <b>Modeling and Simulation</b>			
<b>PO32</b>	<b>Optimal Design Methodology for Azeotropic Distillation Columns</b> <i>C. Gutiérrez-Antonio, A. Briones-Ramírez, Mexico</i>	<b>PO40</b>	<b>Distillation Boundaries in Ternary Heteroazeotropic Systems</b> <i>A.R. Królikowski, Poland</i>
<b>PO33</b>	<b>Boundary Value Design Method for Complex Demethanizer Columns</b> <i>M. Nawaz, M. Jobson, UK</i>	<b>PO41</b>	<b>CFD Simulations of Flow, Heat and Mass-Transfer in Thin-Film Evaporator</b> <i>A. Kolek, J. Dziak, L. Krolkowski, Poland</i>
<b>PO34</b>	<b>Rate Based Mass Transfer Performance Analysis of [EMIM][EtSO<sub>4</sub>] and Ethylene Glycol in the Extractive Distillation of Water-Ethanol Mixtures</b> <i>E. Quijada, G.W. Meindersma, A.B. de Haan, The Netherlands</i>	<b>PO42</b>	<b>Development &amp; Application of Continuous Thermodynamics for Studying Physicochemical Properties of Petroleum Fractions</b> <i>L.P. Tovar, M.R. Wolf-Maciel, C.B. Batistella, R. Maciel-Filho, A. de O. Gomes, L.C. Medina, Brazil</i>
<b>PO35</b>	<b>A Short Method to Calculate Residue Curve Maps</b> <i>M. Carrera-Rodríguez, J.G. Segovia-Hernández, A. Bonilla-Petriciolet, Mexico</i>	<b>PO43</b>	<b>Design of Feed Distribution System in a Falling Film Distillation using CFD</b> <i>J.G. Teleken, L.O. Werle, I.G.B. Parisotto, C. Marangoni, A.P. Meneguelo, R.A.F. Machado, Brazil</i>
<b>PO36</b>	<b>Geometry Subsets of Optimality in Extractive Distillation of Multicomponent Mixtures</b> <i>A.V. Timoshenko, B.B. Dolmatov, E.A. Anokhina, V.S. Timofeev, Russian Federation</i>	<b>PO44</b>	<b>Shortcut Methods for the Design of Heteroazeotropic Distillation of Multicomponent Mixtures</b> <i>K. Kraemer, A. Harwardt, W. Marquardt, Germany</i>
<b>PO37</b>	<b>Ionic Liquid Selection and Performance Evaluation for the Separation of Methylcyclohexane-Toluene by Extractive Distillation</b> <i>J.P. Gutierrez, G.W. Meindersma, A.B. de Haan, The Netherlands</i>	<b>PO45</b>	<b>Simulation of Anhydrous Bioethanol Production Process using Efficiency Correlation for Conventional and Extractive Distillation</b> <i>T.L. Junqueira, M.O.S. Dias, M.R. Wolf Maciel, R. Maciel Filho, C.E.V. Rossel, Brazil</i>
<b>PO38</b>	<b>A Study on Sieve Tray Lower Operating Limit</b> <i>A. Zarei, R. Rahimi, T. Zarei, N. Naziri, Iran</i>	<b>PO66</b>	<b>Hydrodynamics of Liquid Flow in the Model of Theoretical Stage with Perfect Displacement</b> <i>V. Maleta, V. Taran, B. Maleta, Ukraine</i>
<b>PO39</b>	<b>Novel Minimum Reflux Calculation using Eigenvector Maps</b> <i>R. Abbas, S. Holland, I. Halvorsen, South Africa</i>	<b>PO67</b>	<b>Process Design for Micro-Structured Distillation Devices</b> <i>B. Dercks, G. Schmidt, M. Grünwald, Germany</i>



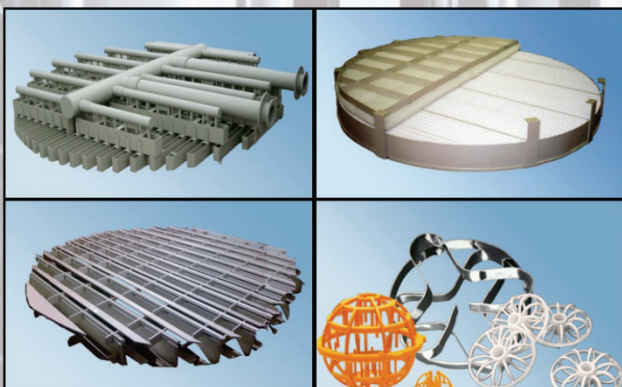
**Plant design**

We are specialised in the development, construction, production, modernisation and maintenance of specific components, equipment and key-ready plants for application in chemical engineering and environmental technology.



**Test facilities for packings**

Our highly automated pilot plants allow standardised fluiddynamic and mass transfer experiments to determine the operation range and separation efficiency of packed columns.



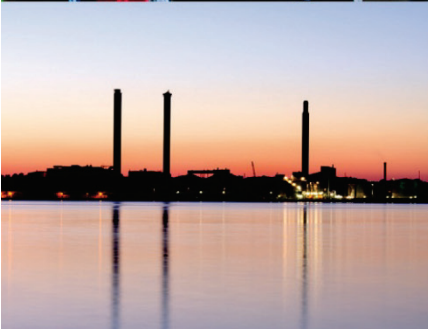
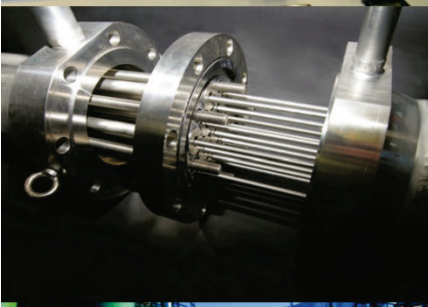
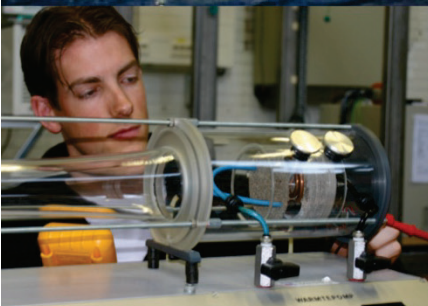
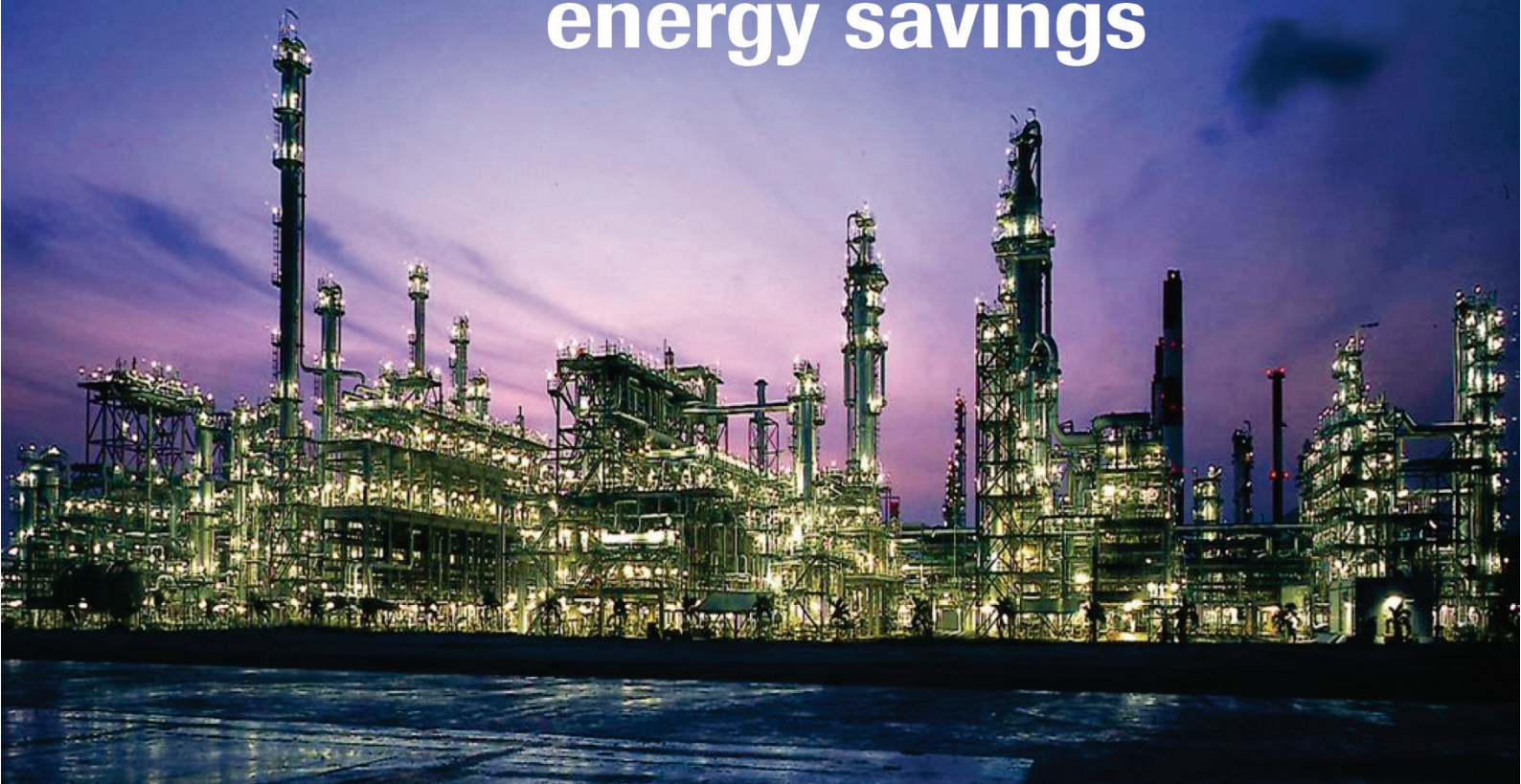
**Column internals**

We offer high-performance random packings, liquid and gas distributors, supporting trays, droplet separators and demisters as well as various software packages for the design of packed and tray columns.



	Theme: <b>Control and Operation</b>		Theme: <b>Equipment Design and Operation</b>
PO46	<b>Double Column Batch Rectifier in Closed Mode for Pressure Swing Batch Distillation</b> <i>G. Modla, Hungary</i>	PO50	<b>Improved High Performance Trays</b> <i>S. Hirsch, M. Pilling, USA</i>
PO47	<b>Product Composition of a Pressure Swing Double Column Batch Rectifier</b> <i>A. Kopasz, G. Modla, P. Lang, Hungary</i>	PO51	<b>Experimental Characterization of Ceramic Sponges as Column Internals</b> <i>J. Grosse, M. Kind, Germany</i>
PO48	<b>Optimal Operation of Thermally Coupled Kaibel Distillation Columns</b> <i>M. Ghadrhan, I. Halvorsen, S. Skogestad, Norway</i>	PO52	<b>Mass Transfer Equipment Design Considerations for Cryogenic Absorbers, Demethanizers and Deethanizers</b> <i>G. Shivelier, D. Egger, T. Oneal, USA</i>
PO49	<b>Development of a System for the Design of Control Structures for Dividing Wall Columns</b> <i>C. Buck, G. Fieg, V. Green, Germany</i>	PO53	<b>Measurement and Correlation of Clear Liquid Height on Small Hole Distillation Sieve Tray</b> <i>L.T. Fan, X.G. Yuan, A.W. Zeng, K.T. Yu, M. Kalbassi, K.E. Porter, China</i>
		PO54	<b>On the Development of an Energy Efficient Packing for Vacuum Distillation</b> <i>A. Shilkin, K. Heinen, C. Großmann, A. Lautenschleger, A. Janzen, E.Y. Kenig, Germany</i>
		PO55	<b>Establishing a Facility for the Hydrodynamic Characterization of Distillation Column Internals</b> <i>E.C. Uys, S.M. Lamprecht, C.E. Schwarz, J.H. Koetze, A.J. Burger, I. Nieuwoudt, A.B. Erasmus, South Africa</i>
		PO56	<b>Commercial Scale Test Validation of Modern High Performance Random and Structured Packings for CO<sub>2</sub> Capture Ranking</b> <i>M. Schultes, S. Chambers, B. Fleming, Germany</i>
		PO57	<b>Experimental Investigations on Biodiesel as Alternative Absorbent for the Recovery of Aromatic Hydrocarbons under Industrial Conditions</b> <i>M.Th. Müller, H. Thielert, D. Richter, J.-U. Repke, G. Wozny, Germany</i>

# Technologies for significant energy savings



To achieve a sustainable energy system, ECN conducts worldwide R&D in the fields of renewable energy, energy efficiency and clean use of fossil fuels.

ECN Efficiency & Infrastructure (E&I) develops technology to reduce energy demand and optimize energy efficiency aimed at achieving:

- minimal use of energy and raw materials in industrial processes and production chains;
- electricity grids that can accommodate a large share of intermittent and decentralized sources as an enabler for a sustainable energy system;
- a sustainable built environment.

ECN E&I has a proven track record in co-development and technology transfer to the industry. Our combination of excellent skills, long-term experience and facilities makes ECN the perfect R&D partner for you.



**Energy research Centre of the Netherlands**

[ei@ecn.nl](mailto:ei@ecn.nl)

[www.ecn.nl](http://www.ecn.nl)

- 09.00 Plenary Lecture: **Heat pumps in distillation**  
*Dolf Bruinsma, Energy Research Centre of the Netherlands (ECN), The Netherlands*  
 Session Chair: Andrzej Górak, TU-Dortmund, Germany

### Parallel Sessions

- |  |  |
|--|--|
| Theme: <b>Integrated, Hybrid and Novel Processes</b><br>Session Chair: Rakesh Agrawal ,<br>Purdue University, USA  | Theme: <b>Equipment Design and Operation</b><br>Session Chair: Elisabetta Brunazzi,<br>University of Pisa, Italy   |
| 09.50 <b>Energy Efficient Hybrid Processes for Ethanol Dehydration – A Comparison of Benchmark and Membrane Assisted Configurations</b><br><i>T. Roth, P. Kreis, A. Górak, Germany</i> | 09.50 <b>Structured Packing Efficiency – Vital Information for Chemical Industry</b><br><i>M. Ottenbacher, Z. Olujic, M. Jödecke, C. Großmann, Germany</i> |
| 10.15 <b>Systematic Synthesis of Dividing Wall Columns for Multicomponent Distillations</b><br><i>B.-G. Rong, Denmark</i>  | 10.15 <b>INTALOX® ULTRA™ Random Packing – Pushing the envelope</b><br><i>J.Nieuwoudt, USA</i>  |
| 10.40 <b>Innovative Biodiesel Production by Heat-Integrated Reactive Absorption</b><br><i>A.A. Kiss, The Netherlands</i>   | 10.40 <b>Characterization and Qualification of the Quality of Gas Flow Distributions</b><br><i>C. Stemich, L. Spiegel, Switzerland</i>                     |
| 11.05 Coffee Break   |  |

### Parallel Sessions

- |   |  |
|---|--|
| Theme: <b>Integrated, Hybrid and Novel Processes</b><br>Session Chair: Alexander Toikka, St.<br>Petersburg State University, Russia   | Theme: <b>Equipment Design and Operation</b><br>Session Chair: Henry Kister, Fluor, USA  |
| 11.30 <b>Development and Modeling of Micro Distillation Column</b><br><i>A. Sundberg, P. Uusi-Kyyny, K. Jakobsson, V. Alopaeus, Finland</i>   | 11.30 <b>Experimental Investigation on the Effect of Packing Material Textures on the Liquid-Side Mass Transfer</b><br><i>M. Kohrt, I. Ausner, J.-U. Repke, Germany</i>                                      |
| 11.55 <b>The D+R Tray: Novel Laboratory Equipment for Studying Heterogeneously Catalyzed Reactive Distillation – Design and Simulation Based Validation</b><br><i>E. von Harbou, M. Schmitt, S. Parada, C. Grossmann, H. Hasse, Germany</i> | 11.55 <b>Measurement of Liquid Hold-Up in Catalytic Structured Packings: Comparison of Different Experimental Techniques</b><br><i>A. Viva, S. Aferka, D. Toye, P. Marchot, M. Crine, E. Brunazzi, Italy</i> |
| 12.20 <b>CO<sub>2</sub> Capture for the Oxidative Coupling of Methane Process – A Case Study on Mini Plant Scale</b><br><i>S. Stünkel, M Brehmer, T. Brinkmann, J.-U. Repke, R. Schomäcker, G. Wozny, Germany</i>                           | 12.20 <b>Maximizing the Performance of Corrugated Sheet Structured Packings</b><br><i>Z. Olujic, T. Rietfort, H. Jansen, B. Kaibel, E. Zich, G. Ruffert, T. Zielke, The Netherlands</i>                      |



## *sasol technology* *technology for tomorrow*



With more than five decades of experience in petrochemical processing, Sasol is at the cutting edge of research & development and uses an array of unique technologies that have taken the beneficiation of hydrocarbons to unprecedented levels. Our prized workforce includes some of the most skilled scientists and engineers in the world.

Sasol Technology (Pty) Ltd - a subsidiary company and strategic business partner to other business units within the Sasol Group - manages Sasol's research & development, technology management & innovation, engineering services and project management portfolios.

We play a vital role in enabling Sasol's growth and sustainability as we direct, acquire, commercialise, install and optimise technology for the group, adding value through leadership in technology innovation and commercialisation, and through the delivery of cleaner technologies. We also help Sasol's fuel and chemical businesses to maintain growth and competitive advantage through optimised technology solutions and services.

**For more information please visit our website at: [www.sasol.com](http://www.sasol.com)**

- 12.45 – 13.30 Lunch Break
- 13.30 Plenary Lecture: **Conceptual design of energy-efficient hybrid separation processes**  
*Wolfgang Marquardt, RWTH-Aachen, Germany*
- 14.15 Plenary Lecture: **Research on Mass Transfer Columns “Old Hat or Still Relevant”**  
*M. Schultes, Rashig GmbH, Germany*  
 Session Chairs: Eva Sorensen, University College London, UK & Zarko Olujic, Delft University of Technology, The Netherlands

## Parallel Sessions

- |   |   |
|---|---|
| <p>Theme: <b>Basic Data</b><br/>         Session Chair: Maria Regina Wolf Maciel, UNICAMP, Brazil</p> <p>14.50 <b>Effect of Nitric and Sulfuric Acids on NO<sub>x</sub> and SO<sub>x</sub> Absorption into Oxidic Acidic Solutions</b><br/> <i>J. Liémans, D. Thomas, Belgium</i></p> <p>15.15 <b>Evaporation in Reacting Systems with Liquid Phase Splitting</b><br/> <i>A. Toikka, Russian Federation</i></p> <p>15.40 <b>Extractive Distillation of Ethylbenzene and Styrene using Sulfolane as Solvent: Low Pressure Isobaric VLE data</b><br/> <i>M.T.G. Jongmans, A. Luijks, J. Maassen, B. Schuur, A.B. de Haan, The Netherlands</i></p> <p>16.05 <b>A Small Static Total Pressure Vapour-Liquid Equilibrium Cell: a Case Study with Methanol + Methyl Formate</b><br/> <i>P. Uusi-Kyyny, A Sundberg, V. Alopaeus, Finland</i></p> | <p>Theme: <b>Control and Operation</b><br/>         Session Chair: Sigurd Skogestad, Norwegian University of Science and Technology, Norway</p> <p>14.50 <b>Practical Control of Dividing Wall Columns</b><br/> <i>J. Strandberg, S. Skogestad, I. Halvorsen, Norway</i></p> <p>15.15 <b>Distillation Pressure Control Troubleshooting – The Hidden Pitfalls of Overdesign</b><br/> <i>J.J. van Merwe, South Africa</i></p> <p>15.40 <b>Study of Control Properties of Intensified Thermally Coupled Distillation Sequences</b><br/> <i>J.G. Segovia-Hernández, R. Murrieta-Dueñas, R. Gutiérrez-Guerra, S. Hernández, H. Hernández, Mexico</i></p> <p>16.05 <b>Improved Control Strategies for Dividing-Wall Columns</b><br/> <i>A.A. Kiss, R.C. van Diggelen, The Netherlands</i></p> |
|---|---|
- 17.30 Departure for celebration event
- 18.00 – 24.00 **50 Years Distillation Absorption Conferences Celebration Event** (optional)
- 00.30 Arrival back in Eindhoven



Who gives electric cars  
such powerful acceleration?

We do.

Tomorrow's cars will run on electricity. Evonik delivers the essentials to make it happen – components that make lithium-ion batteries safer and more powerful with longer life. This winning technology will give our customers in the automotive industry that all-important innovative edge. We are the creative industrial group from Germany active in the fields of Chemicals, Energy and Real Estate.

**Evonik. Power to create.**



- 09.00 Plenary Lecture: **Carbon capture and storage experiences from the Sleipner field**  
*Even Solbraa, Statoil, Norway*  
 Session Chair: Richard Darton, EFCE President, University of Oxford, UK

### Parallel Sessions

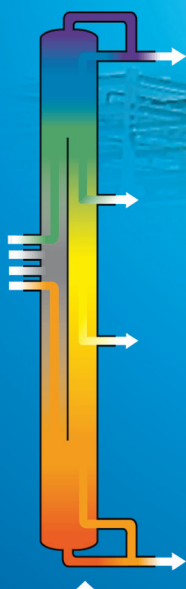
- |  |   |
|--|---|
| <p>09.50 <b>Hyperbranched Polymers in Absorption: Experimental CO<sub>2</sub> Solubilities</b><br/> <i>W. Martini, H. Arellano-Garcia, G. Wozny, Germany</i></p> <p>10.15 <b>Absorption of Carbon Dioxide into Piperazine Activated Aqueous n-Methyldiethanolamine</b><br/> <i>A. Samanta, S.S. Bandyopadhyay, India</i></p> <p>10.40 <b>Benchmarking Solvents for Carbon Capture</b><br/> <i>R.H. Weiland, N.A. Hatcher, J.L. Nava, USA</i></p> | <p>09.50 <b>Design-Troubleshooting of an Absorption Column</b><br/> <i>R. Stockfleth, Germany</i></p> <p>10.15 <b>Diagnostics of High Pressure Depropanizer</b><br/> <i>L. Pless, C. McKeown, S. Xu, USA</i></p> <p>10.40 <b>Vacuum Tower Wash Section: Myth and Reality</b><br/> <i>M. Roza, M. Pilling, Switzerland</i></p> |
| <p>11.05 Coffee Break</p>  |   |

### Parallel Sessions

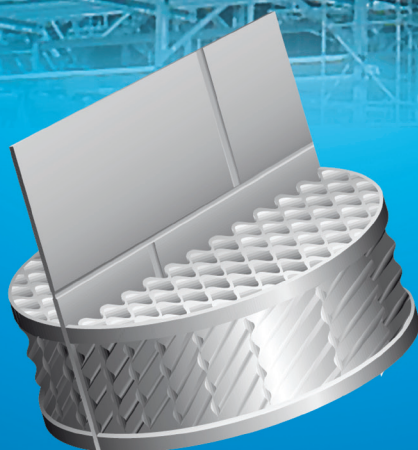
- |   |   |
|---|---|
| <p>11.30 <b>Methodology for Design and Analysis of Reactive Distillation Involving Multi-Element Systems</b><br/> <i>A. Jantharasuk, R. Gani, S. Assabumrungrat, A. Górák, Thailand</i></p> <p>11.55 <b>A Novel Process Concept for the Production of Ethyl Lactate</b><br/> <i>H. Arellano-Garcia, R. Kraus, G. Wozny, Germany</i></p> <p>12.20 <b>Development of a Model for the Synthesis of Unsaturated Polyester by Reactive Distillation</b><br/> <i>M. Shah, E. Zondervan, A.B. de Haan, The Netherlands</i></p> | <p>11.30 <b>Tray Stability at Low Vapor Load</b><br/> <i>D.R. Summers, L. Spiegel, K. Kolesnikov, Switzerland</i></p> <p>11.55 <b>Understanding Maldistribution in 3-Pass Trays</b><br/> <i>H. Kister, M. Olson, A. Viejo, USA</i></p> <p>12.20 <b>Designing Trays for Selective Treating</b><br/> <i>R.H. Weiland, N.A.Hatcher, J.L. Nava, USA</i></p> |
| <p>12.45 Closing Ceremony<br/>             DA2010 best student presentation and poster awards<br/> <i>Jeffrey Felix, Sulzer Chemtech Ltd.</i></p>   |   |
| <p>13.15 – 14.00 Light lunch and departure of participants</p>  |   |

## Dividing wall columns in the process industry

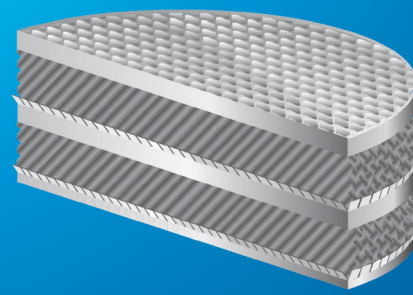
Applying dividing wall columns in rectification processes allows the splitting of multi-component mixtures in 3 or 4 individual product streams in one main column whereas in classic columns a set of 2 or 3 columns was needed to perform such a separation task. Allowing only one dividing wall column enables the chance to use substantial savings in apparatuses investments as well as energy savings – not only for new build columns. Also revamps of existing columns allow savings up to 30%.



Process technology



Non-welded dividing wall



Patented packing solutions

### Technology

Since more than 25 years and over 100 dividing wall columns build, MONTZ offers its wide range of knowledge regarding process and column design

worldwide. Flexibility, efficiency, fast delivery times and the high quality standards are the key values of our MONTZ distillation equipment.

### Julius Montz GmbH

PO box 530, D-40723 Hilden  
Phone: +49 21 03 / 8 94 0  
Fax: +49 21 03 / 8 94 77  
<http://www.montz.de>  
eMail: [hilden@montz.de](mailto:hilden@montz.de)





# Distillation Absorption 2010

12-15 September 2010  
Eindhoven University of Technology  
Eindhoven, The Netherlands  
[www.da2010.nl](http://www.da2010.nl)

## Abstracts

# Are you a good catch?

*"At SABIC, our people are our greatest assets."*  
Mr. Mohamed Al-Mady  
Vice-Chairman and CEO, SABIC

**SABIC is a world leader  
in petrochemicals  
and engineering plastics**

We are a large, diversified organization with 33,000 employees, of which 6,000 are in Europe, and global operations in over 100 countries.

We see it as our task to help you develop a career with us that challenges you in ways that really make you come alive.

Visit us at:  
[www.sabic.com](http://www.sabic.com)



## CELEBRATING 50 YEARS OF DISTILLATION AND ABSORPTION CONFERENCES

Richard Darton

*“Equipment most generally used for Gas Absorption: Tower packed with suitable solid. Types of Tower Packing. A wide variety of types of packing have been suggested at one time or another. These may be classified as follows: 1. Broken Rock...”* (Elements of Chemical Engineering by Badger, Walter L. and McCabe, Warren L. McGraw-Hill 1931)

## SHELL'S RESPONSE TO CLIMATE CHANGE AND THE CHALLENGES IN INNOVATION

Frigyes Lestak, Annet Stones and Jose Bravo

Energy security and climate change are some of the fundamental challenges that industry and society face today and in the future. At Shell, we address the CO<sub>2</sub> challenge through four avenues :

- i. natural gas, a low CO<sub>2</sub> intensity fossil fuel that can reduce emission by 50% when it replaces coal in a power station,
- ii. biofuels, where we are the world's largest supplier of fuels containing renewable components and are developing capabilities to produce sustainable biofuels
- iii. CCS : we will advance technologies in CO<sub>2</sub> capture and transportation, and contribute our capabilities to characterize reservoirs and inject CO<sub>2</sub> underground and
- iv. Efficiency; we will continue improving the energy efficiency of our operations and reducing flaring of natural gas.

Developing new energy sources requires significant effort and typically takes 30 years. The energy industries need to work with governments to create fit for purpose incentives and with technologists to bring about new innovations faster.

## NEW SOLVENT SYSTEMS FOR DISTILLATION AND ABSORPTION INTENSIFICATION

Matthias Seiler

Solvents with an improved price/performance ratio allow for processes with less operating and/or capital expenditure. Therefore, from an industrial perspective, it is worth reviewing the R&D progress in designing new competitive solvents on a regular basis. This paper aims at discussing the potential of new solvent systems applicable as absorbents or entrainers for boosting the performance of absorption and distillation processes. In this context, special focus will be dedicated to solvents like ionic liquids, amines and hyperbranched polymers. In particular, it will be demonstrated how these solvents can contribute to improve the performance of absorption processes such as absorption chillers and CO<sub>2</sub> capture processes as well as distillation processes like the separation of azeotropic mixtures by extractive distillation.

To illustrate the potential value of new solvent systems for the distillation and absorption community, the use of ionic liquids for absorption chillers is worth mentioning here. These sorption systems transform latent heat of the phase change liquid-vapor between different temperature levels by means of two working fluids, the refrigerant and the absorbent (working pair). The systems find use in different areas of application such as chiller applications (gas cooling, solar cooling, waste heat cooling), refrigeration, heat pumping and industrial heat recovery. One of the most prominent areas in which these absorption systems are applied is providing chilled water for air-conditioning by H<sub>2</sub>O/LiBr absorption chillers. In this context, the development has led from single-effect to double-effect systems and from steam-fired to direct-fired generators. The main freedom in designing and improving these kinds of absorption processes lies in the choice of the working pair and in the principle of multistaging.

Thus, a crucial fraction of fixed and/or variable costs for absorption chillers are defined by absorbent and refrigerant properties. Although many innovative working pairs have been suggested over the last decades, only two meet the prevailing industrial requirements: (a)  $\text{H}_2\text{O}/\text{LiBr}$  for water chillers and (b)  $\text{NH}_3/\text{H}_2\text{O}$  for refrigeration. However, these state-of-the-art working pairs show a number of drawbacks, including corrosiveness, a restricted temperature lift due to crystallization ( $\text{H}_2\text{O}/\text{LiBr}$ ), toxicity, high working pressure and/or the need for rectification ( $\text{NH}_3/\text{H}_2\text{O}$ ). Especially for multi-effect cycles with their potential for primary energy savings, selected ionic liquid-based absorbents combining a high capacity with adequate solution viscosities, thermal and chemical stability and a moderate corrosiveness at high process temperatures can substantially contribute to improve the performance of absorption chillers. This example indicates the potential of new solvents and underlines why this contribution will be dedicated to new solvent systems for distillation and absorption intensification. Apart from the use of suitable ionic liquids in absorption chillers, new solvent systems for carbon dioxide capture and extractive distillation will be presented and discussed from an industry perspective.

### HEAT PUMPS IN DISTILLATION

Dolf Bruinsma and Simon Spoelstra

Vapor recompression has become the standard heat pump technology in distillation and substantial energy savings in the order of 50% have been achieved. Economic applications of VRC are limited to column temperature differences of about  $30^\circ\text{C}$ , which is only one fifth of the across the pinch columns in operation. 2<sup>nd</sup> generation heat pump systems based on further heat integration and novel heat pump equipment do not only increase the potential energy savings but also extend the application range to columns with a larger temperature difference.

### SYSTEMATIC OPTIMIZATION-BASED SYNTHESIS OF HYBRID SEPARATION PROCESSES

Wolfgang Marquardt, Korbinian Kraemer, Andreas Harwardt

Hybrid separation processes can offer significant cost-savings over simple distillation processes for close-boiling mixtures. In addition, the separation boundaries of azeotropic mixtures can be overcome. The application of hybrid processes in industry, however, is hindered by the lack of robust and efficient process synthesis tools and methods for these complex and highly integrated processes. In this work, we review an optimization-based framework composed of shortcut and rigorous design steps for the robust and efficient synthesis of separation processes. This synthesis framework is illustrated by an industrial case study for the optimal design of a hybrid process separating a ternary mixture of close-boiling isomers. A multitude of hybrid processes composed of distillation and melt crystallization units are evaluated with powerful shortcut models. A selection of promising process variants is subsequently rigorously optimized by an economic objective function and discrete-continuous optimization techniques. It is shown that the design of the cost-optimal hybrid process within the systematic synthesis framework can be accomplished with paramount robustness and efficiency.

## RESEARCH ON MASS TRANSFER COLUMNS “OLD HAT OR STILL RELEVANT?”

Michael Schultes

Research activities in Universities in the field of mass transfer columns have heavily decreased in the past years. This contribution tries to discuss the question of whether the current knowledge in the field of mass transfer technology for trays, packings and column internals is sufficient to design energy and cost-efficient systems. In the article, various points of view are described which have not been clarified from an industrial point of view and which should play an important role in the field of research in the future. Alongside the thermodynamics of industry relevant systems, this also includes the improved description of fluid dynamics and the mass transfer efficiency in trayed and packed columns. Research should not only deal with idealistic test mixtures, with the help of standardised test equipments and standardised test systems. The industrial parameters such as foams, solids, and chemical and catalytic mass transfer are also of great interest.

## CARBON CAPTURE AND STORAGE EXPERIENCES FROM THE SLEIPNER FIELD

Even Solbraa

The Sleipner West Field, which came on stream in 1996, is the largest gas/condensate field in the Sleipner area. Having a higher carbon dioxide (CO<sub>2</sub>) content (9 mole%) than the gas export quality specifications (2.5 mole%), it was necessary to handle the excess without harming the natural environment. Capture and storage of CO<sub>2</sub> was selected and has got high attention as an option for limiting CO<sub>2</sub> emissions from the use of fossil fuels. CO<sub>2</sub> capture is premised on the safe long-term storage of CO<sub>2</sub> in geological formations. An amine plant was installed at the Sleipner T platform to extract the CO<sub>2</sub> from the reservoir gas, which is injected and stored 800-1000m below sea level and 2.5 km east of the Sleipner A platform in the Utsira Formation - a water-filled aquifer. Until now, about twelve million tonnes of CO<sub>2</sub> have been injected. Selected experiences gained since startup of the CO<sub>2</sub> capture and injection process is presented in this paper. The importance of fundamental knowledge related to thermodynamics and kinetics of chemical absorption at high pressure is highlighted.

## A DESIGN SIMPLIFICATION OF THE IDEAL HEAT-INTEGRATED DISTILLATION COLUMN

Kejin Huang, Haisheng Chen, and Shaofeng Wang

A simplified ideal heat-integrated distillation column, termed the SIHIDiC, is proposed and studied. Only three internal heat exchangers are used to approximate internal heat integration, and their locations and sizes are key decision variables for process synthesis and design and should be considered to enhance thermodynamic efficiency in process development. A stepwise procedure is derived for process synthesis and design and the SIHIDiC is evaluated through intensive comparison with conventional distillation columns and the ideal HIDiC in terms of the separation of an ethylene/ethane binary mixture. The results obtained indicate that the SIHIDiC could be an excellent simplified design to approximate the ideal HIDiC with reduced capital investment and somewhat similar operating cost.

## IDENTIFYING OPTIMAL MIXTURE PROPERTIES FOR HIDiC APPLICATION

Andreas Harwardt, Korbinian Kraemer and Wolfgang Marquardt

Internally heat-integrated distillation columns (HIDiC) are a new design option to provide a sustainable separation system. Although significant energy savings can be achieved using this setup, a considerable increase in investment cost penalizes the application. One major cost driver is the compressor cost, which depends on the relative volatility of the mixture to be separated. While mixtures with large relative volatility are easy to separate in distillation, they require a large pressure increase in the compressor of the HIDiC design, which raises the investment and operating costs of the design. Mixtures with low relative volatility are generally difficult to separate in distillation but favour the application of the HIDiC concept. Although it is clear that close boiling components are favourable from an energetic point of view<sup>10</sup>, the influence of the equipment cost can not be neglected. In this contribution, HIDiC column designs for different mixtures are optimized via rigorous MINLP optimization to identify a relative volatility region which provides optimal operating conditions for maximum cost reduction. The mixtures with a low relative volatility favour a highly integrated design, while for a high relative volatility the conventional design is more cost efficient. The optimal design identified for mixtures with low relative volatility is conceptually very similar to a conventional column with heat pump.

## MULTICOMPONENT DISTILLATION CONFIGURATIONS WITH LARGE ENERGY SAVINGS

Vishesh H. Shah and Rakesh Agrawal

In industry, many separation processes involve the separation of multicomponent mixtures using distillation. There are many distillation configurations that can carry out the same overall separation process. These configurations use an equal number of distillation columns, but they differ significantly in energy consumption. Therefore a major challenge for a practitioner is the identification of energy-optimal configurations for a given application. We describe an easy-to-use matrix-based framework to identify all feasible candidate configurations for the separation of any non-azeotropic multicomponent mixture. We also describe an optimization framework to rank-list all feasible configurations with respect to energy consumption. We have demonstrated the efficacy of these frameworks by identifying more than 70 new configurations that can lower the energy consumption for petroleum crude distillation by 5 – 48%. We also present a framework to analyze operability of distillation sequences.

## MULTI OBJECTIVE OPTIMISATION FOR AN ECONOMICAL DIVIDING WALL COLUMN DESIGN

Christoph Hiller, Sandra Storm, Matthias Leipold and Georg Fieg

The dividing wall column is experiencing a growing interest in industry. The concern about difficult controllability vanishes further and this leads to growing demand of approved guidelines for the design which is indeed time consuming if no expert knowledge is available. In this contribution the design task of a dividing wall column is treated as multi objective optimisation. Backbone of this optimised design method is a mathematical process model verified by an extensive experimental investigation. The optimisation itself allows to identify the best trade-off designs effectively regarding investment and operating costs as well as other constraints without any limitations for a fact based investment decision.

## DESIGNING FOUR-PRODUCT DIVIDING WALL COLUMNS FOR SEPARATION OF A MULTICOMPONENT AROMATICS MIXTURE

I. Halvorsen, I. Dejanović, Lj. Matijašević, Ž. Olujić, S. Skogestad, H. Jansen and B. Kaibel

Preliminary evaluations using a simple but reliable short-cut method indicated that a 15 component aromatic's mixture can be separated very efficiently into four fractions according to given product specifications employing either a single or a multiple partition wall dividing wall column (DWC). The obtained results have been used to initiate rigorous simulations, to determine the number of stages required in different sections, as well as to obtain internal flows of vapour and liquid necessary for dimensioning and adequate (actual delivery prices) cost estimation. Comparison of total annualized costs indicates that more energy efficient complex configuration with three partition walls is a viable option in present case.

In this paper the so called V-min diagram method is used to evaluate potential for energy saving and to indicate most beneficial internal configuration for a single dividing column (DWC) considered as an alternative for conventional three columns configuration used in an aromatics processing plant for separation of a multicomponent feed into four specified product streams. A DWC employing multiple partition walls to separate central part of the column into three sections appeared to be a much more attractive option than its, more practical single partition wall counterpart.

## ENERGY EFFICIENT SYNTHESIS AND DESIGN FOR CARBON CAPTURE

Angelo Lucia, Anirban Roy and Mikhail Sorin

Mononethanolamine (MEA)-based absorption-stripping for CO<sub>2</sub> capture is studied. Energy demands in this process are dominated by the stripping column. The shortest stripping line distance approach is used to determine minimum energy requirements for the MEA stripping column under various lean loadings. Simultaneous reaction and vapor-liquid equilibrium is assumed and modeled by the direct incorporation of experimental data. Results clearly show that the shortest stripping line distance approach easily determines minimum energy requirements and practical designs for the absorption-stripping process.

## PILOT PLANT EXPERIMENTS WITH MEA AND NEW SOLVENTS FOR POST COMBUSTION CO<sub>2</sub> CAPTURE BY REACTIVE ABSORPTION

Hari Prasad Mangalapally, Hans Hasse

Carbon dioxide is a greenhouse gas with a major impact on global climate change. One of the options for reducing CO<sub>2</sub> emissions is post combustion CO<sub>2</sub> capture from power plant flue gases. The main challenge for this process is the reduction of energy requirement for solvent regeneration. In order to reduce the costs of the absorption/desorption process, new tailored solvents for that process are needed. LTD operates a gas-fired pilot plant (column diameters 0.125 m, absorber packing height 4.25 m, flue gas flow 30-100 kg/h, CO<sub>2</sub> partial pressure 35-110 mbar) in which such new solvents were studied in the frame of the EU project CESAR. To obtain a baseline for testing the new solvents, first systematic studies were carried out with MEA in that plant with two different structured packings: Sulzer Mellapak 250.Y and BX 500. The most important process parameters CO<sub>2</sub> removal rate  $\Psi_{\text{CO}_2}$ , fluid dynamic load and solvent flow rate were systematically varied. Besides MEA, two new solvents were studied in the pilot plant. It is shown that a direct comparison of results for different solvents obtained in such pilot plant experiments is not trivial. The comparison of only a few operating points for the new solvents with seemingly corresponding results for MEA can lead to wrong conclusions, since for each solvent an optimisation of the operating conditions is necessary. Only systematic studies allow a meaningful comparison. The technique that was used in the present work for this purpose was measuring data sets at constant CO<sub>2</sub> removal rate of 90% (by adjustment of the regeneration energy in the desorber) and systematically varying the solvent flow rate. A minimal energy requirement for the given removal rate is found from these studies. Only the optima for different solvents should be compared. By this procedure, solvents were identified that show a clear improvement in regeneration energy requirement when compared to MEA.

## OPTIMIZED ABSORBER DESIGN FOR POST-COMBUSTION CCS

Markus Duss and Abhilash Menon

Challenges when capturing CO<sub>2</sub> in post combustion applications using absorption technology are the sheer size of the columns and column internals, the pressure drop requirements to save operating costs, and the overall cost of the packing and internals. This paper addresses these challenges and it can be concluded that structured packing offers the best solution. Based on this outcome, Sulzer has developed a new Mellapak structured packing to reduce CAPEX and OPEX for such applications.



## UPDATE ON AQUEOUS AMMONIA BASED POST COMBUSTION CAPTURE PILOT PLANT AT MUNMORAH

Hai Yu, Scott Morgan, Andrew Allport, Thong Do, Aaron Cottrell, James McGregor and Paul Feron

CSIRO and Delta Electricity have jointly constructed an A\$5 million research scale Post Combustion Capture (PCC) pilot plant at the Munmorah black coal fired power station. The results from the pilot plant trials will be used to assess the potential of using aqueous ammonia solution to capture CO<sub>2</sub> and other acid components such as SO<sub>x</sub> and NO<sub>x</sub> from coal fired power plants under Australian conditions. This paper reports and discusses the experimental results obtained from the pilot plant trials.

## USE OF MULTI-SCALE SIMULATIONS FOR LOWERING THE COST OF CARBON DIOXIDE CAPTURE

Ludovic Raynal, Patrice Font, Tânia Janeiro, Yacine Haroun and Pierre-Antoine Bouillon

Carbon Capture and Storage is one important option for CO<sub>2</sub> mitigation<sup>1</sup>. Post-combustion capture processes using amines are considered as one of the preferred options for CCS. However, the cost of avoided CO<sub>2</sub> is very large and must be reduced. In the present article, it is shown from a macro-scale technico-economic analysis, that Capex represents about one third of the total CO<sub>2</sub> cost. A sensitivity analysis, via Aspen calculations performed at column scale, enables to identify key parameters that control column design. It is shown that the most important mass-transfer parameters is the interfacial area, the gas and liquid mass transfer coefficients having almost no influence. From CFD simulations performed at a finer scale, some insights are given in order to optimize column design.

## HYPERBRANCHED POLYMERS IN ABSORPTION: EXPERIMENTAL CO<sub>2</sub> SOLUBILITIES

Walter Martini, Harvey Arellano-Garcia and Günther Wozny

Oxidative coupling of methane (OCM) is an approach for the direct catalytic conversion of methane to higher hydrocarbons, which is currently being investigated at the Berlin Institute of Technology within the cluster of excellence UniCat (Unifying Concepts of Catalysis). Hereby, the conversion to ethylene is the major goal of the process. In the downstreaming process subsequent to the OCM reaction, a purification step takes place, where carbon dioxide has to be removed from the raw gas. This is done by chemical absorption using an aqueous amine solution, which can have several disadvantages such as a high energy demand for regeneration or solvent losses<sup>1</sup>. However, it has been shown that hyperbranched polymers are promising candidates for gas absorbents with a high capacity for CO<sub>2</sub> and with large selectivities<sup>2</sup>. In this work, a commercially available hyperbranched polymer (Boltorn Perstorp) is investigated. The potential for its use as absorbent in the separation of CO<sub>2</sub> is evaluated by measuring solubilities. The results obtained are reported in terms of Henry constants within the temperature range of 283.15 to 303.15 K. In addition, the densities of the pure polymer or its solution with ethanol are measured in the same temperature range.

## ABSORPTION OF CARBON DIOXIDE INTO PIPERAZINE ACTIVATED AQUEOUS N-METHYLDIETHANOLAMINE

Arunkumar Samanta and [S. S. Bandyopadhyay](#)

This work presents a theoretical and experimental investigation on the absorption of CO<sub>2</sub> into piperazine (PZ) activated aqueous N-methyldiethanolamine (MDEA) solvent. A comprehensive numerical model which is based on Higbie's penetration theory has been developed to analyze the experimental data. The model involving coupled mass transfer–reaction kinetics–chemical equilibrium incorporates the important reversible reactions in the liquid phase. The model is validated with the experimental results of steady state absorption measurements of CO<sub>2</sub> in a 2.81×10<sup>-2</sup> m o.d. stainless steel wetted wall contractor. The rates of absorption of CO<sub>2</sub> into this solvent have been measured over the CO<sub>2</sub> partial pressure range of 2-14 kPa and temperature range of 298 – 313 K under atmospheric pressure. The absorption experiments are performed over the MDEA concentration range of 1.89 - 2.41 kmol.m<sup>-3</sup> along with PZ concentrations of 0.24, 0.60 and 0.95 kmol.m<sup>-3</sup>. Steady state absorption measurements of this work have shown that the CO<sub>2</sub> absorption rates into aqueous MDEA increase significantly with the addition of small amounts of PZ in the solvent. This establishes the potential of the PZ activated aqueous MDEA solvent for industrial gas treating. Good agreement between the model results and experimental results indicates that the combined mass transfer-reaction kinetics-equilibrium model can effectively represent CO<sub>2</sub> mass transfer rates in PZ activated aqueous MDEA for wide range of operating conditions.

## BENCHMARKING SOLVENTS FOR CARBON CAPTURE

[Ralph H. Weiland](#), Nathan A. Hatcher and Jaime L. Nava

Process simulation is used to evaluate the potential of 2-amino-2-methyl-1-propanol (AMP) and sodium glycinate (NaGly) as solvents for CO<sub>2</sub> capture. In terms of regeneration energy (the main energy consumer in capture plants), the performance of a rudimentary MEA-based plant is established first. Pilot plant data on CO<sub>2</sub> absorption into MEA and AMP are shown to be well-reproduced using the ProTreat mass and heat transfer rate process simulation tool. The model is then used to project that (1) AMP should enjoy at least a 15% reboiler energy advantage over MEA and (2) NaGly should carry better than a 40% advantage over MEA under the same conditions.

## ENERGY EFFICIENT HYBRID PROCESSES FOR ETHANOL DEHYDRATION: A COMPARISON OF BENCHMARK AND MEMBRANE ASSISTED CONFIGURATIONS

Tim Roth, Peter Kreis and Andrzej Górak

One of the most promising processes for ethanol dewatering are hybrid separations consisting from different combinations of distillation with adsorption and/or vapour permeation. This paper presents a detailed process analysis showing the influence of decisive parameters on important target variables. The advanced mathematical models have been used for determination of optimal process configuration while using evolutionary algorithms.

## SYSTEMATIC SYNTHESIS OF DIVIDING-WALL COLUMNS FOR MULTICOMPONENT DISTILLATIONS

Ben-Guang Rong

Dividing-wall columns(DWC) are intensified distillation systems for multicomponent separations. They have the potential to save both energy and capital costs significantly than conventional simple column configurations. The several DWC columns for ternary distillations have been figured out by some creative activities from different inventors. Recently they have gained the momentum to be widely implemented in industrial separation processes. As industrial separation problems very often involve four or more components, for such problems, due to complexity, it is impossible to find all the feasible DWC columns by inventive activities. On the other hand, industrial experience shows that the optimal system for a specific application can only be guaranteed by predefining all of the feasible options. In this work, a procedure for systematic synthesis of DWC columns for multicomponent distillation is presented. Starting from the conventional simple column configurations for the separation of a multicomponent mixture, a four-step procedure is formulated which systematically generates all the possible DWC columns. First, the subspace of the possible thermally coupled configurations corresponding to the simple column configurations is generated. Then, the subspace of the possible thermodynamically equivalent structures corresponding to the thermally coupled configurations is produced. Finally, the subspace of the DWC columns corresponding to the thermodynamically equivalent structures is achieved. The method is simple, easy-to-use and can systematically synthesize all the possible DWC columns. An example of quaternary distillation is used to illustrate the synthesis procedure which is applicable to a mixture with any number of components.

## INNOVATIVE BIODIESEL PRODUCTION BY HEAT-INTEGRATED REACTIVE ABSORPTION

Anton A. Kiss

This study proposes an innovative biodiesel technology based on heat-integrated reactive absorption. Rigorous simulations embedding experimental results were performed in AspenTech AspenONE engineering suite to design this novel process and evaluate the technical and economical feasibility. The main results are given for a plant producing 10 ktpy biodiesel from waste vegetable oil with high free fatty acids content, using solid acids as green catalysts. This innovative process eliminates all conventional catalyst related operations, and efficiently uses the raw materials and the reactor volume in an integrated setup that allows significant reduction of both capital and operating costs – with up to 85% energy savings.

## DEVELOPMENT AND MODELING OF MICRO DISTILLATION COLUMN

Aarne Sundberg, Petri Uusi-Kyyny, Kaj Jakobsson and Ville Alopaeus

The design, manufacture, testing and modeling of a novel flat micro-distillation column is presented. Porous metal foam was used as distillation packing. The unit was operated in a horizontal orientation both with total reflux and with continuous feed. The separation efficiency in terms of height to a theoretical plate of 16 mm was determined with a mixture of n-Hexane and Cyclohexane. Operation of the device was stable and results were reproducible. The unit was operated unmanned over extended periods of time. Results were analyzed with McCabe-Thiele –method.

## THE D+R TRAY: NOVEL LABORATORY EQUIPMENT FOR STUDYING HETEROGENEOUSLY CATALYZED REACTIVE DISTILLATION – DESIGN AND SIMULATION-BASED VALIDATION

Erik von Harbou, Markus Schmitt, Sandra Parada, Christoph Grossmann, Hans Hasse

In this paper, novel equipment for laboratory studies of heterogeneously catalyzed reactive distillation is described. The so called D+R tray equipment consists of a combination of conventional bubble cap trays with sections that are filled with catalyst and through which the liquid flows when it passes from one distillation tray down to the next. It is designed so that the catalyst can be easily changed, and its amount can be flexibly chosen. These are important advantages compared to catalytic packings. In the present study, D+R tray equipment built in glass in the 50 mm diameter scale was investigated. In order to proof the general functionality of the D+R tray, the fluid dynamic capacity and the tray efficiency of the distillation section as well as the residence time distribution (RTD) of the reactive section were systematically investigated in a series of preliminary tests. Afterwards, the D+R trays were tested in a comprehensive series of reactive distillation experiments. For these experiments, two test systems were chosen that had been studied thoroughly in previous work in different scales with catalytic packings<sup>1-2</sup>. The most important process parameters such as feed rate and amount of catalyst were systematically varied. High conversions of the reactants and high purities of the products were achieved. The reproducibility of the results is excellent. That proves the general performance and operability of the D+R tray equipment. Process simulations were carried out using a stage-based model. The process model is based on carefully validated models of the physico-chemical properties of the test systems from previous works. The tray efficiency was not adjusted but taken from the independent measurements so that the simulations are predictive. The comparison with the experimental data shows good agreement. With the same model, HCRD experiments carried out in previous work on the same test systems with catalytic packings are well described. This shows that experiments carried out with D+R tray equipment can be used for studying designs of HCRD processes with either catalytic packings or trays.

## CARBON DIOXIDE CAPTURE FOR THE OXIDATIVE COUPLING OF METHANE PROCESS – A CASE STUDY IN MINI-PLANT SCALE

S. Stünkel, M. Brehmer, T. Brinkmann, J.-U. Repke, R. Schomäcker and G. Wozny

The Oxidative Coupling of Methane (OCM) to ethylene is a promising alternative for the oil based industry. In this process, beside the valuable product ethylene, other by-products are produced. Hence the gas stream has to be refined further. The process is not applied in the industry yet, because of high separation costs. This article focuses particular on the CO<sub>2</sub> purification of the OCM product stream. Therefore a case study were done for a design task of the reaction product gas cleaning from 22 mol% CO<sub>2</sub> to 1 mol% on an operating pressure of 32 bar. A state of the art chemical absorption process using Monoethanolamine (MEA) was developed and optimized for the base case. Therefore Aspen Plus<sup>®</sup> with build-in rate based model for the mass transfer with an electrolyte NRTL – approach and chemical equilibrium reactions for the water-MEA-CO<sub>2</sub> system as well as kinetic reactions was applied. In order to improve the energetic performance, gas permeation with dense membranes was studied as alternative process. Therefore a membrane unit was developed in Aspen Custom Modeler<sup>®</sup> (ACM). The solution-diffusion model with the free-volume-theory for gas permeation including Joule-Thomson effect as well as concentration polarisation<sup>2</sup> was applied successfully. Furthermore a rubbery polyethylene oxide (PEO) and a glassy cellulose acetate (CA) composite membrane with

experimentally determined parameters were used in this model. The standard absorption process was developed with 97% CO<sub>2</sub> removal including solvent regeneration and heat integration. Whereas the thermal energy demand results to 2.8 MJ/kg<sub>CO<sub>2</sub></sub> at 53% solvent regeneration in the desorption column for 30 wt% MEA. It was observed, that substitution of the absorption process only by a membrane process causes high product losses, so that the process became uneconomical. Hence the design task can be fulfilled only by a hybrid process, a combination of a membrane unit with an absorption process. This reduces the energy demand down to 1.6 MJ/kg<sub>CO<sub>2</sub></sub> with moderate product loss of 9 %. This article describes the process, as well as the simulation study. Experimental investigations of the process are carried out and results will be given in the presentation.

### **METHODOLOGY FOR DESIGN AND ANALYSIS OF REACTIVE DISTILLATION INVOLVING MULTIELEMENT SYSTEMS**

Amnat Jantharasuk, Rafiqul Gani, Andrzej Górak and Suttichai Assabumrungrat

This work presents a new methodology for design and analysis of reactive distillation. The methodology employing the element-based approach coupled with a driving force diagram for two-element systems is extended to multielement systems commonly involved in most chemical processes. The multielement system is transformed to an equivalent binary (key) element system, and consequently graphical design is carried out to determine the number of stages, the feed stage, the minimum reflux, etc., corresponding to minimal energy consumption, based on a driving force diagram. Two case studies including methyl acetate (MeOAc) synthesis and methyl tertiary butyl ether (MTBE) synthesis are presented. It is shown that the designed column is able to satisfy desired targets with a minimum energy requirement. In addition, an improvement in design is obtained compared to the design without any considerations about nonkey components.

### **A NOVEL PROCESS CONCEPT FOR THE PRODUCTION OF ETHYL LACTATE**

Harvey Arellano-Garcia, Robert Kraus and Günter Wozny

A dynamic model of a reactive divided wall column is presented so as to analyse a novel process concept for the esterification of lactic acid with ethanol to ethyl lactate. The divided wall column is modelled by composing single packing columns to a Petlyuk-structure using different correlations for fluid dynamics and pressure drop. Besides, a variety of side reactions are considered such as the oligomerisation of lactic acid, and the esterification of their oligomers. Moreover, feasibility studies are carried out in order to show in detail the potential of the proposed process concept, in particular, the reactive dividing-wall column. For this purpose, the influence of different parameters like side draw flow rate and the liquid split are simulated to examine their impact on the ethyl lactate production.

### **DEVELOPMENT OF A MODEL FOR THE SYNTHESIS OF UNSATURATED POLYESTER BY REACTIVE DISTILLATION**

M. Shah, E. Zondervan, M.L. Oudshoorn, A.B de Haan

Traditionally polyester production is done in a batch reactor equipped with a separation column for batch distillation. A promising alternative for the intensification of this process is reactive distillation. In this paper, a reactive distillation model is developed for the synthesis of an unsaturated polyester process. The simulation results are compared with the industrial batch reactor output data of the product. It is found that the model predicts the polymer attribute, isomerisation and saturation composition of the polymer in the range of industrial unsaturated polyester production. Industrial unsaturated polyester production time is around 12 hours. However, the simulation study shows that the total production time of unsaturated polyester in a continuous reactive distillation system is between 1.5 hours to 2 hours for the same product quality as during batch production. The equilibrium conversion is also raised by 7% compared to the conventional process. The model demonstrated that reactive distillation has the potential to intensify the process by factor of 6 to 8 in comparison to the batch reactor.

## EFFECT OF NITRIC AND SULFURIC ACIDS ON NO<sub>x</sub> AND SO<sub>x</sub> ABSORPTION INTO OXIDO-ACIDIC SOLUTIONS

Isabelle Liémans and Diane Thomas

SO<sub>2</sub> and NO<sub>x</sub> efficiencies were studied at 293 K and 1 atm, in a cable contactor, up to partial pressures of 2000 ppm, in mixed aqueous solutions containing sulfuric and nitric acids, as products of the wet oxidative removal of SO<sub>x</sub> and NO<sub>x</sub>, and hydrogen peroxide, as oxidizing agent. The carrier gas was essentially carbon dioxide (90% vol). The CO<sub>2</sub> absorption in oxido-acidic conditions was found to be negligible. The SO<sub>2</sub> absorption rate was determined for various SO<sub>2</sub> partial pressures and different concentrations of H<sub>2</sub>SO<sub>4</sub> and HNO<sub>3</sub> (0-4M) and hydrogen peroxide (0.05-1M) in the scrubbing liquid. It was found that the SO<sub>2</sub> absorption rate increases sharply with the hydrogen peroxide concentration and decreases as the H<sub>2</sub>SO<sub>4</sub> concentration increases. This influence of sulfuric acid is preponderant and, in presence of both nitric and sulfuric acids, only a slight influence of HNO<sub>3</sub> is noticed, modifying the properties of the scrubbing liquid but likely involving a negligible effect on the kinetic of the reaction between SO<sub>2</sub> and H<sub>2</sub>O<sub>2</sub>. Similar experiments have been carried out with NO<sub>x</sub> as gas solutes, for different oxidation ratios, showing that an acid medium enhances the NO<sub>x</sub> absorption rates.

## EVAPORATION IN REACTING SYSTEMS WITH LIQUID PHASE SPLITTING

Alexander Toikka

Some theoretical and experimental results on the peculiarities of reacting systems with liquid phase splitting are considered. The evaporation in these systems is a complex process that combines three stages: liquid-vapor phase transition, liquid-liquid phase transition and chemical reaction. Both the simultaneous vapor-liquid equilibrium (VLE), liquid-liquid equilibrium (LLE) and chemical equilibrium (CE) and non-equilibrium cases are of important practical interest, e.g. for reactive distillation. The properties of two-phase liquid solutions with chemical interaction are the main elements that determine the behavior of the system in evaporation process. The main experimental example is a quaternary system with *n*-propyl acetate synthesis reaction.

## EXTRACTIVE DISTILLATION OF ETHYLBENZENE AND STYRENE USING SULFOLANE AS SOLVENT: LOW PRESSURE ISOBARIC VLE DATA

Mark T.G. Jongmans, Adriaan Luijks, Jenny Maassen, Boelo Schuur and André B. de Haan

The distillation of ethylbenzene (EB) from styrene (SM) is very energy intensive. By using extractive distillation instead, both capital and energy expenses are potentially reduced dramatically. Hereto we propose to use sulfolane (SF) as solvent. Currently there is no ternary vapor liquid equilibrium (VLE) data available of the system SM/EB/SF and the binary VLE data sets of EB/SM available in literature are found to be thermodynamically inconsistent. In this study thermodynamically consistent VLE data is obtained for the three binary systems and the ternary system in the pressure range of 50-200 mbar. Both the Wilson and NRTL model can adequately describe the experimental VLE data. The solvent SF increases the relative volatility significantly from 1.3-1.4 up to 2.3. Equilibrium process modeling suggests that an energy reduction of 50% compared to the traditional distillation process can be obtained with the extractive distillation process.

## A SMALL STATIC TOTAL PRESSURE VAPOUR-LIQUID EQUILIBRIUM CELL A CASE STUDY WITH METHANOL-METHYLFORMATE

Petri Uusi-Kyyny, Aarne Sundberg and Ville Alopaeus

A small static total pressure apparatus was developed. Vapour-Liquid Equilibrium was measured for the methanol+methylformate system in the temperature range from 303 K to 353 K. Additionally two isothermal measurements were made with a larger volume apparatus at 342 K and 359 K to validate the small VLE cell measurements. The developed VLE model could describe the literature data. Azeotropic behavior was detected.

## A MEMETIC ALGORITHM FOR THE DESIGN OPTIMIZATION OF REACTIVE DISTILLATION COLUMNS

Maren Urselmann, Sebastian Engell

This contribution deals with the optimization of the design of reactive distillation columns by using a memetic algorithm (MA) which is a combination of an evolution strategy (ES) and a mathematical programming (MP) solver. The standard approach to solve such problems is to formulate them as large MINLPs but then the computational effort needed for the solution process grows substantially if the number of discrete variables increases, e.g. if a restriction on the number of feeds is introduced. Another problem is that the nonlinear solvers only provide a single local optimum. The MA overcomes this problem by addressing the optimization of the discrete and the global search in the space of the continuous design variables, while continuous sub-problems are efficiently solved by an MP solver. A comparison of the results of this new approach with results of commercial MINLP techniques shows that the MA can efficiently handle the global design optimization problem at hand and that it is the only algorithm that found the global solution if the number of discrete variables increases.

## OPTIMAL DESIGN METHODOLOGY FOR DIVIDING WALL COLUMNS

Claudia Gutiérrez-Antonio, Abel Briones-Ramírez

The dividing wall column, DWC, is a thermally coupled sequence that can perform the separation of fluid mixtures with reduced energy consumption, but also decreasing the capital costs associated. Several authors have developed design procedures for this kind of sequence, using short methodologies or optimization strategies. The use of short procedures is easy and fast, but, in the most of the cases, the resulting design is not optimal. On the other hand, the use of optimization procedures allow obtaining optimal designs, but time and complexity required are elevated. In this work, we propose an optimal and short design methodology for DWC. First, we use a multiobjective genetic algorithm with constraints, coupled to Aspen Plus, to obtain Pareto fronts of DWC for different mixtures, feed compositions and recoveries. The analysis of the Pareto fronts brings useful information about the flows and composition of the interconnection flows, key variables in this methodology, which are incorporated in a short method that generates optimal designs with less computational resources.

## EXTENDED CHANNEL MODEL FOR PREDICTION OF HYDRAULICS AND MASS TRANSFER OF RANDOM PACKED COLUMNS FOR GAS-LIQUID SYSTEMS

Jerzy Maćkowiak

The following work presents a new, generally applicable model for description the mass transfer in the liquid phase for packed columns filled with random non-perforated and lattice-type packing with size between 12 and 90 mm for gas-liquid systems in operating range up to flooding point. The new equation was derived on the basis of the assumption that liquid flows down in packed bed, mainly in the form of droplets, and that mass transfer is transient and based on the channel model with a partly open structure. The experimentally derived values for the mass transfer area in different types of random packings  $a_e$  are sufficiently consistent with the calculation based on the new model. It is therefore possible to separate the product  $\beta_L \cdot a_e$  into liquid phase mass transfer coefficient  $\beta_L$  and effective interfacial area  $a_e$ .

## RATE-BASED MODELING OF TWO COMMERCIAL SCALE H<sub>2</sub>S STRIPPING COLUMNS

Ross Taylor, Peter Wilkinson and Harry Kooijman

This paper describes rate-based models<sup>1,2</sup> of two commercial scale H<sub>2</sub>S stripping columns in order to obtain improved prediction of column performance compared to equilibrium stage models that use component efficiencies. For one stripping column for which H<sub>2</sub>S bottom concentrations were available the rate-based column model results are in reasonable agreement with the plant data, whereas the equilibrium stage model predicts H<sub>2</sub>S bottoms concentrations orders of magnitude lower when a constant tray efficiency of 50% is used for all compounds. No plant data was available for the second column but the rate-based model gave results that were well in-line with operating experience. The rate based models simulated both of the columns more or less exactly as they were constructed. The columns were modelled with 20 trays, not with 10 equilibrium stages. The feeds were directed to the appropriate locations in the column; for the equilibrium stage model the H<sub>2</sub>S alone had to be diverted to a lower stage in order to match the plant data. Equilibrium stage models are unable to adequately model the columns under consideration because the efficiencies of different components vary in different ways depending on the component. For example, in one column the heavier components had efficiencies that varied from approximately 40% in the top to 60% in the bottom. For the light components the efficiencies varied from about 20% in the top to around 60% in the bottom. We submit that for columns such as the two H<sub>2</sub>S stripping columns described in this exercise the proper course of action is to use a rate-based model. There were no significant disadvantages concerning calculation speed, convergence, or availability of properties for these processes that contain 60+ components, especially as the predicted efficiencies matched the observed performance.

## A COMPUTATIONAL FLUID DYNAMICS AND AN EXPERIMENTAL APPROACH TO THE EFFECTS OF PUSH VALVES ON SIEVE TRAYS

Rahbar Rahimi, Ali Zarei, Taleb Zarei, Hamed Naziri Firoozsalari, Mortaza Zivdar

In this study to improve hydraulic performance of sieve tray, push valves have been utilized on the sieve tray deck. The hydraulic effects have been investigated using computational fluid dynamics simulation and experimentation. The computational fluid dynamics (CFD) model used 1.213 m diameter Solari and Bell [1] sieve tray. In the CFD model it is found that the ratio of the push valves' open area to the total hole area is approximately 14.31% which is considered as a design parameter. The experimentally investigated sieve tray had 7.039 % hole area and 32 push valves. The ratio of push valves' open area to the total hole area was 14.59%. The dry pressure drop, total pressure drop and weeping were measured. The experimental results of this modified sieve tray and the sieve tray without push valves were compared with each other. Results show that better hydrodynamic behavior of the modified push valve sieve tray than conventional sieve tray.

## DESIGN OF COMPLEX DISTILLATION COLUMNS SEPARATING TERNARY HETEROGENEOUS AZEOTROPIC MIXTURES

Paritta Prayoonpong and Megan Jobson

The boundary value method for design of distillation columns separating ternary heterogeneous azeotropic mixtures is extended to include complex configurations, i.e. columns with integrated decanters and with multiple heterogeneous stages; double-feed columns; columns with intermediate decanters. The methods can be used for establishing product feasibility in a column and evaluating a column design on a basis of cost. Multiple feasible designs can be generated for a given set of product specifications, according to the reflux ratio, number of heterogeneous stages and liquid phase ratio; these designs may be evaluated with respect to operating and equipment costs. Case studies illustrate the design method.



## A GENERALIZED METHODOLOGY FOR OPTIMAL CONFIGURATIONS OF HYBRID DISTILLATION-PERVAPORATION PROCESSES

Yellaiah Naidu and Ranjan K. Malik

The aim of this work is to illustrate the structural and parametric optimization of continuous hybrid distillation-pervaporation process with different configurations such as series, parallel, and series-parallel arrangement of pervaporation modules in the pervaporation network, and to propose a generalized methodology for difficult separations. A superstructure representation of hybrid process is considered and the process is modeled and optimized using an MINLP approach. The optimization strategy is to obtain the desired degree of either the retentate or the distillate purity without violating the composition constraints of products and heat exchange policy which minimizes the required membrane area by increasing the flux through the membrane. The structural and operating parameters such as number of trays required, feed tray location, reflux ratio, retentate recycle location, permeate recycle location, membrane feed location, number of pervaporation modules required, target composition (which is directly related to membrane area), and membrane selectivity are optimized for each configuration by minimizing the total annual cost (TAC) for the separation system. The optimization studies have been carried out with General Algebraic Modeling System software (GAMS/SBB/CONOPT) and the results of different configurations have been compared on the basis of TAC required for the separation. A total of three industrial case studies have been dealt with. The separation of isopropanol-water as an azeotropic mixture, propylene-propane as a close boiling mixture (system with a low relative volatility) and acetone-water as a tangent pinch mixture have been studied as representative examples.

## COLUMN PROFILES FOR MEMBRANE COLUMN SECTIONS

Mark Peters, Shehzaad Kauchali, Diane Hildebrandt, and David Glasser

A novel graphical method of analysing continuous membrane separation systems has been developed. The method is applicable to all counter- and co-current membrane modules – single-stage, cascades, and membrane columns. All configurations can be broken down into “column sections”, no matter how complex the arrangement. Each column section, which resembles a typical single-stage separator, is modelled using the difference point equation. The difference point equation tracks the change in the retentate composition down the length of the column section. For demonstration purposes, a simple constant relative permeability flux model is employed to determine the permeate composition as well as the continually changing retentate flow. All possible operating conditions of a column section are explored. Each condition is a result of the relationships between the flows and compositions at the top of a column section. Using the difference point equation, column profiles for each condition can be plotted. The behaviour of the profiles is discussed both mathematically and graphically. This innovative way of investigating membrane processes provides a unique way of synthesizing and designing them.

## THERMODYNAMIC INSIGHT ON EXTRACTIVE DISTILLATION WITH ENTRAINER FORMING NEW AZEOTROPES

Ivonne Rodriguez Donis, Vincent Gerbaud and Xavier Joulia

This paper deals with the feasibility analysis of batch extractive distillation taking into account the effect of the univolatility lines  $\alpha_{i,j} = 1$  and the shape of residue curves for ternary mixtures involving two binary azeotropes. A general feasibility criterion previously established for ternary mixtures only including one azeotrope is now extended to Serafimov's classification diagrams: 2.0-1, 2.0-2a, 2.0-2b and 2.0-2c. Application of the feasibility criterion hints at which component goes up or down using a rectifying or stripping column. Preliminary feasibility results are verified by computing the map of extractive liquid profiles using a simplified modelling. Examples including batch rectifier are also corroborated by rigorous simulation using ProSim Batch.

## SHORT-CUT METHODS FOR THE OPTIMAL DESIGN OF SIMPLE AND COMPLEX DISTILLATION COLUMNS

Chafika Adiche, Alfons Vogelpohl

New short-cut methods providing optimal design parameters for distillation columns with simple and complex configurations including two-feed and one-feed-one-side-stream columns are presented. The methods assume constant relative volatilities and constant molar flow rates within each distillation section. The constituting design equations are based on the Underwood equations for the calculation of minimum reflux ratio, the analytical formulations of the distillation line, the Eigenfunction and the number of theoretical stages for each mass transfer section<sup>1</sup>. Additional design equations have been established based on the analysis of the geometrical properties for a given separation with respect to the type of split, the configuration of the column (simple or complex) and the mass balance around each feed section for an arbitrary feed quality. Optimization algorithms based on the minimization of the total number of theoretical stages of the column under the constraint of the mass balance at each feed section were elaborated providing the reflux ratio, the minimum number of theoretical stages of the column, the optimal feed location and the product compositions for a given separation. In comparison to the boundary value method<sup>2</sup> the new short-cut methods require a minimum number of specifications, they are completely numerical and provide a lower total number of theoretical stages particularly for complex configurations. The new short-cut methods have been extended to the design of columns separating azeotropic mixtures by approximating the latter by appropriate pseudo-ideal mixtures<sup>3,4</sup>. Several separation examples including ideal and azeotropic mixtures, different types of splits as well as columns with simple and complex configurations were tested and show a very good agreement with the simulation results obtained with Radfrac (Aspenplus).

## PRACTICAL CONTROL OF DIVIDING-WALL COLUMNS

Jens Strandberg, Sigurd Skogestad and Ivar J. Halvorsen

This paper studies the practical implementation of stabilizing control for a Kaibel dividing-wall column. Control configurations with varying number of temperature loops are tested and compared with special attention to the use of the liquid split ratio as a manipulated variable.

## DISTILLATION PRESSURE CONTROL TROUBLESHOOTING – THE HIDDEN PITTFALLS OF OVERDESIGN

Jacques van der Merwe

The operating pressure of a distillation column is one of the main handles with which to control and optimise separation as it affects most other parameters as well as the overall stability of the column. It is therefore one of the most important parameters to control. Controlling a distillation column, designed to be operated under a vacuum, at the intended operating pressure can prove to be much more difficult than for positive pressure columns especially during the initial start-up of the column. Determining the cause of pressure instability can be a daunting task as the column will most likely be under turndown conditions, the inventory might differ from the intended composition, the control loops will be in manual or not tuned yet or the cause might even be from an equipment design perspective. During the initial start-up of a vacuum operated distillation column several problems were encountered that prohibited the column from being operated at its intended pressure. This caused severe instabilities in the column and also affected the downstream sections of the plant. This paper focuses on these problems and the troubleshooting to determine the causes of the pressure instability. During troubleshooting a number of key factors that contributed to the pressure instability were identified, with the main cause being the design and expected air ingress into the column. This influenced the design of several pieces of equipment in and around the column. A deviation from the design air ingress meant that several design parameters had to be re-evaluated in order to eventually reach the intended operating pressure. A conventional pressure control philosophy was implemented, but changes to this were required in order to achieve the necessary stability in the column. The improved control philosophy has several benefits, such as a reduced number of variables to be manipulated by the operator, smoother change over between the primary pressure controller and the setpoint high controller, as well as optimising the product losses to the vacuum system.

## STUDY OF CONTROL PROPERTIES OF INTENSIFIED THERMALLY COUPLED DISTILLATION SEQUENCES

Juan Gabriel Segovia-Hernández, Rodolfo Murrieta-Dueñas, Roberto Gutiérrez-Guerra, Salvador Hernández

In this work, we analyze the control properties of thermally coupled reactive distillation sequences and thermally coupled extractive distillation sequences in comparison with conventional reactive and extractive distillation configurations. All sequences have been designed using a multi objective genetic algorithm with restrictions. We study the theoretical control properties of those schemes using the singular value decomposition technique in all frequency domain and we also present an analysis on the closed loop behavior with dynamic rigorous simulations. The effects of total stages, reactive stages, and extractant/feed ratio on the energy consumption and control properties are obtained for the intensified distillation options. The results show that there are cases in which integrated reactive and extractive sequences do not only provide significant energy savings with respect to the conventional reactive and extractive arrangements, but also may offer dynamic advantages in nonoptimal design conditions.

## IMPROVED CONTROL STRATEGIES FOR DIVIDING-WALL COLUMNS

Anton A. Kiss, Ruben C. van Diggelen

This study investigates the controllability of dividing-wall columns (DWC) and makes an ample comparison of various control strategies based on PID loops, within a multi-loop framework (DB, DV, LB, LV) versus more advanced controllers such as LQG/LQR and high order controllers obtained by  $H_\infty$ -controller synthesis and  $\mu$ -synthesis. All these controllers are applied to a DWC used in an industrial case study – the ternary separation of benzene-toluene-xylene. The performance of these control strategies and the dynamic response of the DWC is investigated in terms of products composition and flow rates, for various persistent disturbances in the feed flow rate and feed composition. Significantly shorter settling times can be achieved using the advanced controllers based on LQG/LQR,  $H_\infty$  and  $\mu$ -synthesis.

## STRUCTURED PACKING EFFICIENCY – VITAL INFORMATION FOR THE CHEMICAL INDUSTRY

Markus Ottenbacher, Žarko Olujić, Michael Jödecke, Christoph Großmann

Distillation is the most important thermal separation process, with separation efficiency as one of the fundamental parameters to influence economy and energy consumption. The precise knowledge of separation efficiency and the ability to compare different types of column internals is vital information for the chemical industry. Still, experimental data is the only significant source of such data. The authors have taken the effort to work out in detail different factors influencing both measurement and interpretation of structured packing separation efficiency data, to provide basis for establishing an open standard in this respect.

## INTALOX® ULTRA™ RANDOM PACKING – PUSHING THE ENVELOPE

Izak Nieuwoudt

INTALOX® ULTRA™ random packing is a new generation random packing that exhibits better efficiency, lower pressure drop and higher capacity than previous generations of random packing. These characteristics translate into savings on new towers, but also open up interesting revamp opportunities.

## CHARACTERIZATION AND QUANTIFICATION OF THE QUALITY OF GAS FLOW DISTRIBUTIONS

Carsten Stemich and Lothar Spiegel

Since the evaluation of the homogeneity of a distribution can be subdivided into two parts (magnitude and spatial distribution), a good key value describing the quality of the distribution has to consider both. The CoV value covers the effects of the fluctuation's magnitude, but any spatial information is lost. Therefore, a complementary key value (Coefficient of Distribution – CoD) was developed to consider both, magnitude and spatial distribution together. The new method is successfully applied to evaluate the vapour velocity distribution at the entrance to the packed bed above the vapour feed of an industrial distillation column with a large diameter.

## EXPERIMENTAL INVESTIGATION ON THE EFFECT OF PACKING MATERIAL TEXTURES ON THE LIQUID-SIDE MASS TRANSFER

Martin Kohrt, Ilja Ausner and Jens-Uwe Repke

In this work, the impact of different packing material textures to liquid-side controlled mass transfer for the CO<sub>2</sub> absorption into silicone oil is analysed. Typical industrially applied textures with bidirectional pyramidal and unidirectional wavy topographies are investigated for a wide range of liquid loads and viscosities. It is found that the texture design has a significant influence on the mass transfer efficiency, e.g. mass transfer intensification up to 80% can be performed by a textured surface compared with a flat plate.

## MEASUREMENT OF LIQUID HOLD-UP IN CATALYTIC STRUCTURED PACKINGS: COMPARISON OF DIFFERENT EXPERIMENTAL TECHNIQUES

Aurora Viva, Said Aferka, Dominique Toye, Pierre Marchot, Michel Crine and Elisabetta Brunazzi

This paper presents the results of an experimental study carried out to examine liquid hold-up in 100 mm diameter catalytic structured packing Katapak-SP. Two versions of the packing have been investigated. Both global and local measurements were carried out on the very same packings, using water at ambient conditions as working liquid. To this scope, traditional methods like draining techniques were used to obtain global hold-up values. A non-intrusive high energy X-ray tomography was used for gathering information on local scale and study axial distribution of the liquid hold-up over the packed column, inside and outside the catalyst containing baskets. The total liquid hold-up of the catalytic packed bed was evaluated by averaging hold-up values obtained at different cross sections over the corresponding volume. Very good agreement was found between global values estimated with the different techniques. The experimental results are useful for supporting theoretical developments in hydrodynamic and mass transfer modeling.

## MAXIMIZING THE PERFORMANCE OF CORRUGATED SHEET STRUCTURED PACKINGS

Žarko Olujić, Thomas Rietfort, Helmut Jansen, Björn Kaibel, Egon Zich, Gerhard Ruffert, Torsten Zielke

Total reflux distillation experiments carried out using state of the art test facilities at Bayer TS with newest generation of J. Montz structured packings indicate that by combining appropriately the dimensions and design of corrugations and the corrugation inclination angle, i.e. by affecting the pressure drop accordingly, either efficiency or capacity, or even both can be enhanced significantly, depending on the type of the packing. This allows leaner columns in new designs and more capacity and other benefits in retrofit situations. Delft model, with appropriate geometry modifications, proved capable of predicting the observed trends. The estimates of the pressure drop seem to be consistently lower than measured and the deviation from experiments tends to increase with increasing specific geometric area of the packing, while the predicted points of onset of loading are close to observed ones. On the efficiency side, the predictions appeared to be conservative; however a fairly good agreement with experiment is obtained if installed specific geometric area is used as effective area.

## TRAY STABILITY AT LOW VAPOR LOAD

Daniel R. Summers, Lothar Spiegel and Ekaterina Kolesnikov

Tower operation at low vapor rates is typically limited by the onset of weeping which can severely hurt tray performance. Many authors have attempted to study the onset of weeping on distillation trays as well as to determine the amount of weeping present. This paper will address this issue from a different perspective which is the uniformity of vapor passage through the tray deck at low vapor loads. It will be shown that there exists a relationship between the onset of weeping, tray performance, dry tray pressure drop and hydrostatic head of liquid on the tray. In addition, this relationship will be addressed with regards to single pass as well as multi-pass trays.

## UNDERSTANDING MALDISTRIBUTION IN 3-PASS TRAYS

Henry Z. Kister and Matthew Olsson

Understanding 3-pass trays is the key to design of 6-pass trays, such as those in the large towers expected in carbon-capture services. This paper presents a hydraulic distribution model for 3-pass trays with no liquid or vapor equalization. The model is verified by comparison with FRI's test data and with one operating tower. Our paper predicts good distribution for the 3-pass trays tested at FRI, and shows that the poor efficiencies in some of the tests were due to losing the downcomer seals and not tray maldistribution. The model predicts good distribution at maximum rates in the operating tower, but finds that at lower rates, where valves open and close, there is an extreme sensitivity of vapor distribution to small pressure drop variations. This sensitivity precludes reliable modeling of distribution in this region and may define an unstable region in the operation of 3-pass trays.

## DESIGNING TRAYS FOR SELECTIVE TREATING

Ralph H. Weiland, Nathan A. Hatcher and Jaime L. Nava

Field performance data from eight different gas treating plants are used to show how certain tray design parameters can be selected to improve contactor performance radically by ensuring the trays operate hydraulically in the spray regime. A case study is also presented in which both CO<sub>2</sub> and H<sub>2</sub>S removal specifications are met by using multi-pass trays even though satisfactory hydraulic performance can be had from a single-pass design.

## DESIGN-TROUBLESHOOTING OF AN ABSORPTION COLUMN – IMPORTANCE OF DETAILS

Ron Stockfleth

An absorption column was suffering from operational problems due to the interaction of gas and liquid in the column bottoms at the total draw-off (chimney) tray. In the bottom of the column one downcomer was discharging liquid directly into the bottoms compartment, which functions as the suction drum for a circulation pump. This caused cavitation of the pump. This problem was solved by installing a “roof” blocking the direct flow of liquid from the downcomer to the pump suction compartment breaking the momentum of the discharged liquid. The liquid and gas interact vigorously in the confined space between the risers of the chimney tray. This interaction causes leakage of the liquid through the risers. This problem was mitigated by reducing the liquid flow. Both problems show that details in the design of Shell calming section multi-downcomer trays are important for proper operation.

## DIAGNOSTICS OF HIGH PRESSURE DEPROPANIZER

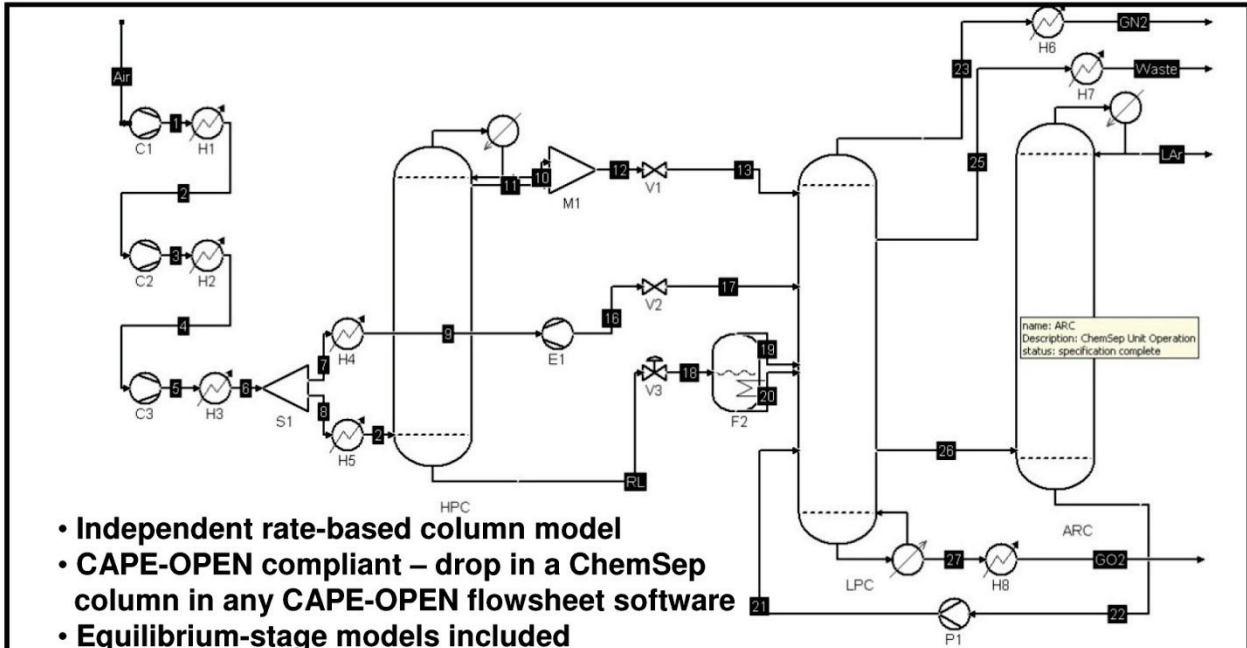
Lowell Pless, Christopher McKeown and Simon Xu

A Depropanizer tower with a large diameter top section and smaller diameter bottom section was field tested and studied for its root cause of flooding. In the diameter transition zone, a two-phase feed was being introduced. Gamma scans identified that the trays in the top section were flooding and liquid accumulation initiated in the transition zone. A neutron backscatter technique was used to investigate downcomer hydraulics and identify the root-cause of flooding. Coupled with the field troubleshooting, a careful analysis of the design revealed likely causes of the flooding problem. Recommendations for modifications were made and installed.

## VACUUM TOWER WASH SECTION DESIGN: MYTH AND REALITY

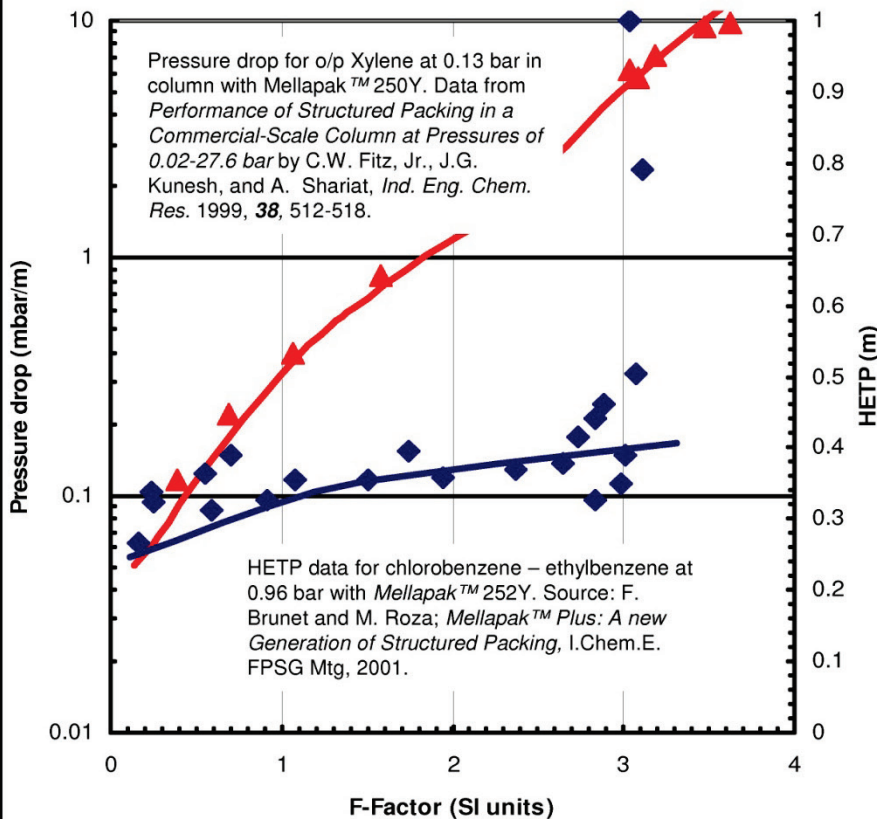
Mario Roza<sup>1</sup> and Mark Pilling<sup>2</sup>

Entrainment from the vacuum tower flash zone is only one aspect which determines the quality and yield of vacuum gas oil which can be obtained for given crudes. All aspects influencing the vacuum gas oil quality must be considered: entrainment from the inlet device, de-entrainment characteristics of the internals in the wash section and entrainment from the wash oil distributor. The importance of all of these factors determine the maximum yield for a given quality of vacuum gas oil.



- Independent rate-based column model
- CAPE-OPEN compliant – drop in a ChemSep column in any CAPE-OPEN flowsheet software
- Equilibrium-stage models included
- Easy to learn interface for Windows
- Total reflux model for validation simulations
- Powerful plotting capabilities
- Export to spreadsheet, text, and web formats
- Residue curve maps and phase diagrams
- Parametric study feature
- Validated design correlations
- Flexible input format

# ChemSep™



This illustration compares *ChemSep* performance predictions (the lines) with data (points) for Sulzer Mellapak™.

It is a combination of two validation plots that can be made in an automated fashion using the parametric study feature.

**ChemSep Lite**  
available FREE!

Download ChemSep  
LITE v6.6

[www.chemsep.com](http://www.chemsep.com)



### EXERGY LOSSES RELATION WITH DRIVING FORCES IN DISTILLATION COLUMN

Seyed Ali Ashrafizadeh, Majid Amidpour, Zohre Heydaricesht

Present investigation involves computation of the exergy losses of the whole column by considering the factors of irreversibility of distillation columns, and comparison of their impact. This included combining the relations of energy-exergy balance with design relations, with impact of various parameters (such as design and operational) on exergy losses of distillation columns. The difference between present method and those carried out elsewhere is the ability to compute exergy losses by applying separate types of irreversibility in the distillation column. This was meant to show comparisons of the sources of irreversibility. Results suggest that the driving forces of mass transfer among other parameters have the most effect on these losses. By the same token reducing these forces can reduce the rate of exergy losses. The paper finally recommends effective methods for reducing the rate of exergy losses in industries in general and the petro-chemicals in particular.

### SYNTHESIS AND OPTIMIZATION OF DEMETHANIZER FLOWSHEETS FOR LOW TEMPERATURE SEPARATION PROCESSES

Muneeb Nawaz and Megan Jobson

Low temperature distillation remains the most important route for the separation and purification of gas mixtures, especially when high throughputs are required. A demethanizer system is an industrially important example of such a process that involves interactions between the separation system, refrigeration system and the heat recovery system. The number of alternative demethanizer flowsheets, both in theory and commercially available, is large. The assessment of all structural alternatives and their operating conditions is a time consuming task requiring many simulations to select the most economic options. Therefore, a systematic approach for synthesis is required to generate effective and economic designs with minimal time and effort. This research extends an existing platform for the design of heat integrated separation systems to address the demethanizer subsystem, characterized by interactions between the complex distillation column and other flowsheet components, including the turbo-expander, flash units, multistream exchangers and external refrigeration system. Heat recovery opportunities are identified to improve the economics of the process. Case studies illustrate that the optimization framework allows energy-efficient and cost-effective gas separation flowsheets to be developed.

### CONCEPTUAL DESIGN AND COMPARISON OF FOUR-PRODUCTS DIVIDING WALL COLUMNS FOR SEPARATION OF A MULTICOMPONENT AROMATICS MIXTURE

Igor Dejanović, Ljubica Matijašević, Žarko Olujić, Ivar Halvorsen, Sigurd Skogestad, Helmut Jansen and Björn Kaibel

Preliminary evaluations using a simple but reliable short-cut method indicated that a 15 component aromatic's mixture can be separated very efficiently into four fractions according to given product specifications employing either a single or a multiple partition wall dividing wall column (DWC). The obtained results have been used to initiate rigorous simulations, to determine the number of stages required in different sections, as well as to obtain internal flows of vapour and liquid necessary for dimensioning and adequate (actual delivery prices) cost estimation. Comparison of total annualized costs indicates that more energy efficient complex configuration with three partition walls is a viable option in present case.

### ESTABLISHING INTERNAL CONFIGURATION OF DIVIDING WALL COLUMN FOR SEPARATION OF A MULTICOMPONENT AROMATICS MIXTURE

Ivar J. Halvorsen, Igor Dejanović, Ljubica Matijašević, Žarko Olujić and Sigurd Skogestad

In this paper the so called V-min diagram method is used to evaluate potential for energy saving and to indicate most beneficial internal configuration for a single dividing column (DWC) considered as an alternative for conventional three columns configuration used in an aromatics processing plant for separation of a multicomponent feed into four specified product streams. A DWC employing multiple partition walls to separate central part of the column into three sections appeared to be a much more attractive option than its, more practical single partition wall counterpart.

### MASS TRANSFER AND PRESSURE DROP OF A NOVEL STRUCTURED PACKING FOR CO<sub>2</sub> POST-COMBUSTION CAPTURE

Pascal ALIX, Ludovic RAYNAL, Aude ROYON-LEBEAUD, François ABBE, Jean-Pierre Maumus, Aras Ahmadi, Michel MEYER, Michel PREVOST, David ROUZINEAU

A novel packing named Sepcarb® 4D had been developed and characterized within 150 mm internal diameter columns in terms of pressure drop, interfacial area ( $a_e$ ) and gas side mass transfer coefficient ( $k_G$ ). The 4D packing consists in a complex arrangement of hollow carbon tubes. Its geometry is given by some geometric parameters, one of which results in the opening fraction,  $\Omega$  (from 30% to 50% for the present study). Pressure drop curves show that the capacity of the present packing is considerably increased when  $\Omega$  increases. Flooding limits become higher than those expected for recent Mellapak 500.Y and 750.Y. The geometric area of the 4D packing,  $a_g$ , is inversely proportional to  $\Omega$ . However the effective area,  $a_e$  is not reduced when  $\Omega$  is increased from 30 to 50% which indicates that  $a_e$  can considerably exceed  $a_g$  for high  $\Omega$ . It appears that  $a_e$  is very sensitive to the gas flowrate, and much higher than those measured for Mellapak 500.Y, 252.Y and 250.Y. Such results can be explained by a non negligible amount of droplets, and are confirmed by  $k_G \cdot a_e$  measurements. The latter are based on water evaporation and require a very sophisticated experimental set-up. In conclusion, the novel 4D packing seems to be very adapted to CO<sub>2</sub> capture.

### CO<sub>2</sub> CAPTURE SOLVENT SELECTION BY COMBINED ABSORPTION-DESORPTION ANALYSIS

Ugochukwu E. Aronu, Hallvard F. Svendsen, Karl Anders Hoff

A method was developed for selection of promising solvents based on CO<sub>2</sub> absorption experiments at 40°C and 9.5 kPa CO<sub>2</sub> partial pressure followed by desorption of same solvents at 80°C down to 1.0 kPa CO<sub>2</sub> partial pressure. The experiments conducted under atmospheric conditions revealed the solvents absorption and desorption characteristics and were compared with 1.0M, 2.5M, 5.0M and 10.0M MEA. Results showed that only absorption or stripping data alone was not sufficient in making robust solvent selection decisions; combined data analysis was necessary. 1.0M tetraethylenepentamine (TEPA) and 5.0M MEA showed the best performance in terms of absorption rate. 1.5M Bis-(3-dimethylaminopropyl) amine (TMBPA) was easy to desorb, has high absorption capacity; and when promoted it has the best performance in terms of CO<sub>2</sub> carrying capacity. At the test conditions, 1.5M TMBPA promoted with 1.0M PZ showed the most outstanding potential for efficient CO<sub>2</sub> removal at reduced cost of all systems tested. Its cyclic capacity in molCO<sub>2</sub>/mol amine was found to be 70% higher than 5M MEA.

### CARBON DIOXIDE CHEMICAL ABSORPTION WITH GLUCOSAMINE IN AIR-LIFT REACTOR

Alicia García-Abuín, Diego Gómez-Díaz, José M. Navaza, Isabel Vidal-Tato

The behaviour of glucosamine aqueous solutions has been studied to be used in carbon dioxide capture through absorption with chemical reaction using an air-lift reactor. Experimental results indicate that this reagent has a similar behavior than other common amines widely used in CO<sub>2</sub> capture, with regard to rate of capture of this acidic gas. The value of mass transfer rate has been determined, and the effect of different operation conditions upon the value of this parameter and gas-liquid interfacial area has been analyzed (amine concentration, pH and gas flow rate).

### RATE BASED MODELING AND VALIDATION OF A CARBON-DIOXIDE PILOT PLANT ABSORPTION COLUMN OPERATING ON MONOETHANOLAMINE

Levente L. Simon, Yannick Elias, Graeme Puxty, Yuli Artanto and Konrad Hungerbuhler

In-silico amine screening is a fast, low-cost and promising way of efficiently evaluating new amine molecules which are proposed for carbon-dioxide capture purposes. In order to implement the screening environment, reliable and robust absorber models are required. This contribution presents the modeling and validation results of a CO<sub>2</sub> capture pilot absorber operated with monoethanolamine (MEA), as the first step of the in-silico solvent screening framework. The simulation results have shown that the outlet amine loading and CO<sub>2</sub> partial pressure can be predicted with a 10% deviation from the experimental values for one column, with larger deviations for the second. Note that no parameter fitting was performed and the model relies entirely on engineering and property correlations available in the scientific literature. In addition the model was extended to include the calculation of the overall mass transfer coefficient from laboratory based wetted-wall experiments completed at CSIRO. This further improved the model prediction and significantly reduced the prediction error for the other column.

### CARBON DIOXIDE ABSORPTION INTO BIPHASIC AMINE SOLVENT WITH SOLVENT LOSS REDUCTION

Jiafei Zhang, Onyekachi Nwani and David W. Agar

The main challenge in the CO<sub>2</sub> capture from flue gases is to reduce the energy consumption required for solvent regeneration. Lipophilic amines exhibit a thermomorphic phase transition upon heating, giving rise to autoextractive behaviour, which enhances desorption at temperatures well below the solvent boiling point. The low regeneration temperature of less than 80°C together with the high cyclic CO<sub>2</sub> loading capacity (c. 0.9 mol<sub>-CO<sub>2</sub></sub>/mol<sub>-absorbent</sub>) of such biphasic amine systems permit the use of low temperature and even waste heat for desorption purposes. In order to improve the capture process and reduce the commensurate energy demand still further, desorption experiments were carried out at 70°C and techniques for enhancing CO<sub>2</sub> release without gas stripping were also studied. The comparison of various amines at a concentration of 3M and for a 15 mol% CO<sub>2</sub> feed gas demonstrates the considerable potential of lipophilic amines for the CO<sub>2</sub> absorption process. Chemical stability is a decisive factor for the industrial application of amine absorbents. Degradation of the novel lipophilic amine absorbents was shown to be minor, while volatility losses represent a major shortcoming of the biphasic solvent systems. Appropriate countermeasures to limit solvent losses were examined experimentally.

**AQUEOUS SOLUTIONS OF PYRROLIDINE FOR CARBON DIOXIDE CAPTURE**

Antonio Blanco, Alicia García-Abuín, Diego Gómez-Díaz, José M. Navaza, Isabel Vidal-Tato

Present study analyses absorption process with chemical reaction between carbon dioxide and aqueous solutions of pyrrolidine. The determination of kinetic has been carried out in order to determine the regime of process, and then the process has been performed in a bubble column reactor and the rate of capture of acidic gases has been analyzed.

**DEVELOPMENT OF TASK SPECIFIC HYPERBRANCHED POLYMERS FOR THE SEPARATION OF CARBON DIOXIDE: CARBON CAPTURE AND BIOGAS UPGRADE**

Johannes Völkl, Jörn Rolker and Wolfgang Arlt

Hyperbranched polymers are a group of components which have been successfully used in several applications in chemical engineering. The structure of these molecules is very flexible and can be tailored by changing functional groups or the repetitive unit. In this work the application of hyperbranched polymer for the upgrade of biogas is investigated. To limit the large numbers of possible polymer structures the a-priori predictive method COSMO-RS is used. The goal was to find the most suited molecules for the separation of carbon dioxide and methane. These optimized components are synthesized and used for further investigation. Results of the a-priori calculations and comparison with measured data are presented. Also the requirements for a solvent for the biogas upgrade and the relation to the chemical structure of a hyperbranched polymer are shown.

**PRELIMINARY ANALYSIS OF PROCESS FLOW SHEET MODIFICATIONS FOR ENERGY EFFICIENT CO<sub>2</sub> CAPTURE FROM FLUE GASES USING CHEMICAL ABSORPTION**

Ashleigh Cousins, Leigh T. Wardhaugh and Paul H.M. Feron

The energy penalty associated with solvent based capture of CO<sub>2</sub> from power station flue gases can be reduced by incorporating process flow sheet modifications into the standard process. A review of modifications suggested in the open and patent literature identified several options, primarily intended for use in the gas processing industry. It was not immediately clear whether these options would have the same benefits when applied to CO<sub>2</sub> capture from near atmospheric pressure flue gases. Process flow sheet modifications, including split flow, rich split, vapour recompression, and inter-stage cooling, were therefore modelled using a commercial rate-based simulation package. The preliminary modelling results showed considerable benefits in reducing the energy penalty of capturing CO<sub>2</sub> from combustion flue gases. Further work will focus on optimising and validating the most relevant process flow sheet modifications in a pilot plant.

## CAPITAL COSTS AND ENERGY CONSIDERATIONS OF DIFFERENT ALTERNATIVE STRIPPER CONFIGURATIONS FOR POST COMBUSTION CO<sub>2</sub> CAPTURE

Mehdi Karimi, Magne Hillestad, Hallvard F. Svendsen

Capturing and storing the greenhouse gas carbon dioxide (CO<sub>2</sub>) produced by power plants and factories before it is emitted to the atmosphere could play a major role in minimizing climate change. Among of the different technologies, aqueous amine absorption/stripping is a promising one. In this study 5 different configurations for aqueous absorption/stripping have been compared with regard to capital investment and energy consumption. The process simulations are made with the use of Unisim and ProTreat, while for the cost calculation relations from Turton et.al.<sup>4</sup> were used.

We can't identify that one single configuration is the best for all cases, because it depends on many parameters like energy and material costs, plant complexity, etc. The split-stream configuration with cooling of semi-lean amine stream has the minimum energy consumption, but the vapor recompression configuration is the optimum one because with a small increase in investment we can save significant amount of energy. The effect of heat integration between the compression section and the stripper also is considered for vapor recompression configuration. Reboiler energy may be saved with heat integration, however because of high temperature into the compressors the compression efficiency decreases. Also the capital cost and the complexity of the plant will increase. Heat integration between compression section and reboiler cause to increase water in produced CO<sub>2</sub> and increase the corrosion problem.

## REACTIVE DIVIDING-WALL COLUMNS: TOWARDS ENHANCED PROCESS INTEGRATION

Anton A. Kiss, J. J. Pragt, C. J. G. van Strien

This work presents an integrated reactive-distillation design based on a dividing-wall column (DWC) applied to an industrial case study within AkzoNobel. Remarkably, it is among the first industrial application of a reactive DWC reported in literature. The benefits of this novel integrated design are the ability to overcome VLE and chemical equilibrium limitations, as well as to separate the main product as high purity side-stream. To solve the problem of a production shift required by market demand changes, we developed an innovative integrated design that combines reaction and separations into one reactive DWC that allows significant savings in capital and operating costs – up to 36% and 15%, respectively. Two scenarios are analyzed and the results of the rigorous simulations are presented.

## NOVEL GRAPHICAL DESIGN METHOD FOR HYBRID PROCESSES

Mark Peters, Shehzaad Kauchali, Diane Hildebrandt, and David Glasser

Shortcut methods for the design and synthesis of separation systems are useful, especially in the conceptual stages of a process design. However, current approaches incorporated in these techniques result in them being suitable for traditional designs only, and unable to manage novel or complex configurations. Using column profile trajectories to describe the compositional behaviour of material in both distillation and membrane sections, it will be shown how any configuration, no matter how complex, can be modelled. With this comes an overall deeper understanding of the operation of the chosen system. As an example, a Petlyuk-type arrangement will be considered – firstly incorporating membrane permeation units as the only means of separation, and then secondly linking membrane units with distillation thereby forming a hybrid. The feasibility of each design is discussed, and compositional regions of feasibility are established, where necessary. Although the nature of column profiles may appear to be complicated, this method allows one to quickly and easily understand complex configurations, thus saving time, money and potentially reducing energy consumption.

## **SYNTHESIS OF NOVEL TERNARY HETEROGENEOUS AZEOTROPIC DISTILLATION FLOWSHEETS**

Paritta Prayoonyong and Megan Jobson

An algorithmic approach is presented for synthesising novel sequences for separating, by distillation and decanting, ternary heterogeneous azeotropic mixtures. Existing synthesis procedures that consider only simple single-feed columns with decanters and integrated decanters are extended to include more industrially relevant options such as columns with several heterogeneous stages, double-feed columns, columns with intermediate decanters, and those accepting a heterogeneous liquid feed. With these advanced column configurations included in the synthesis method, a wider range of sequences may be considered systematically, allowing sequences that are more economically attractive than conventional designs to be identified. A case study illustrates the application of the sequence synthesis approach and the novel flowsheets it can generate.

## **AN INTRODUCTION TO NEW HIGEE DEVICE AND ITS INDUSTRIAL APPLICATIONS**

Wang G. Q., Xu Z. C., Li X. H., Ji J. B.

A new HIGEE device-rotating zigzag bed (RZB) was developed in the context of process intensification. The RZB is structurally featured by a combinatorial rotor of one series of baffles attached to a rotating disk with another series to a stationary disk. The novel structure of the RZB determines its many advantages over the other HIGEE devices. The RZB is free of dynamic seal, capable of intermediate feed and simple coaxial multi-rotor configuration. These advantages qualify the RZB for utilization in continuous distillation. Three cases in different common processes were presented here to illustrate its industrial application. So the RZB is a kind of high efficiency gas-liquid contactor and opens up broad prospects for HIGEE technology commercialized in industrial continuous distillation processes.

## **CATALYTICALLY ACTIVATED SIC FOAM FOR REACTIVE DISTILLATION**

Julien Lévêque, David Rouzineau, Michel Prevost and Michel Meyer

The application of ceramic foam as a packing for distillation has been demonstrated in a previous work<sup>1</sup> but limited due to the low capacity. Nevertheless, the flow employed in reactive distillation are lower, it does not represent a major drawback. Moreover, the application of foam as a catalyst support has shown good activity<sup>2</sup> which let foresee an interesting application for reactive distillation. So, this paper describes the kinetic study of coating foam in a batch reactor on the target reaction application which is the esterification of acetic acid by methanol. Different catalyst coating methods have been tested to choose the most convenient.

## **EFFECT OF HYDRODYNAMIC CONDITIONS ON MASS AND HEAT TRANSFER IN A NOVEL MEMBRANE BASED CONTINUOUS MICRO-DISTILLATION DEVICE: EXPERIMENTAL APPROACH**

Chafika Adiche, Kai Sundmacher

In this work the influence of hydrodynamic conditions on the mass and heat transfer in a novel micro-separator combining membrane distillation concept with micro-fluidic structures has been investigated. In both feed and permeate channels laminar flow conditions have been established. The temperature polarization effect was localized in both the feed and permeate channels and was found to be strongly dependent on the feed composition and the hydrodynamic conditions in both channels. On the other hand, the inert gas flow rate was identified as a crucial operating parameter influencing both the mass and heat transfer in the micro-separator. In addition, the selection of an appropriate membrane liquid-vapor/gas contactor was found to be an important design parameter for the reduction of temperature polarization effects. As compared to existing membrane distillation processes, the new membrane distillation based micro-separator offers a substantial potential to enhance the separation performance particularly for mixtures with high methanol concentration.

### EXPERIMENTAL VALIDATION OF A NEW DOUBLE-COLUMN SYSTEM FOR HETEROAZEOTROPIC BATCH DISTILLATION

Ferenc Denes, Peter Lang and Xavier Joulia

A new double-column batch heteroazeotropic distillation system (DCS) operating in closed mode is studied by laboratory experiments. Our primary aim is the experimental validation of the DCS for the separation of the heteroazeotropic mixture 1-butanol – water in a simple laboratory equipment (glass columns packed by Raschig rings). We compare its performance with that of the conventional batch rectifier (BR). Rigorous simulations are done by using a professional dynamic flowsheet simulator. In the case studied the separation by the DCS proved to be feasible and competitive with that of the BR: By using the DCS higher recovery for 1-butanol was reached during practically the same time.

### SOLVENT RECOVERY FROM A MULTICOMPONENT MIXTURE BY BATCH EXTRACTIVE DISTILLATION AND HYBRID PROCESS

P. Lang, L. Hegely, G. Kovacs, J. Gaal-Szilagyi and B. Kotai

The performance of the basic and a modified operational policy of batch extractive distillation (BED) and the hybrid process (HP; absorption+distillation) for the recovery of tetrahydrofuran (THF) from a five-component industrial waste solvent mixture were investigated with laboratory experiments and rigorous simulations. The components (methanol, THF, acetonitrile, water, pyridine) of the mixture form seven azeotropes. The prescribed separation task (production of aqueous THF with limited content of organic pollutants) was not feasible with batch rectification, but we were able to produce THF of desired quality by BED and HP using water as entrainer. The highest recovery and production rate were achieved with the HP, while the least efficient process was the basic policy of BED.

### REACTIVE PACKED BUBBLE COLUMN FOR THE SYNTHESIS OF ISOPROPYL MYRISTATE

M.C. de Jong, E. Zondervan, A.C. Dimian and A.B. de Haan

In this paper conceptual designs for the esterification of myristic acid with isopropanol through reactive distillation (packed and tray column) and bubble column are constructed, which are evaluated against the batch process based on required reaction volumes. The required reactor volume can be decreased with 27 or 79 %, allowing a maximum temperature of respectively 170 and 220C, using a packed reactive distillation column. Using a tray reactive distillation column and a maximum temperature of 220C, the required reactor volume can be decreased with 93 %. Due to the less favourable mass transfer characteristics of the bubble column, in here the required reactor volume can only be decreased with 78%. When a temperature of 220C is allowed in the column, the tray reactive distillation is the preferable process for the esterification of myristic acid isopropanol, based on the required reaction volumes. The influence of the maximum column temperature and the influence of a larger liquid hold-up per stage as a result of a different column configuration are of equal importance for the required reaction volume.

## BIODIESEL PRODUCTION FROM REACTIVE DISTILLATION PROCESS: A COMPARATIVE STUDY BETWEEN EXPERIMENTAL RESULTS AND SIMULATION

Nívea de Lima da Silva, Carlos Mario Garcia Santander, César Benedito Batistella, Rubens Maciel Filho, María Regina Wolf Maciel.

Biodiesel is a fuel made from vegetable oils, animal fats and microbial oil (algae, bacteria and fungi). The raw materials are converted to biodiesel through a chemical reaction involving alcohol and catalyst. The purpose of the present work is to present an efficient process using reactive distillation columns applied to biodiesel production. Reactive distillation is the simultaneous implementation of reaction and separation within a single unit of column. Nowadays, it is appropriated called "Intensified Process". This combined operation is especially suited for the chemical reaction limited by equilibrium constraints, since one or more of the products of the reaction are continuously separated from the reactants. This work presents the biodiesel production from soy oil oil and bioethanol by reactive distillation. The RD process was carried out in a semi-batch system. The RD column used in this process was a packed column filled with glass rings and equipped with water condenser, temperature controller and reflux controller. The system design was based on the relative volatilities of the raw materials and products. A simulation of the reactive distillation process was carried out in Aspen Plus. Different variables affect the conventional biodiesel production process such as: catalyst concentration, reaction temperature, level of agitation, ethanol:soy oil oil molar ratio, reaction time, and raw material type. In this study, the experimental design was used to optimize the following process variables: the catalyst concentration (from 0.5 %wt to 1.5%wt), and the ethanol:soy oil oil molar ratio (from 3:1 to 9:1). The reactive column reflux rate was 83 ml/min, and the reaction time was 6 minutes. The difference between the boiling temperature of ethanol and the product mixture, ethyl esters and glycerol, is so large that the separation of the alcohol from the product mixture became easy. The use of reactive distillation process to biodiesel production leads to a more efficient process than the conventional transesterification one. The results showed many advantages of the integration process as compared with the conventional biodiesel production such: decrease of the ethanol excess, decrease of the reaction time, and decrease of the equipment units. The best ester conversion was 98.18%wt with 0.65%wt of sodium hydroxide, ethanol:soy oil oil molar ratio of 8:1 and reaction time of 6 minutes. The process simulation results are in agreement with the experimental ones.

## SELECTIVE REMOVAL OF CARBON DIOXIDE FROM AQUEOUS AMMONIA SOLUTIONS

Jan F. Maćkowiak and Andrzej Górak

In this work modelling and experimental validation of an integrated process for the removal of carbon dioxide from ammonia solutions is presented (decarbonisation). In this process, carbon dioxide is stripped out from the solution simultaneously with small amounts of ammonia at ambient pressure in a packed column. Recovery of the stripped ammonia can be reached by combining absorption of ammonia and condensation of stripping steam. The interaction of the different unit operations of stripping, absorption and direct-contact condensation (DCC) can be arranged in one single packed column where stripping takes place in the lower part of the column, and the DCC and ammonia absorption in the upper part. To describe the process a rigorous model based on the film theory which considers heat and mass transfer as well as reaction rates directly has been adapted to the requirements of multicomponent reactive stripping, absorption and direct-contact condensation in packed columns<sup>1</sup>. Extensive experimental investigations have been performed for both, the stripping and for the direct-contact condensation in a pilot scale packed column with diameters of 0.15 and 0.32 m. Relevant operation parameters as well as column dimensions were varied during the experiments in order to achieve a broad data base for the validation. Experimental validation of the two sub-processes and the entire decarbonisation shows good agreement between calculated and experimental values. Based on the validated model a successful optimisation of the decarbonisation process has been performed, leading to increased carbon dioxide removal and reduction of ammonia losses.



### CYCLOHEXANOL PRODUCTION FROM CYCLOHEXENE IN A REACTIVE DIVIDED WALL COLUMN: A FEASIBILITY STUDY

Suman Thotla, Amit Katariya, Hannsjoerg Freund, Kai Sundmacher

In this paper, applicability of reactive divided wall column for two step reactions is investigated. Reactive divided wall column is designed conceptually and simulation studies show that cyclohexanol production from cyclohexene using formic acid as a reactive entrainer in reactive divided wall column is feasible.

### THE SIMULATION OF VAPOR-LIQUID EQUILIBRIUM IN TERNARY SYSTEMS WITH TWO TERNARY AZEOTROPES

Alla K. Frolkova, Tatiana V. Chelyuskina

Theoretical substantiation of biazeotropy phenomenon in ternary systems is presented. The mathematical models of vapor-liquid equilibrium in benzene–perfluorobenzene–methyl propionate and benzene–perfluorobenzene–tert–amyl alcohol systems at various pressures had been developed.

### ABSORPTION RATES OF CO<sub>2</sub> INTO SOLUTIONS OF MEA/2-PROPANOL

L.J. du Preez, C.E. Schwarz, J.H. Knoetze\*

Effective interfacial mass transfer area is a parameter of great importance in evaluating and determining the efficiency of separation column internals. A viable chemical method identified for determining this parameter is the reactive absorption of CO<sub>2</sub> into solutions of primary amines. The experiments were conducted on a wetted wall experimental set-up, which was verified with data obtained from a previous study. The absolute and specific absorption rates of CO<sub>2</sub> into solutions of MEA/2-propanol as functions of surface area and column height at various CO<sub>2</sub> and MEA concentrations and system pressures were determined. The specific absorption rate expression proposed by the previous study<sup>4</sup> is insufficient in predicting the absorption rates at higher CO<sub>2</sub> gas concentrations and it is recommended that a non-linear rate expression derived from fundamental kinetics should be developed.

### EXPERIMENTAL STUDY ON CONTACT ANGLE OF ETHANOL AND N-PROPANOL AQUEOUS SOLUTIONS ON METAL SURFACES

C. X. Zhou, X.G. Yuan, L. T. Fan, A. W. Zeng, K.T. Yu, M. Kalbassi and K. E. Porter

Experimental studies on the contact angles of aqueous solution of ethanol and that of n-propanol on copper, aluminum and stainless steel surfaces are reported in this paper. The contact angles were measured under atmospheric condition, and then under vapor-liquid equilibrium conditions at different temperatures. The results showed the variations of the contact angles with concentrations of aqueous solutions on different metal material surfaces with different roughness. Some unstable behaviours of the wetting ability around the azeotropic point of a binary solution are reported. The influences of concentration, kind of materials and the surface roughness on the wetting ability are discussed.

### PHASE EQUILIBRIA OF ORGANIC SULFUR COMPOUNDS FOR CLEANER FUELS

Erlin Sapei, Petri Uusi-Kyyny, Kari I. Keskinen, Juhani Aittamaa

### NEW METHODOLOGY OF DETERMINATION OF BOILING POINT AT VERY LOW PRESSURE: PETROLEUM CASE

M.S. Lopes, P. Sbaite, C.B. Batistella, M.R. Wolf Maciel, R. Maciel Filho, A. de Oliveira Gomes, L.C. Medina

Molecular distillation is a specific separation process which occurs at reduced pressure, exposing, hence, the material at reduced temperatures. This technique involves, basically, two stages: evaporation and condensation, in which vapor molecules escape from the evaporator in direction to the condenser, where condensation occurs. It is necessary that these generated molecules find a free path between the evaporator and the condenser, and then it is necessary that the condenser be separated from the evaporator by a smaller distance than the mean free path of the evaporating molecules. Since heavy petroleum residues can be easily cracked by thermal heating, the process mentioned above allowed the development of a new methodology for characterization of these types of residues. Usually, the evaluation of the TBP (True Boiling Point) curve of crude oils has been carried out through ASTM D 2892 and D 5236 methods; these methods are so important because at the same time that the TBP Curve is defined, petroleum fractions are obtained, but values of final temperatures are limited to 565 °C. For higher temperatures, a well established method which makes possible to get both objectives, to extend the TBP Curve and to get heavier fractions does not exist, although this is a very important issue to be studied. So, the innovative technique shown here presents large potential for the determination of boiling point of heavy oils using low pressure system. Its potential can be verified in works which uses molecular distiller<sup>1-3</sup>. The aim of this work is to apply this new methodology for the determination of the TBP of petroleum above 565 °C, getting and characterizing extra-heavy fractions at the same time. Experiments using Falling Film Molecular Distiller were carried out using two residues of Brazilian petroleum, where operating temperatures were increased systematically. According to the results, it was obtained an improvement of percentage of distillate (above 10%) and it was possible to reach values up to 720 °C, representing a considerable progress in the analyses of heavy petroleum fractions. Distillate and residue streams obtained were characterized through gas chromatography distillation (SIMDIS), specific gravity and vapor pressure osmometry. It is important to mention that the results of this work are concerned with Boiling Point, True Boiling Point, development of a robust correlation and with experimental data.

### MODELING AND EXPERIMENTAL STUDY OF CARBON DIOXIDE ABSORPTION INTO AQUEOUS AMINE BASED SOLVENTS

Lionel Dubois and Diane Thomas

This work focused on the CO<sub>2</sub> capture by absorption into amines based absorbents. Aqueous mixtures containing different types of amines (MEA, MDEA, AMP, PZ and PZEA) are experimentally compared in a special gas-liquid contactor (a cables-bundle contactor) with respect to the CO<sub>2</sub> removal performances at 25°C and atmospheric pressure. This absorption process was also simulated with the use of published data on physico-chemical properties (densities, viscosities, diffusivities, Henry coefficients) of the CO<sub>2</sub>-amines systems. The different experiments clearly highlighted the positive effect of activators such as PZ and PZEA on the absorption performances measured with MEA, MDEA and AMP solutions. Regarding the simulation results, they matched quite satisfactorily the experimental values concerning individual amines solutions, but improvements should be envisaged in order to simulate successfully the CO<sub>2</sub> absorption into amines mixtures.

## OPTIMAL DESIGN METHODOLOGY FOR AZEOTROPIC DISTILLATION COLUMNS

Claudia Gutiérrez-Antonio, Abel Briones-Ramírez

We develop a short and optimal design methodology for multicomponent mixtures, based on the concept of minimum difference in composition. The minimum reflux ratio is calculated through an analytical procedure, which allowing their use in multicomponent mixtures. The procedure also includes a simple criterion to optimize the structural design of the column, without increasing energy consumption. The method is tested with different azeotropic mixtures, and it is compared with the results of a multiobjective genetic algorithm with constraints. Results show that designs obtained with the new and stochastic methods are quite similar, but less time and computational resources are required.

## BOUNDARY VALUE DESIGN METHOD FOR COMPLEX DEMETHANIZER COLUMNS

Muneeb Nawaz and Megan Jobson

When a design problem dealing with demethanizer flowsheets is approached in a systematic way, the number of separation alternatives to be studied is generally very large. Repetitive simulation studies to evaluate the economic viability of the process can be facilitated by combining shortcut design models with rigorous optimization. These shortcut models are useful at the initial design stage, when there is little information about the separation tasks beyond the design specifications. A demethanizer column has many degrees of freedom, including the operating pressure, the location and the order of feeds, the number and duty of side reboilers and the flow rate of the external reflux stream. An appropriate design model for the demethanizer is needed for the development of an optimization framework for process synthesis and evaluation. Such a column design model should be computationally relatively undemanding yet accurate and allow evaluation of both energy demand and equipment requirements. The complexity of the demethanizer column precludes the use of the Fenske–Underwood–Gilliland shortcut design method. A semi-rigorous boundary value method is proposed for the design of complex demethanizer columns separating multicomponent mixtures. The method has been implemented within MATLAB and linked to HYSYS for prediction of physical and thermodynamic properties. The results of the proposed design methodology are shown to be in good agreement with those of rigorous simulation.

## RATE-BASED MASS TRANSFER PERFORMANCE ANALYSIS OF [EMIM][EtSO<sub>4</sub>] AND ETHYLENE GLYCOL IN THE EXTRACTIVE DISTILLATION OF WATER-ETHANOL MIXTURES

Esteban Quijada, Wytze Meindersma and André de Haan

The mass transfer efficiency of an extractive distillation column was compared for the ionic liquid 1-Ethyl-3-methylimidazolium ethyl sulfate and ethylene glycol as solvents for the separation of water-ethanol. A rate based model was established in ASPEN Plus. Tray efficiency profiles along the column showed a reduction in mass transfer performance when the ionic liquid was used due to its relatively high viscosity. Indeed, this reduction was more pronounced when the liquid phase viscosity was increased by means of a higher solvent-to-feed ratio. Finally, a sharp decline in efficiency was observed at high liquid phase viscosities, approaching the flooding point.

### A SHORT METHOD TO CALCULATE REACTIVE RESIDUE CURVE MAPS

M. Carrera-Rodríguez, J. G. Segovia-Hernández and A. Bonilla-Petriciolet

Reactive residue curve maps (RRCM) are useful for the design of reactive distillation columns as a tool to establish feasible zones of reaction-separation. The calculation of RRCM usually involves great computational effort due to the nonlinearity of the model equations and its iterative nature for the determination of reactive phase equilibrium. In this study, a simplified method for the generation of RRCM is presented. This method is based on the application of reaction-invariant composition variables and assumes that the phase equilibrium constants and the relative volatilities are independent of the temperature. These assumptions allow avoiding iterative calculations for obtaining a good approximation of RRCM. Several case studies are used to show the effectiveness of the proposed method.

### GEOMETRY OF SUBSETS OF OPTIMALITY IN EXTRACTIVE DISTILLATION OF MULTICOMPONENT MIXTURES

Andrey V. Timoshenko, Boris B. Dolmatov, Elena A. Anokhina and Vladimir S. Timofeev

Extractive distillation was investigated of the multicomponent mixtures: methanol – n-propylacetate – toluene (I); acetone – chloroform – n-butanol(II); benzene – n-butanol – ethylbenzene(III). Aniline was selected as entrainer for the I and III mixtures and dimethylformamide for the II mixture separation. The possible three columns distillation flowsheets were constructed for separation of each mixture. Then they were transformed into the partially thermally coupled complexes. Eight points were selected in each simplex of initial feed composition. All flowsheets were simulated and optimized for each composition on the criteria of minimum energy consumption. These results gave an ability to construct the energy consumption surfaces for each flowsheet under the initial feed compositions simplex. The mapping of these surfaces intersection into the initial feed compositions simplex gives the borders which separate different fields of initial feed composition. The each field is characterized by the existence of a single optimal flowsheet and can be described as the region or subset of optimality. The geometry of those subsets was detected for the different classes of flowsheets and for full flowsheets manifold. It was developed that the maximum of energy saving in the investigated field of initial feed compositions are about 14 % for mixture (I), more than 22% for mixture (II) and more than 36% for mixture (III). The best thermally coupled complex is better than the best three-column extractive distillation flowsheet.

### IONIC LIQUID SELECTION AND PERFORMANCE EVALUATION FOR THE SEPARATION OF METHYLCYCLOHEXANE/TOLUENE BY EXTRACTIVE DISTILLATION

Juan Pablo Gutierrez, Wytze Meindersma and André B. de Haan

The effectiveness of an extractive distillation process relies on the choice of the extractive solvent. The conventional methodology to select solvents is based on Group Contribution Methods. Ionic liquids have shown several advantages over conventional solvents used in extractive distillation and liquid-liquid extraction processes. However, there is no existing methodology to select ILs as solvents for ED processes due to the lack of experimental data, their low capacity and unavailability of group contribution parameters for most IL systems. The objective of this work is to establish a systematic solvent selection methodology for ED processes for the separation of aromatics/non-aromatics mixtures employing ionic liquids.

### A STUDY ON SIEVE TRAY LOWER OPERATING LIMIT

Ali Zarei, Rahbar Rahimi, Taleb Zarei, Nader Naziri

Sieve trays are widely used fractionating devices in separation and purification industries involving tray towers. According to the importance of trays, it is vital to predict lower operating range limits for such gas-liquid contacting devices. Weeping phenomenon observed in bubbling regime and occurs at low vapor flow rates. The experimental set up includes a 1.22 m diameter column with two test trays and two chimney trays. Hydraulic parameters and weeping rates were measured in sieve trays with 7.04 percent holes area. The model considers the tray's thickness and is able to calculate the dry tray pressure drop, total pressure drop, clear liquid height, froth height, and weeping rate simultaneously. Predicted results were in good agreement with the experimental data. This model is able to predict the trend of weeping even in higher rates where efficiency is reduced significantly.

### NOVEL MINIMUM REFLUX CALCULATION USING EIGENVECTOR MAPS

Ronald Abbas, Simon Holland and Ivar Halvorsen

Column Profile Map Eigenvectors (CPM-E) technique is introduced to determine the minimum energy demand for multicomponent feed in two-product distillation processes. The technique is a short cut, geometrical, non-iterative method and can be used to predict how the minimum reflux solution is related to the feed-component distribution for all possible operating conditions. The new method makes use of Column Profile Maps and the concept of "moving triangles" and develops co-linearity criteria based on the eigenvectors of the Jacobian of the separation vector evaluated at the feed composition. The CPM-E technique is a powerful tool that can be applied to complex column arrangements, such as Petlyuk or Kaibel Columns. The CPM-E approach is non-exclusive and can therefore be applied to any type of split, sharp or non-sharp, irrespective of the number of components. It will be shown that the CPM-E technique can be used to determine minimum reflux solutions quickly and effectively. From this, it is shown that three limiting product composition regions under minimum reflux conditions are present. The links between the CPM-E technique and the determination of minimum energy demand using Underwood's methods are explored.

### DISTILLATION BOUNDARIES IN TERNARY HETEROAZEOTROPIC SYSTEMS

Andrzej R. Królikowski

Distillation boundaries are created by saddle azeotropes and divide the composition space into distillation regions. In homogeneous mixtures the distillation regions overlap. The common area of two distillation regions is parametrically sensitive, and it determines the possibilities of crossing (at a finite reflux) the distillation boundaries defined for a total reflux or reboil ratio. In this study was scrutinized whether the distillation regions overlap in heteroazeotropic systems like in homoazeotropic systems. In order to see whether distillation regions overlap, such composition points of the products should be found, for which the rectifying profiles will end in different distillation regions. Calculations were performed for mixture classified under Serafimov's<sup>1</sup> topological class 3.1-2: ethanol – benzene – water.

### CFD SIMULATIONS OF FLOW, HEAT AND MASS TRANSFER IN THIN-FILM EVAPORATOR

Andrzej Kolek, Janusz Dziak and Lechoslaw Krolkowski

Mathematical model of the process that takes place during liquid solution evaporation in the vertical thin-film evaporator of static type was developed. The model consists of differential equations of flow, heat and mass transfer as well as boundary conditions. The model was applied for CFD simulations of water-propylene glycol solutions evaporation under reduced pressure. Axial symmetry approach was adopted. Two-dimensional distributions of water concentrations, temperature, pressure and velocities of liquid and gas were obtained.

## DEVELOPMENT & APPLICATION OF CONTINUOUS THERMODYNAMICS FOR STUDYING PHYSICOCHEMICAL PROPERTIES OF PETROLEUM FRACTIONS

Laura P. Tovar, Maria R. Wolf-Maciel, Cesar B. Batistella, Rubens Maciel-Filho, Alexandre de O. Gomes, Lilian C. Medina

Such a general practice in the petroleum industry, petroleum fractions (mixture of hydrocarbons) are divided into a group of narrow boiling range which enables to assign properties to these pseudocomponents. However, the tracking of all pseudocomponents of petroleum fractions would involve enormous computational efforts. This work presents an approach for characterizing the petroleum fractions as a continuous distribution functions. Continuous computations are developed where distilled volume data and the specific gravities are the input data; normal boiling point is the distribution variable and the distribution function is the boiling point curve that already had the temperature experimental data converted to atmospheric equivalent temperature – AET. Thermodynamic, transport and thermophysical properties are related to boiling point by well-established petroleum methods proposed by available correlations and industry standard methods. The computational results indicated that the continuous thermodynamic method is an accurate technique for predicting the physicochemical properties of petroleum fractions. Continuous thermodynamics provides a potentially useful tool for petroleum industry to increase the computational speed and accuracy because it is not necessary to characterize various families of hydrocarbons which may be present in the petroleum fraction.

## DESIGN OF FEED DISTRIBUTION SYSTEM IN A FALLING FILM DISTILLATION USING CFD

Joel G. Teleken, Leandro O. Werle, Iaçanã G. B. Parisotto, Cintia Marangoni, Ana Paula Meneguelo, Ricardo A. F. Machado.

This paper is about the analysis of the liquid discharge by falling film within a distillation tube. Specifically about some flow rates that can be used in this process, when we talk about film's discharge and maintenance. This aim of this paper is to study through simulations in CFD (Computational Fluid Dynamics) what influence the feeding flow rate has on the film's formation, its stability and thickness. This distillation process has low resistance to the liquid flow and high capability of separation, besides a simple construction unity. The commercial code used in order to solve the mathematical modeling was ANSYS CFX 12.0. The results obtained show that the best results achieved were low feeding flow rates, which provided a rather stable and continuous film and lower values of vapor superficial velocity.

## SHORTCUT METHODS FOR THE DESIGN OF HETEROAZEOTROPIC DISTILLATION OF MULTICOMPONENT MIXTURES

Korbinian Kraemer, Andreas Harwardt and Wolfgang Marquardt

Shortcut methods are valuable tools in the early stages of chemical process design, where numerous flowsheet alternatives need to be evaluated to determine the most energy-efficient, feasible flowsheet. Various shortcut methods based on tray-to-tray calculation and pinch point analysis for the inspection of feasibility and the determination of the minimum energy demand (MED) for homogeneous nonideal distillation have been published in the literature. Recently, Kraemer et al.<sup>1</sup> presented the feed pinch method (FPM) for heterogeneous azeotropic mixtures of any number of components. While the FPM returns an accurate representation of the MED, it still requires tray-to-tray calculations for one column section and it can only be applied to separations with a feed pinch, i.e. usually direct or indirect splits. In this work, we propose the feed angle method (FAM) which resolves both of these issues as it does not rely on numerous tray-to-tray calculations and can be applied to any kind of sharp split. The FAM is illustrated by ternary and quaternary heteroazeotropic separations with direct, indirect and intermediate splits.

### **SIMULATION OF ANHYDROUS BIOETHANOL PRODUCTION PROCESS USING EFFICIENCY CORRELATIONS FOR CONVENTIONAL AND EXTRACTIVE DISTILLATION**

Tassia L. Junqueira, Marina O. S. Dias, Maria Regina Wolf-Maciel, Rubens Maciel Filho and Carlos E. V. Rossell

In this work, simulations of the complete separation process in anhydrous bioethanol production were carried out in Aspen Plus<sup>®</sup>. This process comprises distillation and rectification columns as well as an extractive column. Equilibrium stage model and Barros & Wolf efficiency correlations were used to perform the calculations. Efficiency profiles were obtained for all columns showing that efficiency values significantly vary along the columns. Influence of the introduction of efficiencies was evaluated through comparison with equilibrium stage model (ideal process). Results pointed out that energy requirements are not significantly higher when efficiencies are taken into account; however stream results and temperature profiles were quite different from each other. This reveals that is necessary to consider efficiency changes along the column if reliable predictions are to be made.

### **DOUBLE COLUMN BATCH RECTIFIER IN CLOSED MODE FOR PRESSURE SWING BATCH DISTILLATION**

G. Modla

The double column batch rectifier in closed mode is presented for pressure swing batch distillation and it is investigated by feasibility studies and rigorous simulation using a professional dynamic simulator moreover it is compared with double column batch stripper in open mode. The calculations are performed for a binary minimum (acetone - methanol) azeotropic mixture. Results show that by the application of the closed mode energy saving can be realised.

### **PRODUCT COMPOSITION CONTROL OF A PRESSURE SWING DOUBLE COLUMN BATCH RECTIFIER**

Arpad Kopasz, Gabor Modla, Peter Lang

The pressure swing separation of a binary maximum azeotrope (water-EDA) in a double column batch rectifier is studied by rigorous simulation. For controlling the product compositions a simple scheme is presented. On the basis of temperatures of the top products PID controllers manipulate their flow rates varying the reflux ratios. The influence of the most important operational parameter (division ratio for the stream leaving the common bottom vessel) is investigated. For rigorous simulation calculations a professional dynamic flowsheet simulator is applied.

### **OPTIONAL OPERATION OF THERMALLY-COUPLED KAIBEL DISTILLATION COLUMNS**

Maryam Ghadrán, Ivar Halvorsen and Sigurd Skogestad

The objective of this paper is to study the Kaibel distillation column from operability point of view. Two different objectives, namely minimizing energy requirement at fixed product purities and maximizing product purities with a fixed boilup are considered. We have visualized the objective functions around the optimum. This can be used to get insight in column behavior and as a basis for control structure design.

## DEVELOPMENT OF A SYSTEM FOR THE DESIGN OF CONTROL STRUCTURES FOR DIVIDING WALL COLUMNS

Christina Buck, Georg Fieg, Virginia Green

The technology of dividing wall columns offers the possibility to save energy and investment costs compared to conventional distillation columns and their configurations. The practical use of the technology is still limited due to a lack of experience and high interactions between the process variables. The contribution focuses on a new developed appliance, named *ConStruct DWC*, for the model based and automated design of control systems for dividing wall columns. The architecture of *ConStruct DWC* is explained and the effectiveness is shown by the exemplary design and test of a control system.

## IMPROVED HIGH PERFORMANCE TRAYS

Stefan Hirsch and Mark Pilling

From a design and hydraulic standpoint, trays are relatively complex distillation internals. In the ongoing search for higher performance trays, one first must understand the hydraulic and mass transfer aspects of the tray operation such as entrainment, downcomer flooding, and vapor liquid contact. When this is well understood, then various aspects of the deck and/or downcomer designs can more easily be modified to achieve performance improvements. As a result of this process, Sulzer has developed a promising new design for a high performance distillation tray that demonstrates significant improvements in capacity over a broad range of air/water simulator operating rates. Depending on the operating region, capacity gains in excess of 10% have been verified in comparison to existing high performance trays. This paper will discuss design strategies and important tray operating parameters. Design characteristics of the new high performance tray will be presented and discussed. Test data from this new tray will be shown to demonstrate its improved performance.

## EXPERIMENTAL CHARACTERIZATION OF CERAMIC SPONGES AS COLUMN INTERNALS

Julia Große and Matthias Kind

Ceramic sponges are monolithic network structures with high specific surface areas at a low pressure drop compared to other ceramic column internals. The characterization of hydrodynamics as well as mass transfer in two phase counter-current flow is the basis for the comparison of sponges with other packings. Sponges of different material, pore size and porosity are thus evaluated concerning holdup, pressure drop and flooding behavior as well as gas and liquid side mass transfer coefficients and interfacial surface areas.

## MASS TRANSFER EQUIPMENT DESIGN CONSIDERATIONS FOR CRYOGENIC ABSORBERS, DEMETHANIZERS AND DEETHANIZERS

Glenn Shivelor, Daniel Egger, Tim Oneal

Cryogenic fractionators for natural gas liquids recovery plants have special design considerations for the mass transfer equipment owing to the fluid physical properties for fractionators that operate at high-pressure near the critical point. Over the years, the industry has equipped these NGL recovery units with trays and packings for tower revamps and new vessels. This paper considers the selection of packing, towers internals and trays for NGL recovery units. The mass transfer efficiency and hydraulic flow parameter of packing is shown for high-pressure distillation tests and plant operating data. The design of feed inlet devices and draws for the unusual fluid physical properties for these units is considered. The paper provides a comparison of equipment design strategies to cope with process issues such as sub-cooled feeds and hydrates.



### MEASUREMENT AND CORRELATION OF CLEAR LIQUID HEIGHT ON SMALL HOLE DISTILLATION SIEVE TRAY

L. T. Fan, X.G. Yuan, A. W. Zeng, K.T. Yu, M. Kalbassi and K. E. Porter

The present paper reports an experimental study in measuring the clear liquid height and its gradient along the flowing path direction of the liquid on an experimental tray with small sieve holes and of industrial-scale. The experiments were performed with water and air in a rectangular tray installed within a column of 1.2m inner diameter. The experimental results under various operating conditions are compared with a number of published empirical and semi-theoretical correlations. The models are recorrelated and suitable correlations for predicting the clear liquid height on small-hole sieve trays are recommended.

### ON THE DEVELOPMENT OF AN ENERGY EFFICIENT PACKING FOR VACUUM DISTILLATION

A. Shilkin, K. Heinen, C. Großmann, A. Lautenschleger, A. Janzen, E.Y. Kenig

This paper describes an approach to develop a novel structured packing for vacuum distillation, with superior characteristics compared to the conventional packings. The contribution of elementary pressure drop mechanisms to the heat and mass transfer is investigated using the complementary modelling at different levels of detailisation. The main objective of this study is to identify the "useful" and to eliminate the "useless" pressure drop mechanisms, thus reducing the energy input while keeping the same packing heat and mass transfer efficiency.

### ESTABLISHING A FACILITY FOR THE HYDRODYNAMIC CHARACTERISATION OF DISTILLATION COLUMN INTERNALS

E.C. Uys, S.M. Lamprecht, C.E. Schwarz, A.J. Burger, I. Nieuwoudt and A.B. Erasmus, J.H. Knoetze

A better understanding of the hydrodynamics related to flooding conditions in distillation columns is required in order to provide optimised designs for new plants and plant retrofits. Current flooding prediction correlations are predominantly based on air/water systems and tend to diverge at high vapour capacities. In this work an experimental setup was designed and constructed to test the hydrodynamic characteristics of random – and structured packing as well as sieve – and valve trays. The experimental setup is used to develop a better understanding of the influence of gas and liquid properties on entrainment and column flooding. The experimental setup was tested with an air/water system and the tray entrainment data followed the trends from Bennett *et al.* **Fout! Verwijzingsbron niet gevonden.** quite well. The packed column yielded the correct trends on both pressure drop and liquid hold-up data which correlated reasonably well with the general model proposed by Piché *et al.* **Fout! Verwijzingsbron niet gevonden.**

### COMMERCIAL SCALE TEST VALIDATION OF MODERN HIGH PERFORMANCE RANDOM AND STRUCTURED PACKINGS FOR CO<sub>2</sub>-CAPTURE RANKING

Michael Schultes, Simon Chambers, Brad Fleming

To meet the goal of optimized CO<sub>2</sub>-Capture performance from Power Plant flue gas, high capacity/high mass-transfer-efficiency/low pressure drop modern packings are required. To support this claim, hydraulics-efficiency research from Total Reflux Distillation tests in the Commercial/Pilot Test Columns at Fractionation Research Incorporated (F.R.I.) and at the Separations Research Program (SRP) was performed. Additional research to measure pressure drop with the air-water system and mass transfer measurements from CO<sub>2</sub> absorption supplement the findings from distillation testing.. The results show distinct performance advantages of modern high performance metal random and structured packings over the current state-of-the-art packings. The data presented will validate the necessity of such test campaigns so as to rank packings most suitable in CO<sub>2</sub> Absorption/Stripping processes. The packings involved in the comparison studies are Raschig Super-Ring<sup>®</sup> random packings, various sized Pall Rings<sup>®</sup> and Third Generation random packings; Raschig Super-Pak<sup>®</sup> structured packings, Sulzer Mellapak<sup>®</sup> including Mellapak-Plus<sup>®</sup>, and the Montz B1<sup>®</sup> packing types.

### EXPERIMENTAL INVESTIGATIONS ON BIODIESEL AS AN ALTERNATIVE ABSORBENT FOR THE RECOVERY OF AROMATIC HYDROCARBONS UNDER INDUSTRIAL CONDITIONS

Michael Th. Müller, Holger Thielert, Diethmar Richter, Jens-Uwe Repke, Günter Wozny

The recovery of aromatic hydrocarbons from coke oven gas is of great economic interest. Therefore experimental investigations on a promising alternative absorbent, biodiesel were carried out under industrial conditions with the aim of determining the performance and proving its applicability for the BTX-removal. For this purpose a mobile mini plant was constructed at the Berlin Institute of Technology and installed at the coking plant ZKS at Dillingen/Saar, where it was integrated into the industrial process and set into operation. Some of the main experimental results proving the applicability of biodiesel are shown in this contribution.

### REACTIVE ABSORPTION OF CO<sub>2</sub> IN MEA: A SCALE-UP STUDY

Chinmay Kale, Anja Müller, Inga Tönnies, Hans Hasse, Andrzej Górak

Post combustion capture of CO<sub>2</sub> is an important method to combat global warming. Reactive absorption of CO<sub>2</sub> using amines is one of the most attractive options for CO<sub>2</sub> removal in flue gases. Absorption of CO<sub>2</sub> in aqueous MEA (mono ethanolamine) is a widely studied reaction system for many years now, although the studies are limited to laboratory scale and in-silico analysis. Hence, a scale-up study is undertaken in order to commercialise the technology for a broader application. In this respect, a rate based model in Aspen Custom Modeller<sup>®</sup> (ACM) was modified and is being validated with experimental results taken from TU Kaiserslautern. A rate based model was used to simulate the CO<sub>2</sub> absorption in a packed column. Model considers actual chemical kinetics and its effects in absorption process. In the model, each stage is described using two film theory. On each stage, thermodynamic non-idealities, heat transfer, mass transfer of multi-component systems, cooling effects and influence of column internals were taken into account. It was assumed that reaction is taking place only in liquid phase and the liquid film is discretised into small segments for detailed analysis. The model is validated using experimental results in a pilot absorption column at TU Kaiserslautern. It was found that the model can predict the results of experiments with good accuracy. A good agreement was seen for temperature and concentration profiles over the height of the column. Agreement of the model results with experimental results is an important step in scale-up study of the reactive absorption of CO<sub>2</sub>. Thus, the model can further be used for scale-up studies and to validate the experimental results in the scale-up studies.

### AN EQUILIBRIUM BEHAVIOUR OF A NOVEL GAS SEPARATION PROCESS, WITH APPLICATION TO CARBON CAPTURE

Martin Sweatman

A novel gas separation process<sup>1</sup> is described and analysed in the context of carbon capture. It involves a highly selective absorbent fluid below its saturation pressure pre-mixed with the gas to be separated and adsorbed into a porous solid. This fluid mixture simultaneously forms gas-like and liquid-like regions within the porous solid depending on the pore size. The gas component to be separated is selectively absorbed by the liquid-like regions, and a novel 'pressure-swing wetting layer absorption' process is used to recover the absorbed gas. This work examines the equilibrium behaviour of this process in the context of carbon capture using the density functional theory (DFT) of classical fluids. The DFT model employed represents the porous solid in terms of ideal graphitic slit-pores, and a ternary fluid model is calibrated to represent mixtures of tetrahydrofuran (the absorbent fluid), carbon dioxide and nitrogen. Under the conditions investigated here we find that the equilibrium behaviour of this system is superior to the analogous pressure-swing adsorption process without solvent. More accurate studies involving Monte-Carlo molecular simulations confirm this behavior. These results motivate further experimental and dynamical process modeling studies of this system.

## CHALLENGES AND OPPORTUNITIES FOR POST-COMBUSTION CO<sub>2</sub> CAPTURE IN AUSTRALIA

Paul H. M. Feron

CSIRO has developed a post-combustion CO<sub>2</sub> capture (PCC) R&D program consisting of two major components which are operated in an integrated manner: The pilot plant program is aimed at providing hands-on-experience for future operators of PCC plants. The application of emission controls (DeNOx and FGD) in the EU, USA and Japan has given those power station operators a familiarity with chemical process technology. There have been no large scale chemical processes applied in the Australian power industry for chemical process experience to be developed. The pilot plants will provide an important opportunity for the industry to gain experience in these types of technologies before going to a large scale. In addition to this the pilot plant program will result in the identification of operational issues and detailed understanding of the technology requirement. These issues can be resolved at an early stage and if not straightforward they will lead to the specification of research tasks. A pilot plant operating on real flue gas will also be a testing ground for novel technologies/solvents brought forward by laboratory based research, as these technologies can be tested under realistic flue gas conditions (temperature and composition). The laboratory research program includes the development of novel chemical absorbents and novel processes for post-combustion capture including the integration with the power plants. Overall, the program is designed to reduce both the capital and operating costs of CO<sub>2</sub> capture under Australian conditions by determining optimum liquid absorbent and process configurations. The laboratory based research program will also support the pilot plant program operation through the provision of analytical services. It provides support to the interpretation of research results through e.g. process modeling and detailed chemical analysis and results assessment. The research program is also the starting point for the development of novel chemical absorbents and novel process concepts, which when deemed to be sufficiently qualified can be rolled out to the pilot plants. Within this research the Australian specific requirements related to the flue gas quality and the water limitations are also addressed.

## OPTIMISATION BASED DESIGN OF MEMBRANE ASSISTED HYBRID SEPARATION PROCESSES USING AN EVOLUTIONARY ALGORITHM

Katharina Koch, Daniel Sudhoff, Stefan Kreiß, Peter Kreis

Separation of non-ideal multicomponent mixtures is an immanent part of most of the processes in the chemical industry. By combining distillation and membrane separation to a hybrid process, limitations of at least one of the unit operations involved can be overcome and therefore investment and operational costs can be reduced. In this paper, the development of a generic process design method for the separation of an azeotropic ternary system is shown and demonstrated for a mixture of acetone, isopropyl alcohol and water. The optimisation approach is based on a sophisticated model of distillation considering multicomponent mass and heat transfer and fluid dynamics, and a rate-based model for membrane separation, which is based on the solution-diffusion-model and accounts for all transport resistances. The parameters for prediction of transmembrane flux are determined in lab-scale experiments. The parameter determination using an empirical correlation for the calculation of permeances using the difference of fugacities as driving force shows a very good agreement between calculated and measured permeate fluxes. Using these results for the description of the membrane separation, a superstructure for a hybrid separation process consisting of one distillation column and one pervaporation module was developed and optimised with the above described method. The optimisation criterion are the costs for the purification of one ton of acetone as objective function. The results show, that the developed optimisation methodology is already applicable for a complex design problem with the simultaneous optimisation of 3 discontinuous and 9 continuous variables.

## HOW TO SEPARATE TWO NEAR AZEOTROPES. CASE OF THE SEPARATION OF THE MIXTURE PHENOL – HYDROCARBONS

Florin Oprea

The paper presents a new process for phenol separation from the mixture phenol-hydrocarbons using azeotropic distillation with water. The mixture phenol-hydrocarbons is obtained at the top of one column in the separation system of an acetone-phenol plant. In this moment, there are three processes for this separation: (1) extraction with NaOH aqueous solution, (2) process for simultaneously phenol removal/recovery from the mixture phenol-hydrocarbons and aqueous solution (phenol waters) and, (3) extractive distillation with DEG. Like an alternative at these processes, it is proposed a new process with a very simple flow sheet. It is used only one column, at atmospheric pressure, with a small number of trays and like entrainer, water, easy to find and, practically, free of charge. The proposed process is based on idea of separation of the two azeotropes formed by water with phenol and hydrocarbons. Even if the difference between boiling temperature of these azeotropes is small, their separation is easy. In addition, the separation of water from the two azeotropes is easy (practically, the aqueous solution of phenol is recycled in the process, and the hetero-azeotropes water-hydrocarbons are separated in water and hydrocarbons, water being the entrainer). Based on NRTL parameters obtained from experimental vapor liquid equilibrium in the system cumene-alpha-methyl styrene, it done a complete simulation model using PRO/II programe. The great numbers of simulations lead to an optimum concerning number of trays and water/entrainer consumption. In addition, linking simulation and experimental results, it was determined the HETP for a Sulzer packing used in this column. The results of the process simulation were verified on a lab column and on an industrial column. The proposed process is simple, easy to put in practice, easy to control. The necessary number of trays is small, the entrainer is very common. The process can replace older processes. A Romanian patent was granted.

## REACTIVE DISTILLATION FOR SELECTIVITY IMPROVEMENT IN THE TRANSESTERIFICATION OF DIMETHYL CARBONATE

Tobias Keller, Alexander Niesbach, Achim Hoffmann, Andrzej Górak

Reactive distillation (RD), where reaction and separation are integrated in one single unit operation, is one of the most known examples of process intensification. In this work, the reversible consecutive second-order transesterification of dimethyl carbonate (DMC) with ethanol via ethyl methyl carbonate (EMC) to diethyl carbonate (DEC) was investigated. Up to now only theoretical investigations about the transesterification of DMC in a RD column have been published<sup>1</sup>. In this work, the potential of RD to enhance the selectivity of consecutive reactions has been demonstrated experimentally. Since no suitable heterogeneous catalyst for DEC synthesis has been found yet, a homogeneously catalysed transesterification of DMC using sodium ethoxide was selected for our study. Due to the high activity of the catalyst, chemical equilibrium is reached after a few minutes at reaction temperature (6 min at 70°C). A rate-based approach<sup>2</sup> was used for a modelling of the DEC synthesis in a reactive distillation column. The homogeneously catalysed transesterification was carried out in a packed column. Because of the considerable liquid holdup in distributors the model takes also the chemical reaction in distributors into account. It has been experimentally proven that they behave like ideal continuous stirred tank reactors. Temperature and concentration profiles along the pilot RD column were measured. The column has an inner diameter of 50 mm, is equipped with Sulzer BX packing elements providing a total packing height of 5.4 m. The steady-state condition was monitored by an 'online data reconciliation' and was reached after 12 h. Since the temperature in the vapour phase is measured and there are eight samples taken along the column height, the experimental setup provides a detailed internal column profile to properly validate the process model. A satisfactory agreement between experiment and simulation was achieved.

## MODELLING AND SIMULATION OF THE TAEЕ SYNTHESIS BY CATALYTIC DISTILLATION

C. A. González-Rugerio, W. Sałacki, J. Pilarczyk, P. Kreis, A. Górak

Tertiary ethers have become important additives for gasoline over the last decades. They are mainly used to enhance the octane number of gasoline, but they also improve the combustion and reduce emissions. Methyl tert-butyl ether (MTBE) is the most common oxygenate used in gasoline blending. However, it has been detected in groundwater and therefore, the production of other oxygenated compounds, such as tertiary-amyl ethyl ether (TAEЕ) is of present interest. The modelling and simulation of the TAEЕ synthesis from isoamylenes (IA) fraction and ethanol in a reactive distillation (RD) column is carried out. Components of the fraction were merged into groups and were represented by one chemical compound. 18 components and 6 chemical reactions were selected to represent the system, based on their content in the fraction, reactivity and ability to create azeotropes. Kinetics were taken from literature<sup>1,2</sup>. Besides the reactions of TAEЕ synthesis, the formation of tert-hexyl ethyl ether and the dimerization of IA were considered. A non-equilibrium stage model based on the Maxwell-Stefan approach was applied<sup>1</sup>. Hydrodynamic influences were taken into account by using packing-specific correlations. Non-idealities of the liquid phase were described with the UNIFAC method. An excellent agreement between experiments and simulation results for the main components was obtained. Somewhat more significant deviations appear in the composition profiles of inert hydrocarbons. Neither IA nor ethanol was present in the bottom of the column. The composition of TAEЕ in the bottom is low (~ 23% mole) due to its low reaction rate and high composition of inert components in the system. Optimal operating conditions were found to obtain the highest conversion (based in the inlet to the column) of IA (~ 40%) for the investigated column configuration. Multiplicity of steady states (MSS) has been detected. The modelling and simulation of the TAEЕ synthesis in a RD column was carried out. Simulation studies revealed a maximum conversion for different operating parameters, such as pressure, distillate to feed, reflux and molar ethanol/IA ratios. It was found that the influence of reflux in the system is relatively small but not the influence of the other parameters. MSS was found.

## MULTI-EFFECT DISTILLATION – WETTABILITY OF POLYMERIC FALLING FILM HEAT TRANSFER SURFACES

Jochen B. P. Christmann, Lorenz J. Krätz and Hans-Jörg Bart

Multi-effect distillation (MED) with falling film evaporators is a well-established process in seawater desalination. Against the background of increasing prices for metals and shortage of resources, polymeric materials might be a low cost and less corrodible alternative to metals for energy efficient falling film heat transfer. One drawback of polymers for falling film applications, with regard to the MED-plants, is their poor water-wettability. Moreover, wettability of polymer surfaces is also an important aspect in distillation columns and trickle bed reactors with polymer packings. The high performance polymer polyetheretherketone (PEEK) was chosen as test material. The main research focus was set on water-wettability of the surface. Therefore, the PEEK film wettability was characterised by contact angle measurements with water, ethylene glycol and diiodomethane. Consecutive calculations of surface free energies were performed with the model of Owens<sup>2</sup>, Wendt<sup>2</sup>, Rabel<sup>3</sup> and Kaelble<sup>4</sup> (OWRK) as well as with the more sophisticated model of van Oss et al.<sup>5,6</sup>. These calculation results were utilised to create wetting envelope diagrams. The obtained results show that pre-treatment by conditioning of PEEK films in water leads to an effect similar to plasma pre-treatment. Both result in an improved surface wettability with water. The OWRK surface free energy model shows an increase of surface free energy's polar part due to pre-treatment. Furthermore the surface free energy model of van Oss et al. reveal that the acidic contribution of surface free energy is negligible and stays almost the same after plasma treatment and conditioning in water, respectively. However, the basic contribution of surface free energy is increasing in both cases. In the case of pre-treatment by conditioning in water, this is an indication for a structural rearrangement of polymer chains at the polymer surface. It could be explained by reorientation of benzene rings, which exhibit a monopolar basic character due to the electron donor behaviour of their  $\pi$  electrons.

## HYDRODYNAMICS OF LIQUID FLOW IN THE MODEL OF THEORETICAL STAGE WITH PERFECT DISPLACEMENT

Vladimir Maleta, Vitaliy Taran and Bogdan Maleta

According to Lewis [1], the theoretical use of combinations of various hydrodynamic models of liquid and steam stages enhances the efficiency of components separation on the tray. The highest effect is achieved upon perfect displacement by liquid and vapor and single-direction movement of liquid on adjacent contact stages. The objective of the present work is determination of interrelation between hydrodynamic models of contacting phases for both modes with theoretical models of mass transfer in column apparatuses. It is generally accepted that the theoretical stage of McCabe-Thiele's contact is depicted in coordinates  $(x, y)$ . In this case the hydrodynamic model of liquid flow is reduced to the perfect mixing model. The process operating line is discrete, and the operating line points (trays) coordinates shall be recorded as  $(x_i, y_i)$ . For determination of concentration fields in steam and liquid phase upon perfect displacement (cyclic mode) and balance between vapor and liquid the numeric solutions of non-linear system of the material balance differential equations is used. The obvious functions received as a result of calculation  $(x, y)$ , shall be depicted in coordinates  $(x, y)$  as the perfect displacement operating line. The operating line coordinate points shall be determined  $(x_i, y_i)$  for random time  $t_i$  at the vapor supply time period  $\tau$ . Therefore, the line shall be depicted by definition as a line of points of meeting of vapor rising from the below tray with liquid on the above tray. The line is uninterrupted and straight for the case of  $\tau \rightarrow 0$ . The tangent of inclination of the perfect displacement operating line is less than the values  $\tan \alpha$  which determines the process efficiency. The contact stage built on this line is a theoretical stage of perfect displacement contact. The difference between cyclic and stationary processes consists in change of the coordinate system upon separation. The hydrodynamic model of the liquid flow in cyclic mode during vapor supply is determined solely as a perfect displacement model. Upon overflow of liquid from tray to tray the liquid flow hydrodynamics determines only distribution of components on the trays as of the beginning of vapor supply period. The theoretical contact stage and theoretical stage of the perfect displacement contact are the ultimate cases of the liquid flows hydrodynamic models of the same name. In industrial conditions the adequacy of Lewis' model cyclic process with separation efficiency according to Murphree as 200-300%, significantly exceeds any constructive solutions for stationary process.

## PROCESS DESIGN FOR MICRO-STRUCTURED DISTILLATION DEVICES

B. Dercks, G. Schmidt, M. Grünwald

Micro process technology is based on the processing of fluids inside small volumina, typically inside channels with diameters of less than 1 mm. Previous research activities concentrate on the area of micro reactors, micro mixers and micro heat exchangers. Only few publications deal with the topic of separation processes in micro structured devices, although unit operations like absorption, extraction and distillation conducted in micro channels are inevitable to realize a complete chemical production process. Our contribution will review the limits and opportunities of fluid-fluid based unit operations in micro channels and will focus on distillation in particular. The analysis is based on simulation studies with a rigorous process model assuming laminar flow behavior in both phases, mass transfer from and to the interphase by diffusion and pressure drop along the flow through the channels. The set of model equations allows the computation of both the more or less direct contact of the phases and the indirect contact through a membrane. The results reveal that the width of the operating window depends on the design of the micro-channels. Especially the pressure drop resulting from the choice of height and wide of the cross-sectional area limits the achievable number of transfer units per device due to Gibbs phase rule. Accordingly simulation studies have been carried out to design promising sequences of single distillation devices for the separation of a two component mixture.