Conference Program

20-22 November, 2018

Abu Dhabi, UAE

ICFMCE 2018

2018 2nd International Conference on Functional Materials and Chemical Engineering

Welcome

Dear Distinguished Participants,

Welcome to 2018 2nd International Conference on Functional Materials and Chemical Engineering (ICFMCE 2018)

After one-year painstaking preparation, we're delighted to declare that ICFMCE 2018 organized by IASED will be held at Khalifa University, Abu Dhabi, UAE as scheduled.

First of all, we'd like to express our sincere gratitude for your participation, which is the vital note to make the conference a great forum for the collision and fusion of ideas and knowledge. Besides, we'd like to say that the kind help and great efforts offered to our conference by our conference chair Prof. Rafiqul Gani is greatly appreciated. Meanwhile, we also appreciate our local chair, Prof. Ali El Kamel, plenary speakers, Dr. Steven Griffiths, Prof. Jay H Lee and Prof. Stratos Pistikopoulos and our Keynote Speakers who will share their newest and outstanding research achievements on the conference site.

In this big data age, the ever-changing information technology has updated and revolutionized the structure and content of our knowledge. The aim as well as the objective of ICFMCE 2018 is to present the latest research and results of Functional Materials and Chemical Engineering. By providing opportunities for the delegates to exchange new ideas face-to-face, to establish business or research relations as well as to find global partners for future collaborations, we do hope that the conference will intensify mutual improvement and facilitate academic exchange, as a result that leading to significant contributions to the knowledge in these up-to-date scientific fields.

Finally, we wish ICFMCE will be held with a complete success. At the same time, we wish you enjoy a very splendid time during the conference days in the impressive city of Abu Dhabi, UAE!

Thank you!

Sincerely,

ICFMCE 2018 Committee

❖**Registration**

The registration desk will be situated at **Room 1013, Building 1, the Petroleum Institute, Khalifa University, Abu Dhabi** during the following time:

13:00-17:00, Tuesday, 20 November, 2018.

❖**Remarks:** Conference will provide free coffee breaks**,** lunch and dinner, beyond the fixed menu will be on bill.

❖**A Polite Request to All Participants**

Participants are requested to arrive in a timely fashion for all addresses. Presenters are reminded that the time slots should be divided fairly and equally by the number of presentations, and that they should not overrun. The session chair is asked to assume this timekeeping role and to summarize key issues in each topic.

❖**Prayer Room**

There is a prayer room (Room 103). There is another prayer room in the next building (Building 2) and there is a Mosque on campus.

❖**Dress Code for Conference:** Formal or National Custom

❖**Dress Code in Khalifa University:**

Visitors, irrespective of religion or nationality should dress in a modest and appropriate manner on campus. It is required that every visitor respects the norms of UAE society and he/she should not dress in a way that may offend cultural sensitivities and/or may not be within acceptable general taste.

The following points must be observed regarding visitors dress at the University campus. It is noted,however, that special protective clothing for laboratories shall be worn as necessary.

Male Visitors Dress Code

1. Male visitors must wear a shirt and long trousers/jeans. Shorts and sleeveless shirts must be avoided.

2. Clothes displaying offensive/objectionable writings/drawings/pictures must be avoided.

3. Visible tattoos and piercings must be avoided.

Female Visitors Dress Code

1. Female visitors must dress conservatively wearing long-sleeved shirts/blouses with long and loose fitting skirts/slacks, or a long-sleeve loose fitting long dress.

2. Shorts, short skirts and sleeveless/low-cut neckline shirts must be avoided.

3. Clothing that is tight, transparent, or short and shows too much skin or exposes the waist, back, or legs must be avoided.

4. Clothes displaying offensive/objectionable writings/drawings/pictures must be avoided.

5. Visible tattoos and piercings must be avoided. This does not include generally acceptable items such as earrings and henna.

❖Certificate

Certificate of Attendance

A certificate of presentation indicates a presenter's name, affiliation and the paper title that is presented in the scheduled session, certifying the paper has been presented on the conference site.

Certificate of Best Paper & Best Student Paper & Best Poster

Presenters who presents a great oral presentation or poster presentation will be awarded as the Best Paper, the Best Student Paper or the Best Poster. The conference chair or the session chair will award a certificate of Best for them in the award ceremony on 22 November, 2018.

Certificate Distribution

Oral presenters will receive a certificate of presentation from the session chair at the end of your presentation.

Poster presenters will receive a certificate of presentation from the conference chair at the poster session.

Listener will receive a certificate from the conference chair at the end of the conference.

❖**Preparation for Oral Presentations**

All presentation rooms are equipped with a screen, an LCD projector, and a laptop computer installed with Microsoft Power Point. You will be able to insert your USB flash drive into the computer and double check your file in PowerPoint. We recommend you to bring two copies of the file in case that one fails. You may also connect your own laptop to the provided projector; however please ensure you have the requisite connector.

Regular Oral Session: about 10 minutes of Presentation, 2-5 minutes of Q&A.

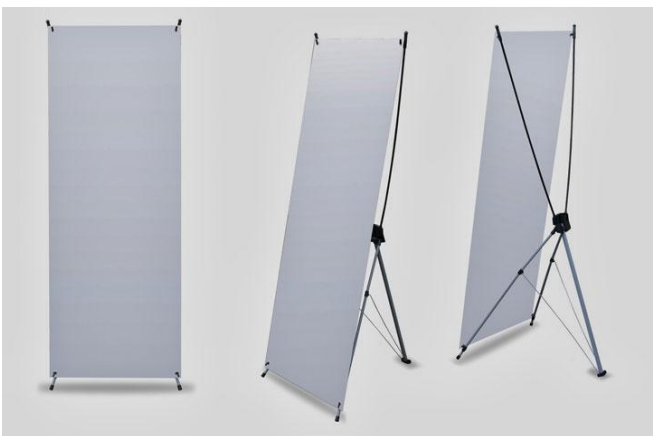
❖**Preparation for Poster Presentation**

Materials Prepared by the Conference Organizer:

Adhesive tapes

Materials Prepared by the Presenters:

Home-made poster (s)
Material: not limited, can be posted on the canvases.
Recommended poster size: weight*height: 56*86cm..



Building 1 (Zarkuh), Petroleum Institute(SAN Campus), Khalifa University (جامعة خليفة)

Address: Umm Al Nar, Near Al Maqta Bridge, Abu Dhabi, UAE

SAN Campus, Khalifa University (Umm Al Nar, Near Al Maqta Bridge, Abu Dhabi)

The Petroleum Institute University and Research Center (PI), as it was initially known, was established in 2001 to support the oil and gas industry of Abu Dhabi and the wider UAE. To achieve that goal it developed and offered undergraduate and graduate engineering and research programs in areas of significance to the oil, gas and broader energy industries.

The Petroleum Institute campus is also now rebranded as the Sas Al Nakhl Campus of Khalifa University.

❖

24° 25'12.7"N 54° 30'07.0"E

24.420197, 54.501933

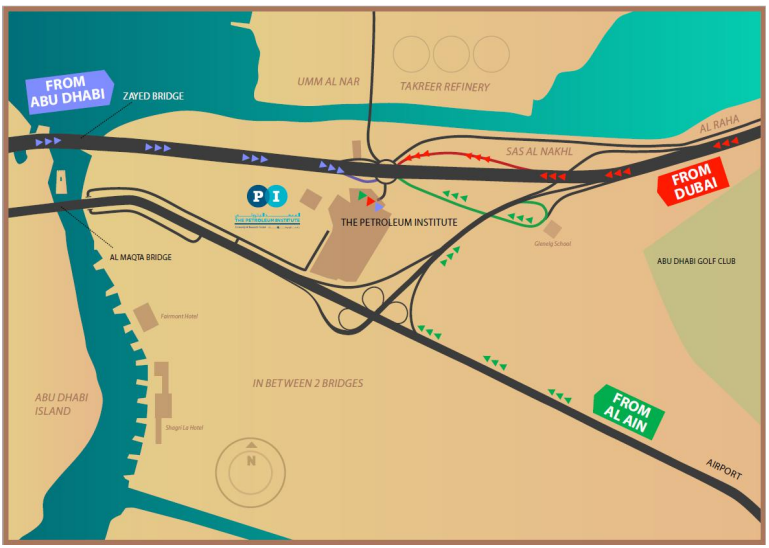
❖**Transportation**

From Abu Dhabi International Airport to the Petroleum Institute, Khalifa University

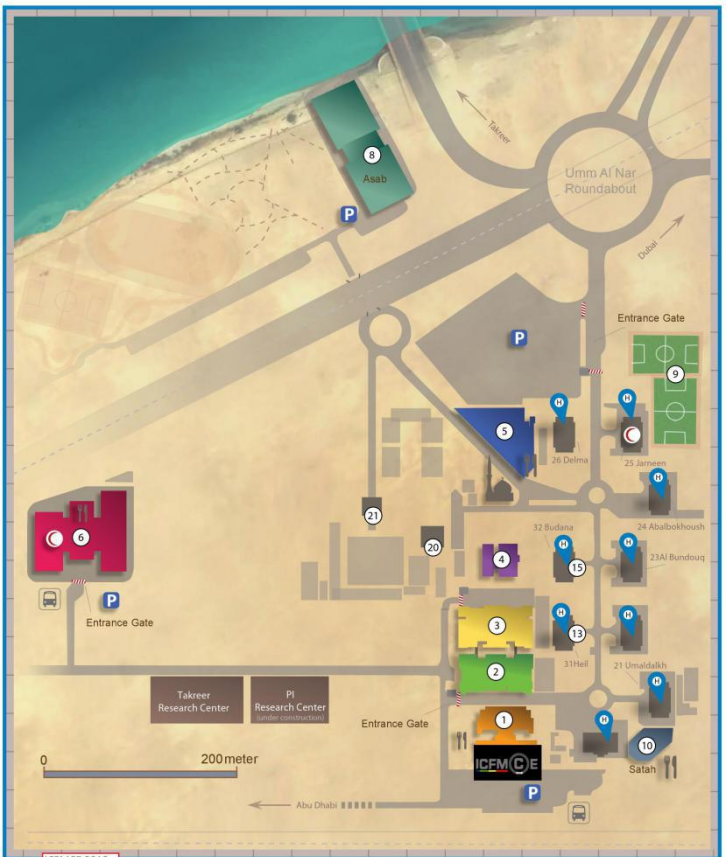
To get to Khalifa University's SAN Campus the trip duration will usually take around 17 minutes from Abu Dhabi International Airport. Note if you are coming from Dubai the travel duration will be around 1 hour and 30 minutes by car.

By Taxi

To get to SAN Campus there are couple of roads to take. Specifically through the two bridges of Al Maqta and Mussafah leading into Abu Dhabi, Capital of the United Arab Emirates.



The Petroleum Institute Campus Map



Time		
1300-1700	Registration (**Room 1013**)	
1645-1745	Reception (**Auditorium and Room 101**)	
1745	**Opening Session (ADCO Auditorium)**	
1745 (Welcome Address)		Dr. Arif Sultan Al Hammadi Executive Vice President Khalifa University
		Prof A Elkamel Local Chair, ICFMCE 2018 Khalifa University
		Prof R Gani ICFMCE 2018 Chair PSE for SPEED Company
1800-1845 (Plenary)	**Session Chair: Prof Gani** **Room 1 (ADCO Auditorium)**	
		Dr S Griffiths Khalifa University of Science & Technology, Abu Dhabi, UAE *System design for achieving very high shares of renewable electricity*
1900	End of Session	

Time	Parallel Session	
0900-1000 (30-min Keynote)	**Session Chair: Prof E Zondervan**	
		Prof E Zondervan University of Bremen *Design of bio-based supply chains*
		Dr B Sarup AlfaLaval-Denmark *Feedstock and pre-treatment processing options for production of HVO biofuels*
1000-1045 (15-min Oral)	F043	LKK Maia Univ Bremen Energy storage in the context of grid flexibility: A Case Study of the German electricity grid
	F040	Dr OW Lukman PT Badak-Indonesia Amine circulation rate optimization of gas purification unit in LNG Plant Bontang
	F064	Shahid Rabbani, Hamid Abderrehmane, Mohamed Sassi Masdar Institute, KU Comparative Study of effect of water, gas and foam flooding on enhanced oil recovery (EOR)
1045-1100	***Break* (ADCO Auditorium and Room 101)**	

1100-1140	**Plenary Lecture**	
	Session Chair: Prof Pistikopoulos	
		Prof JH Lee KAIST, South Korea *Analysis of CO_2 capture and utilization technologies for sustainable carbon management*
1145-1215	5-min oral presentations by poster authors (parallel)	
	Session Chair: Prof P Liu	
	P1 (F001)	Dr. HAMMOUDA Nadia Université du 20 Août 1955- Skikda, Algeria Effect of Surface Treatment by Sandblasting on the Quality and Electrochemical Corrosion Properties of a C-1020 Carbon Steel used by an Algerian Oil Company
	P2 (F013)	Nashwa El.Tahhan University of the Witwatersrand, South Africa Adsorption of Zn (II) and Cu (II) Ions from Wastewater Using Water Hyacinth (Eichhornia Crassipes)
	P3 (F027)	Nicodemus Kure Kaduna State University, Kaduna Nigeria Construction and Synthesis of Carbon Nanostructures via Household Microwave Oven
	P7 (F046)	Amel GHARBI Research Center in Industrial

		Technologies (CRTI), Algeria Abrasion wear behavior of A105N steel after heat treatment at different temperatures (500, 600, 700, and 800 °C)
	P11 (F051)	Sammia Shahid Department of Chemistry, School of Science, University of Management and Technology, Pakistan Antidiabetic Activity of Extracts of Pistachia khinjuk on Alloxan monohydrate Induced Diabetic Mice
	P12 (F058)	Dr. Ozhet Mauit National Laboratory Astana, Nazarbayev University, Kazakhstan Growth of ZnO:Al by atomic layer deposition: Deconvoluting the contribution of hydrogen interstitials and crystallographic texture on the conductivity
	P14 (F056)	Dr. Olzat Toktarbaiuly Department of Chemical Engineering, Khalifa University of Science & Technology, UAE Large scale fabrication of $PtSe_2$ thin film by physical method
	P15 (F016)	Rajakumar Devarapalli Masdar City Campus, Khalifa University, Abu Dhabi, UAE Investigation of Petro-Physical Properties at Different Scales: Numerial and Experimental Approach

1215-1300	***Lunch* (Cafeteria near Building 1)**	
1300-1400	Poster Session (Poster presentation and discussion at the poster display) **(Outside ADCO Auditorium)**	
1400-1530 (30-min Keynote)	**Parallel Session**	
	Session Chair: Prof MH Wang	
		Prof F Manenti Politecnico di Milano *Acid gas to syngas™ (AG2S™) technology for CO_2 utilization: from theory to industrial applications*
		Prof MH Wang University of Sheffield *Process and Energy Systems Engineering: CCUS and beyond …*
		Prof SB Anne National Institute of Technology – Warangal *Energy efficiency and CO_2 management*
1530-1545	***Break* (ADCO Auditorium and Room 101)**	
1545-1645 (15-min Oral)	F019	Dr V Ramsagar NIT Warangal Integration of a Calcium looping system for CO_2 capture in an Indian natural gas fired combined cycle power plant: A feasibility study
	F031	Dr E Oko University of Sheffield

		Experimental study of CO_2 solubility in high concentration MEA solution for intensified solvent-based carbon capture
	F057	HA Balogun Khalifa University Roles of microalgae in CO_2 management: A modeling approach
	F022	D. Bahamon & Lourdes F. Vega Khalifa University Tuning adsorbent materials to optimize CO_2 capture at industrial conditions
1645-1730	**Plenary Lecture**	
	Session Chair: Prof Lee	
		Prof EN Pistikopoulos Texas A&M University, USA *Multi-scale Energy Systems Engineering*

❖**All coffee breaks will be in the ADCO Auditorium and Room 101**

Time	Parallel Session	
0900-1000 (30-min Keynote)	**Session Chair: Prof L Zhang**	
		Prof L Zhang Dalian University of Technology *An optimization-based computer-aided molecular and mixture design framework*
		Prof MR Eden Auburn University *Component based development of computer-aided tools for different applications*
1000-1045 (15-min Oral)	F063	K Rambabu, G Bharath, Anjali Achazhiyath Edathil, Priyabrata Pal, Fawzi Banat Khalifa University Green synthesis of zinc oxide nanoparticles using Tamarindus indica leaves and its application for dye ultrafiltration
	F037	Prof C Kiparissides CERTH, CPERI From molecular to plant scale computer aided design of polymer manufacturing processes
	F067	Samah E.E Warrag Khalifa University Capturing Impurities from Oil and Gas Using Deep Eutectic Solvents

1045-1100	***Break* (ADCO Auditorium and Room 101)**	
1100-1140	**Plenary Lecture (ADCO Auditorium)**	
1145-1215	5-min oral presentations by poster authors (parallel)	
	Session Chair: Prof SB Anne	
	P4 (F042)	Touati Souheila National polytechnic school Constantine (ENPC) Genie Process Department, Algeria Formulation and Caracterisation of Controlled Release Ketoprofen Microsponges
	P5 (F044)	Asst. Prof. Dr. Heungjo An Khalifa University of Science and Technology, UAE Simulation modeling for the closed-loop shipping system to transport petrochemical products from a manufacturing plant to international ports
	P6 (F045)	Yechan Choi KAIST, South Korea Integrated management of chemical product manufacturing and maritime inventory routing in the shipping system under various sources of uncertainty
	P8 (F047)	Oualid GHELLOUDJ Research Center in Industrial Technologies (CRTI), Algeria Structural and tribological behavior of AISI L6 tool steel
	P9 (F049)	Assoc. Prof. Daniele Previtali Politecnico di Milano, Italy

		Hydrogen Recovery by AG2S™ Technology to Improve Hydrofinishing Process in Exhausted Oil Refineries
	P010 (F050)	Asst. Prof. Gowri Sundaram Department of Physics, Cauvery College for Women, India A Study On Second Harmonic Generation Efficiency On Organic Dopant KHP Crystal
	P13 (F061)	Arjun Ravikumar Department of Chemical Engineering, Khalifa University of Science & Technology, UAE Process Simulation and Modelling of Air Cooled Condenser Using Aspen EDR
1215-1300	***Lunch* (Cafeteria near Building 1)**	
1300-1400	Poster Session (Poster presentation and discussion at the poster display) **(Outside ADCO Auditorium)**	
1400-1530 (30-min Keynote)	**Parallel Session**	
	Session Chair: Prof MMF Hassan	
		Prof M M F Hassan Texas A&M University *Designing for small-scale, distributed and unconventional feedstocks*
		Prof P Liu Tsinghua University *Modelling and optimization of power generation and transmission planning: Applications in China*

		Prof M Kroon Khalifa University *Hydrophobic deep eutectic solvents and their applications*
1530-1545	***Break* (ADCO Auditorium and Room 101)**	
1545-1645 (15-min Oral)	F065	Mouna Zaidani, Jehad Abed, Mohamed Sassi Masdar Institute, KU Two-phase flow hydrodynamics of trickle bed reactors at the pore scale using the phase field method
	F026	Dra M Khaleel Khalifa University Amine-functionalized hierarchical Zeolites for Carbon Dioxide capture
	F025	Dra M Khaleel Khalifa University Optimizing hierarchical Zeolites for applications in catalysis
	F004	Prof H Naseh Aerospace Research Institute Catalyst bed multi-objective optimization
1645-1730	**Plenary Lecture (ADCO Auditorium)**	

❖**All Plenary Lectures will be held in ADCO Auditorium**

❖**For the Parallel Sessions in Room 1003, except for the Plenary Lectures, this sessions will be held in Room 1003.**

❖**All coffee breaks will be in the ADCO Auditorium and Room 101.**

Time	Parallel Session	
0900-1000 (30-min Keynote)	**Session Chair: Prof T Majozi**	
		Prof I Mujtaba Bradford University *Water- One of the grand challenges of the world*
		Prof T Majozi University of the Witwatersrand *On Mathematical optimization methods for consideration of water-energy nexus in synthesis of chemical plants*
1000-1100 (15-min Oral)	F012	MK Amosa University of the Witwatersrand Towards sustainable water solutions: Specific cake resistance as a vital index for filtration throughput
	F066	Priyabrata Pal, Aiza Gay Corpuz and Fawzi Banat Khalifa University Removal of Oil from Wastewater using Colloidal Gas Aphrons
	F036	Prof C Kiparidissides CERTH, CPERI Recent Advances in Nanotechnology-based Water

		Purification Methods
	F055	O Ualibek Nazarbayev University Plasmonic metal nanostructures
1100-1115	***Break* (ADCO Auditorium and Room 101)**	
Time	**Plenary (ADCO Auditorium)**	
1115-1215 (Keynote)	**Session Chair: Prof I Mujtaba**	
		Prof A Kokossis National Technical University Athens *An integrated approach for the development of renewable supply chains and industrial symbiosis networks*
		Prof SS Mansouri Technical University of Denmark *Process systems engineering for efficiently achieving circular economy*
1215-1245	**Closing Session & Awards**	
		Prof A Almansoori Khalifa University
		Prof R Gani PSE for SPEED Company
1245-1330	***Lunch* (Cafeteria near Building 1)**	
1400 -	Visit to Khalifa University	

Time	Parallel Session	
0900-1000 (30-min Keynote)	**Session Chair: Prof P Varbanov**	
		Prof P Varbanov Brno University of Technology *Process Integration, Saving Energy, Resources And Emissions*
		Prof S Macchietto Imperial College *Optimal cleaning scheduling and flow control of heat exchanger networks under fouling: recent advances*
1000-1100 (15-min Oral)	F015	Dr J Zhu South-East University of China Generalized active disturbance rejection control for the boiler-turbine unit using multi-objective optimization and extended state observer
	F017	Dr P Sha South-East University of China Data-driven state monitoring of thermal power plant devices using density peaks clustering and evidential K-nearest neighbor classifier
	F062	Dr. Falah Alhameli Khalifa University, UAE A Mixed-Integer Programming Approach for Data Clustering in

		Support of Scheduling and Planning Decisions
	F041	X Fan University of South-Eastern Norway Facile synthesis of NFL-$ZnWO_4$ for pseudo-capacitor applications
1100-1115	***Break* (ADCO Auditorium and Room 101)**	
1115-1215	**Plenary Session (ADCO Auditorium)**	
1215-1245	**Closing Session (ADCO Auditorium)**	
1245-1330	***Lunch* (Cafeteria near Building 1)**	
1400 -	Visit to Khalifa University	

- **Sessions in Room 1003 will just held at 09:00-11:00**
- **Closing Session & Awards will be held in ADCO Auditorium**
- **Coffee breaks will be in the ADCO Auditorium and Room 101.**

ICFMCE 2018

Abstracts

System Design for Achieving Very High Shares of Renewable Electricity

Dr. Steven Griffiths
Senior Vice President, Research and Development, Professor of Practice
Khalifa University of Science and Technology, UAE

Abstract.
Our global energy system will look much different in the future relative to the recent past because of both political and technological factors. Among the most significant changes will be widespread deployment of renewable energy technologies, distribution of energy supply, sector coupling through electrification and the adoption of digital technologies. The opportunity for renewable energy is strongest in the electricity sector given the significant cost reductions observed for solar and wind energy technologies over the course of the past decade. Although solar and wind energy have experienced very strong growth in recent years, continued advancement will require technologies and operational practices that overcome the inherent limitations imposed by the intermittent nature of the electricity they supply. This is a systems level challenge that is context dependent and requires both temporal and spatial considerations to achieve adequate system flexibility. Here, flexibility refers to the ability of a power system to respond to variability of the net load, which is the load less variable energy sources like solar and wind.
Many technological and operational options can be leveraged for electricity system flexibility. These options, which relate to energy supply, energy demand, energy storage and grid infrastructure, must be assembled to ensure that electrical power grids are able to achieve balanced supply and demand at time scales ranging from seconds to years. The appropriate selection of measures requires intricate knowledge of the power system in which they will be utilized. In this talk, a model-based case study of power system transformation in the United Arab Emirates (UAE) demonstrates the tailoring of power

system flexibility to context. The results show that long-duration and seasonal energy storage can be play a key role in helping the UAE achieve more than 40% of electricity from intermittent sources by 2050. Further, the UAE case study demonstrates that context-specific load shifting, and potentially other modes of intelligent demand side management, are integral to developing an electricity system that is capable of cost-effectively incorporating a very-high share of intermittent renewables.

Analysis of CO_2 Capture and Utilization Technologies for Sustainable Carbon Management

Prof. Jay H. Lee
Professor of Department of Chemical and Biomolecular Engineering
Director of Aramco-KAIST CO_2 Management Center
Korea Advanced Institute of Science and Technology (KAIST)
Daejeon, Korea

Abstract.
The biomass feedstock is geographically dispersed and subject to variability. Therefore, strategic supply chain design can significantly influence the economic viability of bio-derived products. Preprocessing through decentralized fast pyrolysis facilities followed by centralized upgrading has recently gained a lot of attention because it limits costly biomass transportation. In this work, a modeling framework that captures the main characteristics of bio-based supply chains has been developed to investigate cost-optimal system configurations. The model provides a valuable tool to determine the optimal area that the supply chain must cover. Furthermore, optimisation results indicate that through the geographical concentration of biomass sources the profitability of the supply chain is increased enormously, and that preprocessing followed by upgrading is no longer by definition the preferred processing strategy. However, further analysis revealed that under uncertain scenarios the clustering of biomass sources has a slight

adverse effect on the robustness of the supply chain.

Multi-scale Energy Systems Engineering

Prof. Stratos Pistikopoulos FREng
Director, Texas A&M Energy Institute, TEES Eminent Professor
Artie McFerrin Department of Chemical Engineering
Texas A&M University, USA

Abstract.
Multi-scale energy systems engineering is a methodologic and generic framework to address complex energy and environmental problems via a holistic and system-based approach and arrive at realistic integrated solutions. This framework is used to tackle the problems existing in design, control, and operation of energy systems and their supply chains in an integrated manner. Optimal solutions are provided to the decision-makers for systems ranging from nanoscale, micro-scale, meso-scale to mega-scale levels over horizons that range from milliseconds to months or year.
Methodologies in energy systems engineering include, superstructure optimization with high-fidelity and data-driven modeling, mixed-integer linear or nonlinear programming, global optimization, optimal design and control under uncertainty, and life-cycle assessment. These concepts and methods are illustrated by presenting their application to natural gas utilization examples, including (i) optimal flowsheet design of ammonia-methanol coproduction from natural gas by using process synthesis techniques with simultaneous heat, power, and water integration, and (ii) supply chain optimization of natural gas to liquid transportation fuels (GTL) for nationwide, regional, and state-wide scales.

Acid Gas to Syngas™ (AG2S™) technology for CO_2 utilization: from theory to industrial applications

Prof. Flavio Manenti
Politecnico di Milano, CMIC Dept. "Giulio Natta", Piazza Leonardo da Vinci 32, 20133, Milano, Italy

Abstract.
The Acid Gas to Syngas™ (AG2S™) technology is an innovative process to produce syngas starting from two emissions, CO_2 and H_2S. The technology kernel is a regenerative thermal reactor that favors the overall oxy-reduction reaction:

$$2\ H_2S + CO_2 \rightarrow H_2 + CO + S_2 + H_2O$$

The regenerative thermal reactor is energetically self-sustainable thanks to a minor injection of air or oxygen, according to the final syngas uses, which is fed in premixed mode with the acid gases.
Acid gases undergo a thermal treatment in the regenerative part of the reactor (temperature preferably higher than 1000 °C); hot effluents are partially quenched to remove radical species by recombination reactions and a gas-gas feed/effluent heat exchange recovers the largest part of the heat at the end. The process generates syngas for the largest part, together with elemental sulfur, which has a market, and water, both innocuous byproducts.
If opportunely coupled with conventional technologies, AG2S™allows converting acid gases into liquids such as methanol, ammonia and all the other syngas-based derivatives (Acid Gas to Liquid™ AG2L™ technology).
Due to the low invasiveness of the AG2S™technology, plant refurbishing are cheap and relatively fast. First industrial applications are ongoing in Europe on oil refineries, geothermal power generation plants, and methanol synthesis plants.

Designing for Small-scale, Distributed and Unconventional Feedstocks

Dr. M.M. Faruque Hasan
Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, USA

Abstract.
Modular processes show significant promise for the utilization of distributed and unconventional feedstocks such as stranded natural gas, associated gas, shale gas, biogas, landfill gas, and even flue gas. Their advantages come from simple plug-and-play operation, responsiveness to fluctuations in market conditions, low waste, and low investment risks. However, most modular processes are designed to perform a single task (e.g., air separation, fuel cell, cold box). When included in a larger plant, these modules increase the energy consumption and cost due to the lack of proper integration with other units. They also suffer from poor economies-of-scale. These limitations can be overcome through process intensification, which combines separation, conversion and/or other operations in "multi-tasking" units. Conceptually it is possible to intensify a process using a multifunctional material, but these materials may not always exist. In this presentation, we will present a multiscale framework for modular process intensification using existing single-functional materials. Significant opportunities exist for integrated processes that use multiple materials in a single unit (e.g., sorption-enhanced reaction processes). Specifically, we will discuss new contributions in the following areas: (i) Conceptual Design: how to select materials and their functions to create and exploit new process dynamics and trade-offs introduced by different functional materials in an intensified unit, (ii) Modular Process Synthesis: how to systematically arrange materials and configure operational cycles in cyclic/periodic, material-enhanced modular processes, and (iii) Multiscale Optimization: how to integrate the development of materials and process systems in a single framework.

Design of Bio-Based Supply Chains

Edwin Zondervan and Jelle Adan
Bremen University, Leobener Straße D 28359 Bremen, Germany

Abstract.
The biomass feedstock is geographically dispersed and subject to variability. Therefore, strategic supply chain design can significantly influence the economic viability of bio-derived products. Preprocessing through decentralized fast pyrolysis facilities followed by centralized upgrading has recently gained a lot of attention because it limits costly biomass transportation. In this work, a modeling framework that captures the main characteristics of bio-based supply chains has been developed to investigate cost-optimal system configurations. The model provides a valuable tool to determine the optimal area that the supply chain must cover. Furthermore, optimisation results indicate that through the geographical concentration of biomass sources the profitability of the supply chain is increased enormously, and that preprocessing followed by upgrading is no longer by definition the preferred processing strategy. However, further analysis revealed that under uncertain scenarios the clustering of biomass sources has a slight adverse effect on the robustness of the supply chain.

Water-One of the grand challenges of the world

Iqbal M. Mujtaba
Chemical Engineering Division, Faculty of Engineering & Informatics, University of Bradford. Bradford, West Yorkshire BD7 1DP, UK

Abstract.
After air, water is the most essential commodity to all living species on the earth and quality water must be available in abundance to all species. In addition, agriculture and industry require sustainable water supplies throughout the world. Global water shortages will become so catastrophic over the next decades that two in three people on the planet

will face regular depletion of water supplies. Global thirst will turn millions into water refugees. Meeting the exponentially growing water demand that are required to improve the quality of life, and securing sustainable water supply is one of the global challenges of today's scientists and engineers. Certainly, the chemical engineers can play a vital and increasing role in meeting the current and future needs of the planet Earth: from water supply to waste water management.

As more than 94 percent of the world's water is saline, desalination technology is vital for sustaining human habitation (including agriculture and industry) in many parts of today's world. The commonly used industrial desalination processes can be classified broadly into two groups: (a) Heat consuming or thermal processes (b) Power consuming or membrane processes. Although thermal process is the oldest and still dominating for large scale production of freshwater, Reverse Osmosis (RO) process, due to advancement in membrane technology, has been continuously increasing its market share.

Increasing use of water also results in the increase of wastewater. Wastewater is also becoming a supplementary source of producing high quality recycled water. Wastewater is composed of organic, inorganic compounds and dissolved gases. A major problem over the last decades is the groundwater (including rivers) contamination via organic chemical compounds resulting in huge public health concern. These compounds constitute a very large group of toxic contaminants. A number of different techniques are being employed to treat wastewater including membrane and oxidation processes. In recent years, Reverse osmosis (RO) process has been successfully implemented to produce recycled water from wastewater containing toxic and harmful pollutants. Also, Catalytic Wet Air Oxidation (CWAO) using Trickle Bed Reactor (TBR) process has been considered as a useful and powerful method for removing toxic compounds such as phenol from wastewater.

While there have been no shortage of research work in desalination and in wastewater treatment for the last few decades, the ongoing objective has still been to improve the design, operation and control of these processes to ensure quality water at cheaper price with lower

environmental impact. In this lecture both Desalination Technology and Wastewater Treatment methods will be explored. Opportunity for energy savings in these processes will also be highlighted.

Hydrophobic deep eutectic solvents and their applications

Samah E. E. Warrag[a], Carin H. J. T. Dietz[b], Dannie J. G. P. van Osch[b], Maaike C. Kroon[a,*]

[a]*Khalifa University, Dept. Chemical Engineering, P.O. Box 127788, Abu Dhabi, UAE*

[b]*Eindhoven University of Technology, Dept. Chemical Engineering, P.O. Box 513, 5600 MB Eindhoven, Netherlands*

Abstract.

Deep eutectic solvents (DESs) are often considered as a new generation of innovative, tunable, low-volatile and sustainable solvents. DESs are mixtures of two solid compounds, a hydrogen bond donor (HBD) and a hydrogen bond acceptor (HBA), which form liquids upon mixing with melting points far below that of the individual compounds. The potential use of DESs covers a wide range of applications in separation technology, such as extraction, absorption, distillation and chromatography.

However, all presented DESs so far are hydrophilic. Recently, we published the first ever hydrophobic DESs consisting of decanoic acid as HBD and a range of quaternary ammonium salts as HBAs. These hydrophobic DESs were evaluated for the extraction of volatile fatty acids, biomolecules (e.g. furfural and hydromethylfurfural) and metal ions from water. The results showed that the hydrophobic DESs had superior extraction behavior in comparison with conventionally used extractants. Moreover, the regeneration of the DES phase was investigated. The impregnation of the DES onto a polymeric support was found to be a new cost-effective membrane technology. We also investigated the new hydrophobic DESs for other applications, including

the desulfurization of diesel, the separation of azeotropic mixtures and their capacity for CO_2 capture. These results will be presented at the congress.

An Optimization-based Computer-Aided Molecular and Mixture Design Framework

Dr. Lei Zhang
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Abstract.
The sustainability of modern society depends on the continuous availability of chemical-based products. Nowadays, product design and development has become a key topic in chemical engineering since high value-added products, green chemistry and product-process sustainability have started to receive increasing focus. Various requirements have to be satisfied for different product design problems, which are hard to be determined from limited number of experiments, considering the cost of time and money. Therefore, it is important to develop a systematic way to determine the optimal products based on the appropriate product attributes that need to be converted to property constraints.
In this talk, an optimization-based framework for molecular and mixture product design is presented. The molecular product design problem is decomposed into preliminary design, isomer generation and evaluation and verification steps. In the preliminary design step, an optimization-based mathematical programming model is established to generate feasible sets of molecular groups. Then, a SMILES-based isomer generation strategy is proposed to generate all isomers. In the evaluation and verification step, the generated isomers are verified using database and rigorous property models, to evaluate the availability of the generated molecules and accuracy of the properties. In the case of mixture design, a MILP/MINLP problem is formulated to find the optimal mixture (chemical identity and their composition) that satisfy a

set of desired target properties. Case studies including the design extraction/crystallization/reaction solvents, fragrance products, polymers, tailor-made fuel blends and lubricants will be presented to illustrate the application of the developed molecular and mixture design framework.

Process Systems Engineering for Efficiently Achieving Circular Economy

Dr. Seyed Soheil Mansouri
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Abstract.
This talk will highlight the benefits of systems thinking and process systems engineering incorporated in decision-making to achieve circular economy. Process systems engineering is an interdisciplinary field within Chemical Engineering that its main objective is the development of systematic procedures based on mathematical models and computational techniques for the analysis, design, operation, control and optimization of process systems. The ability to systematically evaluate the opportunities to create revenue streams from waste streams helps in efficiently achieving a circular economy. Various examples and latest developments will be shown to demonstrate the importance of systematic evaluation and identification of these opportunities and planning for developing new processes to realize them.

Component based development of computer-aided tools for different applications

Prof. Mario Eden
Chemical Engineering Department, Auburn University, Auburn, USA

Abstract.
Chemical engineering is in constant evolution and access to computational resources are changing the way chemical engineering

problems are addressed. Process simulation, which emerged in the 1960s, has become one of the great success stories in the use of computing in the chemical industry. Parallel with the development of new process-product development technologies, associated computer aided tools are needed for faster dissemination. However, the current unit-operation based process simulators, although having great success and wide applications, are not able to satisfy the demands for the new technologies (multiscale, multipurpose, new concepts leading to new algorithms, visualization, etc.). Therefore, the demand for a new class of computer-aided software has increased, especially for new areas of chemical engineering in which there are no standard software tools. For example, computer tools are developed to target and accelerate the half life of product innovation (time to market) due to competitive global economy and increasing consumer demands.

This work focuses on generic component-based architecture for development of tailor-made computer-aided tools for specific application objectives. The architecture is based on “components”, which can be model-objects that are stored in a library; collection of property models; databases; numerical solvers; and design-algorithms. The main idea of these components is to incorporate a plug & play framework, where for a specific purpose, after the work-flow and associated data-flow are established, a specific computer-aided tool can be configured without too much additional programming work. That is, after implementing through an interface, the work-flow and data-flow associated with the new tool, retrieve and connect the necessary components for step of the work-flow.

This presentation will focus on the architecture, components and the generic main user interface through which different components are connected based on the identified data and work flows. Tailor-made tool development based on this component-based architecture will be illustrated to emphasize the power of true "plug & play".

On Mathematical Optimization Methods for Consideration of Water-Energy Nexus in Synthesis of Chemical Plants

Prof. Thokozani Majozi
School of Chemical and Metallurgical Engineering, University of the Witwatersrand, Johannesburg, South Africa

Abstract.
The lecture presents recent developments in the exploration of water-energy nexus as it pertains to both batch and continuous processes. In particular, the application of advanced mathematical modelling as an optimization tool is demonstrated through real-life case studies and practical results. The systematic mathematical framework is based on a comprehensive superstructure for an integrated membrane network with a background network of water using operations. The water-energy nexus character of such a system emanates from the fact that the integrated membrane network is an energy sink, whilst the background water using process is a water sink. Increasing partial treatment of process water through the membrane network increases reusability water within the process, thereby reducing freshwater intake. However, increased partial treatment of water requires more energy for the membrane network, hence the trade-off between energy and water. The adopted approach deviates from the established black-box techniques and considers detailed design of the selected types of membranes. Electrodialysis and reverse osmosis membrane systems are considered in this lecture. Also presented, is a recent continuous-time scheduling framework that captures time in its exact form in multipurpose batch chemical plants. The latter is capable of addressing all the known idiosyncratic features of batch plants, stemming from various combinations of operational philosophies, including Process Intermediate Storage (PIS) and Finite Intermediate Storage (FIS) operational philosophies. Case studies drawn from different chemical industrial sectors are presented to illustrate applicability of the

developed mathematical framework.

Feedstock and pre-treatment processing options for production of HVO biofuels

Dr. Bent Sarup
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Abstract.
World production of fats and oils is presently around 225 mill ton/year, the main part being being used as food. However, about 35 mill tons/year is being used as fuel, mainly being converted to diesel fuel. Common feedstocks are fats and oils from palm, soya, rapeseed and tallow. Diesel fuel produced via hydrotreating (HVO) has a number of advantages, including the ability to produce a sustainable jet fuel, not possible with the traditional fatty acid methyl ester route to biodiesel. This presentation will provide an overview of the feedstock challenges and the pretreatment options available to safeguard the performance of the downstream hydrotreating catalyst.

Process and Energy Systems Engineering: CCUS and beyond …

Prof. Meihong Wang
Department of Chemical and Biological Engineering, The University of Sheffield, Sheffield S1 3QJ, UK

Abstract.
The talk starts with a brief introduction to Systems Engineering. It is aimed to emphasise that Process and Energy Systems Engineering is interdisciplinary and can deal with multi-scale industrial and physical systems. This is followed by motivations of our research. Energy security, emission reduction and affordability form the energy trilemma. Neither fossil fuels nor renewables can solve the energy problem from the above three aspects. Carbon dioxide is the main greenhouse gas.

Global concentration of CO_2 in the atmosphere currently stands at 409 ppm. Atmosphere CO_2 must remain 450 ppm to ensure that global warming stays below 2 °C. Therefore, it is essential to pursue carbon capture, utilisation and storage (CCUS).
The main part of this talk will be our research (funded projects and published work) in carbon capture for power plants and industry, and CO_2 transport in the context of CCUS. Our research on carbon capture is mainly based on solvent-based post-combustion carbon capture. Pilot plants and commercial development of this technology worldwide were reviewed. Coal-fired subcritical and supercritical power plants were modelled based on first principles. More attention will be given to detailed modelling of solvent-based post-combustion carbon capture using monoethanolamine (MEA), its implementation in gPROMS, steady state validation and dynamic validation and scale-up. Process analysis using validated models for integrated coal-fired power plant and solvent-based carbon capture plant indicated the reduction in thermal efficiency of the power plant and the challenges for operating such an integrated plant. To reduce capture plant footprint and energy consumption, process intensification was proposed to improve mass transfer using rotating packed bed (RPB) instead of packed bed. Model-based analysis was used to quantify such a potential in packing volume and column size reduction. In summary, first principle modelling of these processes, model validation and model-based process analysis provide many insights regarding how to improve mass transfer and chemical reaction (in order to reduce the CO_2 avoidance cost).
In the end, the topic will be extended to the use of Systems Engineering methods for study in Energy Storage (mainly liquid air energy storage and/or compressed air energy storage working with wind electricity) and Bio-Energy (biomass pyrolysis/gasification and syngas cleaning).

Modelling and optimization of power generation and transmission planning: Applications in China

Dr. Pei Liu

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Abstract.
Increasing global energy consumption and consequent greenhouse gas emissions pose great challenges to the sustainable development of international human society. Electricity constitutes the largest part of energy carriers, and the power sector is identified as the key sector with great carbon dioxide mitigation potential. Therefore, power generation expansion planning (GEP) problem has drawn great attention due to its important role in global energy supply, renewable energy utilization and carbon dioxide mitigation. Several important issues, including renewable energy sources integration, operating reserve, deregulated power market, demand response and carbon pricing mechanism should be incorporated in a GEP problem. Energy system engineering provides a methodological framework to address the complex energy, economic and environmental problems by adopting an integrated systematic approach, featuring superstructure-based modeling, mixed-integer programming, multi-objective optimization, and optimization under uncertainty. Moreover, China has made a commitment to reach its greenhouse gas emissions peak around 2030. This poses great challenge and uncertainty to the development of its power sector. Power supply and demand in China has already exhibited a feature of uneven spatial distribution, and this may be largely exaggerated if some constraint on greenhouse gas emissions is set on the sector. In this talk, we present scenario analyses of China's power sector with environmental and greenhouse gas emissions constraints based on a multi-regional and multi-period power sector planning model.

Optimal cleaning scheduling and flow control of heat exchanger networks under fouling: recent advances

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Abstract.
Fouling in heat exchangers is a major source of energy recovery inefficiencies. The unwanted deposition of material over transfer surfaces decreases heat duties, increases pressure drops, reduces energy recovery, causes lower throughputs and eventually, shut downs. An economically important case is crude oil refining, where large heat exchanger networks (pre-heat trains) at the front-end of every crude distillation unit (CDU) process essentially the entire world crude oil. Similar issues arise in the chemical, food and water industries.
Two common fouling mitigation alternatives are i) the control of flow distribution in the network (by manipulating bypasses and flow splits to parallel branches) and ii) the periodic cleaning of selected units. Flow control has a rather fast dynamic response which needs to be addressed using detailed dynamic models, while fouling is a slow dynamic process which is typically addressed using scheduling methods with highly simplified (pseudo) steady-state models. The two problems are traditionally approached independently and using distinct techniques. It is speculated there are synergistic effects arising from optimising flow control and cleaning schedules simultaneously, but it is not obvious whether this is beneficial and to which extent, hence whether a simultaneous solution, which is very challenging, is worth tackling in the first place.
Here, a simultaneous solution is proposed based on the formulation and solution of a MINLP optimization problem that considers both short and long term dynamics, with realistically complex models, over a long operating horizon (from months to a few years).
Two key aspects are addressed: i) a realistic representation of the problem, and ii) the efficient solution of the optimal cleaning scheduling and control problems. The starting point is a compact, radially distributed, but axially lumped, nonlinear dynamic heat exchanger model which accounts for fouling as a growth rate of the deposit, its

composition and impact on thermal and hydraulic performance. An efficient formulation is obtained via a time horizon discretization into periods, and a continue time approach is used to model the transitions between discrete states (e.g. “operating”, “being cleaned”) in the units. This approach allows solving simultaneously the scheduling and control problems. We also describe how scheduling decisions are modelled and how this general formulation can handle simultaneous cleanings of multiple units and different types of cleanings (e.g. mechanical, chemical, which have different effectiveness in restoring thermal and hydraulic performance).

The second key aspect deals with two main numerical difficulties: i) the complexity arising from the combinatorial nature of the problem due to the large number of possible cleaning schedules over long operating horizons, and ii) the large problem size and large number of nonlinearities that arise from the use of realistic heat exchanger and fouling models. Mathematically, this translates into a large number of binary variables, complicating variables and constraint in the formulation. We propose a reformulation and relaxation of the binary variables and scheduling constraints using complementarity constraints. This allows solving the optimal cleaning scheduling problem in a reasonable computational time, with general and flexible applications of a variety of operational constraints.

A case study of industrial significance is presented that demonstrates that i) the proposed formulation and solution strategy can solve realistically large heat exchanger networks and ii) there are indeed substantial synergies and potential economic savings resulting from the simultaneous optimisation of cleaning schedules and flow rate control, over and above the optimisation of either aspect individually. This is well explained in terms of thermal and hydraulic interactions caused by fouling, flow and cleaning, and their otherwise hard to predict propagation through the network.

The significance of the work and applicability to other industries are briefly considered.

An Integrated Approach for the Development of Renewable Supply Chains and Industrial Symbiosis Networks

Prof. Antonis Kokossis
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Abstract.
The design of renewable supply chains from pilots and installed facilities bears tremendous social and economic benefits. By 2020, Bloomberg predicts that, only in Europe, there would be around 1,000 of such new units bringing €32.3 trillion revenues and 1 million new jobs. Process systems engineering has a pivotal and critical role in the development of bio-renewable supply chains. The general view is increasingly supported by results and analysis that prove the significance of systems engineering in future developments. The designs are required to match maximum efficiencies in the use of materials/energy and to assess uncertainties in processing and economic parameters that may affect the selected designs and the level of integration. The presentation explains a systems framework tested on real-life applications. The work combines methods in process synthesis and integration, optimization and process modelling. At a conceptual level, process synthesis determines process and products to use, enabling a systematic screening with a simultaneous approach and the systematic use of optimization. Process integration, integrates for maximum efficiency in raw materials and energy, as well as for the maximum performance against environmental targets. Process flowsheeting validates with process simulation and enables improvements with parametric optimization. The coordinated use of the systems methods constitutes a significant advancement in the state of the art, currently relying on case-by-case analysis (flowsheeting) or the experimentation with commercial simulators.
Applications include a range of real-life applications featuring the

processing of organic substrates, algo-refineries and waste processing refineries. Applications involve chemistry paths with 70-odd chemicals that include basic intermediates (sugars, lignin, ethylene, oils), bulk chemicals (ethanol, butanol, propanol, isopropanol), bio-based polymers (PVC, resins, polyamides, PEIF, polyacrylates, PUs), and a wide range of chemicals (xylitol, xylonic acid, itaconic acid, sorbitol, isosorbide, hydrogel etc). Preliminary results are often impressive. Other than systematically screening and scoping integrated paths for the plant, the analysis reduces energy by 70% and the water use by 50-60%. Research is strongly coordinated with LCA. Results demonstrate that, unless fully integrated, biorefineries remain unsustainable. Instead, fully integrated biorefineries stand as viable and operational options, offering a strong promise to the development of sustainable industries in the future. The methodology is particularly tested in the context of Industrial Symbiosis where the systems methods are deployed to explore links (mass and energy exchanges) between industries and resources available at urban sites. Results and applications in that context will be presented from recent work to evaluate the renewable energy potential at four different EU ports.

Review of Energy Usage and Carbon Dioxide Management

Ramsagar Vooradi, Venkata Suresh Patnaikuni and Sarath Babu Anne
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Abstract.
Energy is not only a crucial but an inevitable driving force for sustaining human life. Around 200 years ago, the human population was limited to one billion only. With a consistent rise in energy consumption and remarkable technological advancements, today the population has grown over seven billion. Approximately 80% of the global energy requirement of this oversized human population is predominantly met by fossil fuels

such as oil, gas and coal. Though these sources are available in plenty, the major concern of using them is the release of greenhouse gases which in turn leads to global warming. In this article a brief review of different energy resources available for consumption, their impact in terms of carbon emissions as well as management, and sustainable chemical processing is presented. It is observed from the data that most of the energy resources are not utilized in an effective and sustainable manner. To mitigate CO_2 emission due to fuel combustion, preventive measures such as development of new energy efficient processes, sustainable storage technologies for excess renewable energy, retrofit redesign of current energy intensive operations that significantly reduce the energy consumption, etc. are analyzed as promising options to explore for minimization of energy requirement. The state of the art on integration of "curing" measures such as CCS, CCU or their combination with energy harvesting technologies from fossil fuels is presented. A sustainable energy & CO_2 management is discussed along with few case studies (i) hybrid technologies: hybrid separation scheme for separation of benzene-cyclohexane mixture, (ii) post combustion CO_2 capture: Chemical Looping technology for CO_2 capture from stationary sources and (iii) CO_2 utilization: A 3-stage framework for sustainable process design for utilization of CO_2 as feed for multiple products. In the end, some perspectives based upon the present scenario and future directions of CO_2 management are summarized.

Process Integration, Saving Energy, Resources and Emissions

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Abstract.
Energy – its efficient use in production is key to ensuring the healthy

functioning of the world economies. Climate change, together with the haze in growing megalopolises, and water scarcity in many areas are the key environmental challenges of our time. Polluted air and water, especially in places with high population density and high resource demands, have been posing an increasing threat to the mankind. To solve those issues, a complex thinking is very much needed. Traditionally, the involvement of process, mechanical and chemical engineering was considered as a cornerstone of a successful outcome. The close and strategic collaboration from most fields is a strong requirement. The complex systems thinking requires a close synergy of technologists, managers and economists, policymakers and politicians and related social scientists. In this context, ensuring cleaner energy is the necessary condition for cleaner production, especially for reducing the emissions of greenhouse gases and other pollutants, which are directly related to the types and loads of the energy sources used.

They are various emerging methodologies of sustainability assessment. The footprint methodology is one of gaining considerable attention. Greenhouse Gases (GHG – rather than just carbon) Footprint becomes a widely accepted environmental accounting tool for business managers, policy makers and non-governmental organisations, attempting to identify mitigation measures that reduce the threat of climate change. The industry is increasingly engaged as a part of policy development and product design.

This presentation offers a review of the main lessons recently learned in the field of more efficient energy use, the recent development of Process Integration, cleaner fuels and biofuels, cleaner production, CO_2 capture, optimisation, water and waste management, including process-level emission minimisation, self-sufficient regions, and industrial symbiosis for optimising usage of waste heat and waste material flows.

As an illustrative case study of a toll following complex systems thinking presents the development of Process Integration. It originatesd from Heat Integration to target the minimum heat requirements and following the demand being extended to Total Sites, Locally Integrated energy systems and even to self-sufficient regions methodology. To

cover the complexity with wider scope targeting GHG and haze creating emissions, integration of renewable energy sources, biofuels, waste and effluents supply chains, investment, property and material recovery targeting.

The presentation will be concluded by suggestions for future research and the discussion and exchange of ideas are most welcome.

F004: Catalyst Bed Multi-objective Optimization

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Abstract.
The main aim of this paper is to present of hydrazine monopropellant catalyst bed optimization methodology. To this end, the main parameters of hydrazine catalyst bed in optimization are decomposition products properties, molecular weight, specific heat ratio and their temperature as function of hydrazine decomposition and ammonia dissociation. These parameters are function of catalyst type, size, and geometry, reaction chamber pressure, and propellant dwell time. Also the objective functions in the optimization are catalyst bed's weight and performance. First one, a parametric study on hydrazine decomposition products as a function of catalyst bed design has been done. Catalyst bed output temperature, specific heat ratio and molecular weight were calculated as hydrazine and Ammonia dissociation ratio. Thermo chemical result shows that best specific velocity is attained when %25 of ammonia is allowed to dissociate. Pellet diameter, bed loading factor and thrust chamber pressure are assumed as the preliminary design parameters of the catalyst bed to find the catalyst bed length and pressure drop. Finally a numerical simulations, one dimensional, steady state, adiabatic, homogeneous, creeping and uniform flow at axial sections or Plug flow that has chemical reaction across a constant cross-sections catalytic bed, for different pellet diameters, loading factor and chamber pressure, have been carried out with the help of a validated formulations. According to this study, catalyst bed length and pressure drop will increase as the pellet diameter or bed loading increases. However the increase of chamber pressure will lead to the lessening catalyst bed length and pressure drop, but this influence is ignorable.

F012: Towards Sustainable Water Solutions: Specific Cake Resistance as a Vital Index for Filtration Throughput

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Abstract.
In the calculation of solid-liquid separation processes, the specific cake resistance (α) is always used as a measure of difficulty of the fluid permeation through the filter. This parameter is thus a vital productivity index towards a sustainable water security since it is required for the measurement of compressibility (γ) and fouling (ϑ) indices. In this work, the effect of porosity on α has been discussed based on experimental results from the filtration of the suspended solids laden wastewater from an oil milling process. Since the effect of porosity is dependent on the applied pressure, varying pressures and membranes with different porosity were used for the evaluation. The requisite data is provided from a bench-scale wastewater reclamation set-up consisting of, amongst other separation trains, a cross-flow membrane filtration process operated at constant transmembrane pressures (TMP) of 40, 80 and 120 kPa for three ultrafiltration (UF) membranes of porosity measured in terms of molecular weight cut-offs (MWCO) of 1, 5 and 10 kDa. Furthermore, α, γ, and ϑ are evaluated for each UF membrane from a series of filtrate volume vs. time data. The data are then corrected and modelled with the classical Darcy's model for cake filtration using suspended solids as a validation parameter. Results reveal a close correlation of the model and experimental results with R^2 values of 0.9264, 0.9849 and 0.9832 for 1, 5 and 10 kDa UF membranes, respectively. It is also observed that α decreases as the membrane porosity increases with the 10 kDa UF membrane having the lowest α of 2.90E+15 cmg^{-1}. The cakes are observed to be moderately compressible

based on the γ value of 0.35 exhibited by the 10 kDa UF membrane thereby making the membrane the most suitable for such measurement. Besides, the 1 and 5 kDa UF membranes are found to be unsuitable for compressibility measurement due to the negative γ values they both exhibited probably due to the nature of the feed-water utilized in this study. Furthermore, ϑ decreases as the porosity increases with 1, 5 and 10 kDa UF membranes having ϑ values of 5.46E+13, 5.41E+12 and 1.48E+11 cm^{-2}, respectively. Physically at each instant of time, the porosity decreases throughout the cake from the cake surface to the membrane septum where it has the lowest value. With the cake behaviour as observed in this study and since α increases more dramatically with a decrease in porosity, it could be concluded that the cake layer serves as a reliable and permeable secondary layer that sustains the filtration flux for a longer period and bring about higher and sustainable productivity.

F015: Generalized Active Disturbance Rejection Control for the Boiler-Turbine Unit Using Multi-Objective Optimization and Extended State Observer

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Abstract.

This paper proposes a generalized active disturbance rejection controller (GADRC) based hierarchical control structure for the boiler-turbine unit.

In the lower layer, a multivariable extended state observer (MESO) is developed to estimate the values of the lumped disturbances caused by modelling mismatches, fuel quality variation and wide range load variation. The influence of the disturbances is then compensated at the input side as a feedforward control. In the upper layer, the multi-objective optimization is devised to obtain the set-points by removing the plant behaviour variation from the optimized model in a feasible way. The low-pass filter acting on the lumped disturbances is designed to bridge the gap between the lower and upper layer. The impact of the feedthrough item is approximated by a first-order system and a two degree-of-freedom (2-DOF) control strategy is established to illustrate the set-point tracking and disturbance rejection properties of the controller. Simulation studies on a 1000MWe coal-fired ultra-supercritical boiler-turbine unit demonstrate that the proposed control strategy can achieve a satisfactory performance in cases of fuel quality variations, model-plant mismatches and wide range load variation.

F017: Data-Driven State Monitoring of Air Preheater Using Density Peaks Clustering and Evidential K-nearest Neighbour Classifier

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Abstract.
Data-driven state monitoring requiring a little priori knowledge plays a key role for timely fault detection and is therefore of great importance for the safe and economical operation of the thermal power plant. The main drawback for most of the existing data-driven methods is the

complex procedure of data preprocessing and model training especially when unlabelled operating data is used. To overcome this issue, this paper proposes a new framework of data-driven state monitoring approach for the thermal power plant devices. The approach is composed of two steps. In the first step, density peaks clustering(DPC) is performed on the historical data to generate labels for the data. Then in the second step, evidential K-nearest neighbour(EKNN) method is used to monitor the current state based on the labelled historical data and operating data. Verifications on operating data of an air preheater system of a 1000MW thermal power plant show that the proposed method can identify various air leakage states accurately and efficiently.

F019: Integration of a Calcium Looping System for CO_2 Capture in an Indian Natural Gas Fired Combined Cycle Power Plant: A Feasibility Study

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Abstract.

Since 1990's, the Indian energy sector has grown significantly and achieved remarkable progress. At present, most of the country's power generation demands are met by conventional fuels such as coal, oil and gas. The share of natural gas in India is around 9% only to this sector but the recent discoveries of shale gas reserves in Krishna-Godavari, Cauvery and Cambay basins have paved the way to exploit the available native hydrocarbon resource for power generation. Further, the natural gas is considered to be the cleanest fuel among all fossil fuels because of less CO_2 emission during combustion. Being the fourth largest greenhouse gas emitter in the world, India is adopting policies and exploring various carbon mitigation techniques to reduce greenhouse gas (GHG) emissions to 33-35% of 2005 levels by the year 2030.

Integrating natural gas fired combined cycle (NGCC) power plant with CO_2 capture technology may prove to be helpful in achieving this CO_2 reduction target. In recent times, Calcium looping (CaL) has emerged as one of the most promising post-combustion CO_2 capture technologies for decarbonization of power plants. Further, India's self-sufficiency of limestone puts CaL technology as a potential option to capture CO_2 from stationary sources economically. Hence, this study is intended to analyze a CaL system integrated with Indian NGCC power plant in Indian climatic conditions. An integrated model of CaL with Indian NGCC power plant is developed using ASPEN® simulation software. The proposed CaL scheme is based on the double looping technique. In the first calcium loop, the solid CaO stream that circulates between the combustor and calciner acts as a simple heat carrier which can supply heat during calcination process. In the second calcium loop, the CO_2 is captured by the solid CaO sorbent in the carbonator reactor, where the exothermic reaction takes place at 600 ^{0}C. The resulting carbonated solid $CaCO_3$ acts as a CO_2 carrier and is transported to calciner, where concentrated CO_2 is released at around 900 ^{0}C. Apart from the power generation through gas turbine, the high grade available energy in the carbonator and lean CO_2 gas mixture are also utilized to generate the power. A thermodynamic study has been carried out to evaluate the performance of CaL integrated power plant and compared with conventional NGCC power plant without CO_2 capture. Net thermal efficiency for the conventional NGCC power plant has been found to be 39.48% on a higher heating value basis. On the other hand, the CaL integrated Indian NGCC power plant with 91% CO_2 capture rate attains a net thermal efficiency of 33.90%. Hence, the study reveals that the proposed CaL integrated Indian NGCC power plant has an efficiency penalty of 5.6% as compared to conventional Indian NGCC power plant without CO_2 capture.

F022: Tuning Adsorbent Materials to Optimize CO_2 Capture at Industrial Conditions

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Abstract.
In the context of sustainable development, one of the most important alternatives to mitigate anthropogenic CO_2 emissions is to capture and separate CO_2 (CCS) from diluted sources, such as gases emitted from fossil fuel combustion and other industrial processes. By combining molecular simulations (Grand Canonical Monte Carlo) with macroscopic thermodynamics, we have developed a model to explicitly study the influence of impurities on the performance of Swing Adsorption processes for capturing CO_2 at operating conditions. The work focuses on realistic activated carbon structures compared with the MOF-74 family and with FAU-type zeolites tuned at different Si/Al ratio for the effective separation of CO_2 capture from an industrial flue gas. We present a quantitative assessment of the influence of impurities such as H2O, SOx and NOx on the energy requirements and process performance for CCS by adsorption in real swing adsorption processes from the fundamental knowledge of the adsorption. Simulations of pure components were validated with available experimental data in order to determine the accuracy of the model and were used in a predictive manner for multicomponent study. The study includes different evaluation criteria to analyze the CO_2 capture performance for each structure, such as selectivity, working capacity, regenerability, purity, energy for regeneration and exergetic performance. Hotspot regions for each material were identified for different adsorption/desorption technologies (i.e., Pressure Swing Adsorption (PSA), Vacuum Swing Adsorption, (VSA), Temperature Swing Adsorption, (TSA), and hybrid cycles), where high working capacities, and purities and recoveries above 80–90% can be obtained, without incurring in extremely high

energetic requirements.

F025: Optimizing Hierarchical Zeolites for Applications in Catalysis

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Abstract.
Efforts to overcome diffusional limitation in microporous zeolites have been directed towards the design of hierarchical zeolite structures. Hierarchical zeolites contain highly interconnected networks of zeolitic micropores combined with meso- and/or macropores. Interest in these materials stems from the higher reaction rates, improved selectivity, resistance to deactivation, and novel adsorption behavior that they exhibit in comparison to the typical zeolites that only have micropores. Among the synthesis approaches, repetitive branching by rotational intergrowth holds promise for industrial implementation due to its simplicity and lower cost as it is a one-step synthesis which uses simple structure-directing agents or additives compared to hard and dual-soft templating approaches.
Faujasite is one of the most widely used catalysts, mainly in fluid catalytic cracking (FCC) of heavy petroleum, where coking is significant. Hierarchical Faujasite, with enhanced micropore accessibility, can reduce the detrimental effect of coking. Hierarchical Faujasite has been prepared by post synthetic treatment, or by using soft-templates or hard templates, adding extra cost and complexity to the synthesis. House-of-card assembly of Faujasite sheets by repetitive branching has been previously reported using either organosilane surfactants[1] or lithium or zinc salts[2]. Previous work by Khaleel et. al.[3] showed that FAU/EMT intergrowth is responsible for the repetitive branching leading to the development of house-of-card assembly of zeolite X nanosheets. Thus, being able to control the intergrowth of

crystal phases in particles will allow control of mesopore size by controlling sheet thickness and branching frequency. Both FAU and EMT can nucleate from inorganic sols containing only sodium ions. Hence, the development of a house-of-card assembly of Faujasite sheets from sodium aluminosilicate sol is in principle possible, thus avoiding the extra cost of additives. In this work, we demonstrated for the first time a practical and simple strategy for preparing hierarchical house-of-card Faujasite from inorganic sodium aluminosilicate sols.
Attempts are being made to tune the hierarchical Faujasite for catalytic applications by increasing the framework Si/Al ratio, while retaining the house-of-card morphology, using both inorganic bottom up and post treatment approaches. The latter would allow successful ammonium ion exchange for generating Bronsted acidic sites.

F026: Amine-Functionalized Hierarchical Zeolites for Carbon Dioxide Capture

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Abstract.
One of the greatest challenges we are facing in the 21st century is our ability to provide sustainable energy sources to meet the demands for quality of life and economic growth. As most of the energy today is provided from fossil fuels, huge amounts of CO_2 and other greenhouse gases are emitted to the atmosphere, with negative effects on the environment. Depletion of fossil fuels and their associated environmental pollution lead scientists to the pursuit of renewable energy sources and clean energy. However, reducing dependency on fossil fuels is a major challenge for most economically advanced

countries. To make fossil fuels clean, efficient, reliable and scalable technologies for CO_2 capture from large sources should be developed to control CO_2 emission in the short-medium term. Although some technologies for carbon capture are available in the market they still suffer from some limitations to be fully implemented at large scale.

Conventional CO_2 removal using aqueous alkanolamine solutions is energy intensive. This lead researchers to investigate various solid adsorbents for selective CO_2 removal at low pressure ranges while requiring less energy for regeneration compared to alkanoamine solutions [1]. Various porous solids were tested for post-combustion CO_2 capture including activated carbon [2], zeolites [3] and metal–organic frameworks (MOFs) [4]. Solid materials grafted or impregnated with amines were also studied to further increase the CO_2 binding strength and hence CO_2 uptake [5, 6]. Of particular interest are amine grafted zeolites that combine strong CO_2 capturing zeolite micropores with the chemical binding of CO_2 with amines [7]. Hierarchical zeolites, combining zeolite micropores and mesoporous domains, show increased surface area and pore volume compared to conventional zeolites. Functionalizing the mesoporous domains in such materials with amines can result in high CO_2 uptake because both the active sites of the zeolite and the amine groups in the mesopore space can simultaneously capture CO_2. However, there are very few studies of amine grafted hierarchical zeolites and the latter were prepared using expensive organics [7].

In this work we study the performance of amine grafted hierarchical zeolites, prepared from inorganic (i.e. inexpensive) routes, in CO_2 capture. A series of zeolites with varying textural properties are synthesized and grafted with different amines and their performance is tested for CO_2 adsorption. Synthesized materials are characterized using X-ray Diffraction, Nitrogen Physisorption and Scanning Electron Microscopy. CO_2 uptake properties are evaluated by equilibrium gas uptake measurements to study the effect of hierarchy on the performance of the materials. Thermogravimetric Analysis is used to estimate the amount of amine grafted on zeolite samples and Infrared

Spectroscopy is used to study the functionality of the materials.
FT-IR spectroscopy showed successful amine grafting in zeolite. CO_2 isotherms show that the amine modified hierarchical zeolite exhibits enhanced CO_2 uptake at 15 mbar and 60 °C (typical flue gas conditions) compared to conventional zeolite, amine modified conventional zeolite, and bare hierarchical zeolite.

F031: Experimental study of CO_2 solubility in high concentration MEA solution for intensified solvent-based carbon capture

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Abstract.
The solvent-based carbon capture process is the most matured and economical route for decarbonizing the power sector. In this process, aqueous monoethanolamine (MEA) is commonly used as the solvent for CO_2 scrubbing from the power plant flue gases. Generally, aqueous MEA with 30 wt% (or less) concentration is considered the benchmark solvent. The CO_2 solubility data in aqueous MEA solution, used for modelling of the vapour-liquid equilibria (VLE) of CO_2 in MEA solutions, are widely published for 30 wt% (or less) concentration. Aqueous MEA with higher concentrations (from 40 to 100 wt%) is considered in solvent-based carbon capture designs with techniques involving process intensification (PI) [1-2]. PI techniques could improve the process economics and operability of solvent-based carbon capture [2]. Developing PI for application in capture process requires CO_2 solubility data for concentrated MEA solutions. These data are however

limited in literature; Mason and Dodge [3] presented CO_2 solubility data for 56 and 74 wt% MEA solution, Atadan [4] presented data for 45 and 59 wt% MEA solution and Aronu et al. [5] presented data for 45 and 60 wt% MEA solution. The modelling of the vapour-liquid equilibria (VLE) of CO_2 in MEA solutions for PI-based solvent capture techniques involving stronger MEA solution of about 80 wt% concentration requires solubility data at the concentration. In this study, the data for 80 wt% MEA is presented for 40,60, 100 and 120^{o}C. The experimental technique and analytical procedure in this study were validated by comparing the measurements for 30 wt% MEA with data from the literature. The data from this study can be fitted to VLE models such as electrolyte NRTL, extended UNIQUAC etc. which is an important component of solvent-based capture model using MEA as the solvent. More accurate VLE models will improve the prediction accuracy of capture level, rich loading etc. using PI-based solvent-based capture model (e.g. rotating packed beds).

F036: Recent Advances in Nanotechnology-based Water Purification Methods

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Abstract.
Water treatment and purification is undoubtedly the most important topic in the environmental technologies. Membrane technologies and nanosized materials offer a wide range of possibilities and ways for water treatment by means of combined filtration and catalytic degradation processes. Recent advances in nanotechnology-based water purification methods (e.g., nanosorbents, nanocatalysts, bioactive nanoparticles, nanostructured catalytic membranes and nanoparticle

enhanced filtration, etc.) can largely contribute to the improvement of water purification technologies. Moreover, new developments in water desalination methods are among the most exciting and promising ones.
In this brief presentation, current issues related to nanotechnology-based water treatment and purification methods will be reviewed including nanostructured membranes and nano-catalysts, molecularly imprinted materials, nanosorbents, biomimetic membranes and membrane bioreactors (MBR), etc.

F037: From Molecular to Plant Scale Computer Aided Design of Polymer Manufacturing Processes

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Abstract.
A major objective of polymerization process modeling is to quantify the effects of kinetic mechanism, physical transport phenomena (e.g., mass and heat transfer), thermodynamic phase-equilibrium, non-ideal mixing phenomena, residence time distribution, reactor configuration and operating conditions on 'polymer quality'. The last term includes all the polymer microstrucre properties (e.g., molecular weight distribution (MWD), copolymer composition distribution (CCD), sequence length distribution (SLD), long and short chain branching (LCB, SCB) distributions, bivariate molecular weight – long chain branching (MW-LCB) distribution, bivariate molecular weight – copolymer composition (MW-CC) distribution, etc.) as well as the morphological properties of the product (e.g., particle size distribution (PSD), pore size distribution, etc.). Moreover, it is of paramount importance the prediction of polymer end-use properties (i.e., thermal, mechanical, rheological, chemical, etc. properties) and the molecular/topological characteristics of the polymer chain architecture in terms of the polymer chain microstructure.

Thus, control of the polymer chain microstructure in a polymerization process is of profound interest. This presupposes a thorough knowledge of the polymerization kinetics, accurate quantitative descriptions of all thermodynamic, mixing and transport phenomena in a polymerization process and the availability of detailed mathematical models to quantify the effects of process operating conditions (i.e., temperature, monomer to co-monomer molar ratio, initiator concentration, etc.) on the polymer molecular properties. Thus, to simulate the dynamic operation of complex polymerization plants, one needs to develop mathematical models, at different time and length scales, accounting for the physical and chemical phenomena taking place in a polymerization process. The present lecture presents a comprehensive, multi-scale approach for modeling the operation of lab-, pilot- and industrial-scale high- and low-pressure olefin polymerization processes for prediction of molecular and rheological polymer properties of produced polyolefins in multi-reactor configurations.

F040: Amine Circulation Rate Optimization of Gas Purification Unit in LNG Plant Bontang

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Abstract.
PT Badak Natural Gas Liquefaction (NGL) is a world class energy company which is capable to produce liquefied natural gas (LNG) and liquefied petroleum gas (LPG) from the gas well. There are mainly four steps in order to treat the natural gas; purification, dehydration, separation, and liquefaction process. Natural gas from the gas well is purified from any impurities especially acid gas in the gas purification unit. After that, natural gas is dehydrated to remove its water content in the dehydration unit. Treated gas is then separated in the fractionation column and liquefied into LNG or LPG. LNG or LPG is finally stored in the tanks before being shipped.
Due to the leaner feed gas entrance from the gas suppliers, PT Badak NGL is currently facing new operational challenge in LNG and LPG

production. With the leaner feed gas supply, the gas composition significantly changes. Thus, operating conditions in the plant need to be adjusted in order to maintain desired LNG and LPG product specifications. One of the operating conditions should be adjusted is the amine circulation rate which is utilized to remove acid gas components in the feed gas especially CO_2 content. Gas purification is the first step of the natural gas liquefaction. Currently, CO_2 content in the lean gas is also decreasing (approximately 30% of previous condition). With the lower CO_2 content in the feed gas, amine circulation rate can be also optimized in order to get the higher energy saving in the Amine Regenerator Unit.

By evaluating the new feed gas composition, the amine circulation rate in gas purification unit can be optimized from 900 m^3/hr to 700 m^3/hr in each train. The performance test was then performed to implement the new amine circulation rate in all trains running. The result shows that new amine circulation rate can be successfully implemented in PT Badak NGL without any operational issues that should be taken into account. With this amine circulation optimization program, steam consumption in the gas purification unit can be reduced as much as 3 ton/hr per train running (equivalent with 17% steam saving). By implementing new amine circulation rate in all trains running, total steam consumption can be reduced up to 78,840 ton in a year or equals to USD 696,946 per year steam production cost.

F041: Facile synthesis of NFL-$ZnWO_4$ for pseudocapacitor application

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Abstract.

With the development of human society, a large amount of energy sources have been consumed, such as coal, petroleum, and natural gas.

Therefore, novel and suitable energy storage devices need to be developed. Supercapacitors (SCs), the new devices between conventional physical capacitors and lithium-ion batteries, have been extensively studied to serve as one of the most promising candidates for energy storage because of their high-power density, long cycling lifespan and fast charge/discharge process. In general, supercapacitors can be divided into two categories according to the energy storage mechanism: one is the electric double layer capacitors (EDLCs), in which carbonaceous materials have been widely utilized and the other is the Faradaic redox reaction pseudocapacitors(PsCs) usually containing transition metal oxides as the electrode materials. In comparison with electric double layer capacitors, PsCs show much higher specific capacitance performance, making it is of far-reaching significance to focus research on.

So far, nanostructured metal oxides have been intensively explored in order to use them as electrode materials. However, the high cost of some transition metal oxides limited their practical use in commercial supercapacitors. Hence, searching for a low cost pseudocapacitive material and economically affordable generation systems has been a major challenge in supercapacitors research. In recent years, Zinc tungstate ($ZnWO_4$), an environmentally friendly low-cost transition metal oxide and both its constituent elements being relatively earth-abundant, with high technological applications in various fields, such as photocatalysts, optical fibers and gas sensors, have been reported. Because both Zn and W elements can take part in the Faradaic redox reactions, $ZnWO_4$ is of great potential for electrode materials. Unfortunately, $ZnWO_4$ is rarely reported as the composite materials for supercapacitors.

Herein, we employed a simple, facile and effective hydrothermal route to synthesize nanoflower-like $ZnWO_4$(NFL-$ZnWO_4$) and to the best of our knowledge, there are no reports on this morphology. The physical and chemical properties were carried out by SEM, EDS, XRD and XPS, respectively. A series of electrochemical tests including CV, GCD and EIS were conducted. It was demonstrated that the NFL-$ZnWO_4$ exhibits

good electrochemical behaviors with a high specific capacitance of 107.7 F g^{-1} at 5 mV s^{-1}. In the future, efforts of morphology tunnings or synergies with other materials on $ZnWO_4$ can be made to match the superior electrochemical properties need. In view of this, $ZnWO_4$ as an electrode material is well worth being applied to supercapacitors.

F043: Energy storage in the context of grid flexibility: A Case Study of the German electricity grid

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Abstract.
Germany is one of the leaders in the transition to cleaner energy mixes, with strong policies and clear goals for the coming decades, making it an interesting case study. In this work we explore the ramifications of incoming changes brought by the energy transition, most notably the increased penetration of variable renewable energy (VRE) and phase-out of nuclear and other conventional electricity sources. The electricity grid will require additional flexibility capabilities to accommodate such changes, as the mismatch between generation and demand is bound to increase. Through mathematical modelling and optimization, we simulate the German electricity grid and investigate the requirements of on-grid large-scale storage, dispatchable generation, electricity trading between neighboring countries and energy curtailment.
For short- and medium-term storage, electrochemical storage is a strong candidate due to its high efficiencies and fast response times. Different scenarios are evaluated up to 2050. Dispatchable generation will still be relevant, even in high VRE scenarios. 3.5 GW to 90 GW of large-scale storage are required until 2050, depending on the scenario. Between the electrochemical technologies evaluated, lithium-ion was the best candidate. A strong reliance on electricity imports was observed, in case commissioning of VRE plants does not go as quickly as planned. Energy

curtailment increases with VRE shares, with up to 22 TWh curtailed in high VRE scenarios in 2050.

F055: Self-assembled plasmonic nanostructures by glancing angle deposition technique for sensing and electronic applications

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Abstract.
Plasmonic metal nanostructures have attracted significant scientific attention in the last decades. In particular, Plasmonic nanostructures are potentially interested in optical circuits, plasmonic solar cells, phase-change memory, surface enhanced Raman spectroscopy, second harmonic generation, biosensors and etc. Recently, we developed a novel fabrication method based on deposition at a glancing angle on a stepped template and flat surfaces. This is a simple method based on self-assembly that can produce highly ordered plasmonic nanostructures. Adatoms are evaporated towards a surface at shallow angles of incidence. The principle, often referred to as glancing angle deposition (GLAD), is simple and is mainly based on geometrical considerations, rendering it largely independent of the deposited material in the case of step shadowing. The shape of nanostructures can be tuned by tuning the deposition parameters. In this work, we demonstrate various applications of plamonic nanostructures such as 2D materials based plasmonic solar cells, phase change memory from Ga nanoparticle arrays and sensing applications of Ag nanoparticle arrays in surface enhanced Raman spectroscopy.

F057: Roles of Microalgae in CO_2 Management: A Modeling Approach

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Abstract.
The world increase in energy demand has been simultaneously met with an upsurge in fossil fuel production which pose a lot of environmental challenges via the enormous release of carbon dioxide (CO_2) emissions. Abatement technologies such as carbon capture and storage (CCS) has been demonstrated to sequester CO_2 over a definite period of time. Whilst CCS proves to be expensive in terms of capture cost and net environmental footprint, the need to utilize CO_2 via chemical and/or biological means is paramount. To mitigate climate change and utilize CO_2 simultaneously, microalgae – abundantly available photosynthetic organism that are able to survive under extremely harsh conditions, can convert CO_2 into complex sugars and other metabolites such as carotenes, antioxidants and toxins. In microalgae, CO_2 from any source is first concentrated via active bicarbonate uptake transporters, pyrenoid within their chloroplasts or suite of carbonic anhydrases within their cells before fixation through Calvin-Benson-Bassham cycle. Via the CO_2 utilization mechanism, high-value products useful in food, energy, pharmaceuticals, cosmetic and agricultural industries such as biofuel, biochemical, bioplastics etc. can be synthesized. This study presents the various bio-activities of microalgae in an economic and environmental CO_2 management system. With the advent of DNA sequencing and genomic profiling of microorganisms, metabolic networks are designed to capture every of their bioactivities. Herein, a dynamic flux balance analysis (DFBA) model–constructed from metabolic network, is employed to understand the various roles played by microalgae from CO_2 capturing to utilization and conversion. Performance indices such yearly CO_2 avoided, capture efficiency and annual productivities of proteins and lipids (essential feedstock) are employed to understand these contributions via the cultivation of microalgae in 1hectare open raceway pond. Within the CO_2 network, microalgae act as bio-fixation

agents; utilizing dissolved CO_2 within their culture to produce biomass and bio-based products. For a scenario of flue gas from a combined cycle gas turbine with an influx of 121165 kg/hr of CO_2 distributed among 1000 ponds, results show that 2.86 x 10^8 kg of CO_2 can be avoided per annum yielding a capture efficiency of 37.31%. Likewise, at this sparging rate, the model predicts that annual productivity of biomass totaling 1.08 x 10^8 kgDW/ha with proteins and lipids content of 26.3% and 43.2% respectively. As compared to other players (CCS technologies and other CCU options) in the CO_2 management systems, microalgae cultivation is a standalone technology with lower net CO_2 emission and less energy requirement. As more efficient cultivation systems are designed, microalgae stand the chance of efficiently abating CO_2 environmental pollution at significant reduction in technological cost.

F062: A Mixed-Integer Programming Approach for Data Clustering in Support of Scheduling and Planning Decisions

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Abstract.

Integration across decision levels of a supply chain is a key point in improving returns on investment. For example, planning and scheduling are usually carried out separately although they are interdependent of each other. Integration of planning and scheduling results in better coordination between decision levels and a reduction in operating costs. Integration of different time scales leads to large scale problems which

are usually computationally intractable. Different approaches have been proposed to tackle the problem in terms of modeling and solution methods. However, most of them are problem specific or applicable only to short time horizons. Clustering has the potential to handle such a problem by grouping similar input parameters (like demand or price) together. This will considerably shrink the model size and make it more computationally tractable while at the same time not compromising solution accuracy.

Therefore, the aim of this work is to develop a new class of clustering algorithms that are based on mathematical programming techniques in order to support the integration of planning applications of different time scales (strategic, tactical, and operational) in process systems engineering. The clustering algorithms were formulated using integer programming with IAE (integral absolute error) as a similarity measure. The initial formulation was a Mixed Integer Nonlinear Program (MINLP) and then reduced to a Mixed Integer Linear Program (MILP) using exact linearization techniques. The model resulted in two different clustering algorithms: normal and sequence clustering. Two case studies were presented to assess outputs and computational performance of the algorithms. Electricity demand and solar radiation data were clustered in these case studies. Both clustering algorithms captured the trend in the data. However, the computational burden of the model was prohibitive to tackle large planning horizons.

In order to deal with computational complexity, a heuristic algorithm was developed utilizing an iterative scheme, which was first applied to clustering the electricity demand in the original cases studied for validation purposes. The quality of the solutions from this algorithm were checked against the MILP optimal solutions and it was found that the heuristic algorithm is able to provide good quality solutions and even succeeded in finding the optimal solution for simulation runs carried out. The heuristic algorithm was applied to clustering the electricity demand for a whole year with a small computational effort and providing clusters with high intra-cluster similarity and low inter-cluster similarity.

In order to illustrate the use of the clustering procedure in solving large scale planning model, the clustered electricity demand was used as input to a Unit Commitment (UC) model with the objective to evaluate the solution quality when clustered demand is applied. The UC problem is a classical problem in electrical power production where the production of a set of electrical generators is coordinated in order to meet the energy demand at minimum cost or maximize revenues from energy production. The results showed a great advantage in term of solution time for the clustering technique compared to the regular solution when no clustering of demand was applied. Moreover, the error of objective function was within 0.5 % of the non-clustered demand for all cases. In addition, a sensitivity analysis study suggested that high quality solutions could still be achieved with smaller number of clusters.

The clustering algorithm was extended in order to take into account multiple attributes at the same time such as clustering simultaneously demand for electricity and heat. In this respect, the objective function had different scales due to the different units of measurements of the attributes, and the problem was dealt with as a multi-objective optimization problem. The weighting method was chosen as the optimization approach and to be able to scale appropriately the different attributes. The clustering algorithm was successfully applied to simultaneously cluster hourly electricity and heat demands for the whole year. The Pareto front was captured for all runs with the weight factor combinations considered in this study. The results show that a better objective function is achieved when the number of clusters increases for both normal and sequence clustering. Normal clustering and as expected lead to a better objective function, error average and standard deviation than sequential clustering due to the additional restrictions of sequencing requirements imposed on the model. Clusters that take into account the time of occurrence of events and abide to certain minimum sequencing restrictions are also needed in planning operations in order to minimize the number of set-ups and inconvenience to operators. The statistical analysis of the heat demand was challenging as suggested by the results, due to the huge fluctuation in the heat demand. Moreover,

calculations of relative error were problematic for the demand that was close to zero. The results indicated that in the case when operations are flexible or in the case of just classifying demand patterns, normal clustering should be used since it has a major advantage in terms of solution quality over sequence clustering. For the case of simultaneously clustering heat and electricity, it was required to employ many clusters of electricity that sometimes overlap with each other. These clusters could not be merged since they correspond to different days and the clusters of heat demand for these days are different. Nevertheless, the proposed algorithm was able to obtain groups that simultaneously cluster the two attributes and hence can provide computational advantages when solving integrated planning models that deal with more than one demand attribute.

The clustered electricity and heat demands were used as inputs to an energy hub model, with the objective of evaluating the solution quality when multiple clustered demand attributes are applied to planning models. The average error of objective function was -1.7 % for normal clustering while for sequence clustering it was -4.2 %. Increasing the number of clusters was found to enhance the solution quality for both normal and sequence clustering. For this particular example, varying the weight factors did not have a drastic effect on the values of the objective function. This is due mainly to a symmetry or inverse similarity in the heat and electricity demands.

F063: Green synthesis of zinc oxide nanoparticles using *Tamarindus indica* leaves and its application for dye ultrafiltration

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Abstract.

In this study, green synthesis of zinc oxide (ZnO) nanoparticles using leaf extract of *Tamarindus indica* (Tamarind) and zinc nitrate as a precursor was carried out. The bio-synthesized ZnO nanoparticles were characterized by Ultraviolet-visible spectroscopy (UV-vis), Fourier Transform Infrared Spectroscopy (FTIR), X-ray Diffraction (XRD), Transmission Electron Microscope (TEM), Scanning Electron Microscope (SEM) and Brunauer-Emmett-Teller (BET) analysis. The synthesized ZnO nanoparticles were pure, predominantly spherical in shape with size ranging from 36.9 to 89.3nm. These ZnO nanoparticles were blended with polyethersulfone (PES) membranes to study the performance enhancement of the ultrafiltration of dye separation from aqueous streams. ZnO blended PES membranes showed enhanced flux, improved dye rejection and better antifouling effect. Anti-bacterial studies on the PES/ZnO blend membranes indicated the decrease in bacterial activity with increase in the ZnO concentration in the membrane. Comparison studies with commercial ZnO nanoparticles showed the competitive performance of the prepared bio-synthesised ZnO nanoparticles for the dye ultrafiltration studies.

F064: Comparative Study of effect of water, gas and foam Flooding on Enhanced Oil Recovery (EOR)

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Abstract.
For decades, Enhanced Oil Recovery (EOR) has been posing an exigent task for researchers in the oil and industry. Traditionally water and gas are used as displacing fluids for oil recovery. More recently foam, which is a dispersion of liquid in gas, has proved to be highly successful than traditional fluid displacement methods to recover trapped oil in the porous medium. Foam increases oil sweep efficiency by controlling gas

mobility and gravity override. In this work oil recovery efficiency using water, gas and foam flooding is compared. We perform upscaling for two phase immiscible flows in porous media and perform numerical simulations to determine oil recovery from water, gas and foam flooding. 2D two phase and three phase models are created in COMSOL and effects viscous instabilities and permeability of different ground layers on recovery factor are investigated.

F065: Two-phase flow hydrodynamics of trickle bed reactors at the pore scale using the phase field method

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Abstract.
Pore scale modeling of multiphase flow of trickle bed reactor through a porous media is a true challenge for engineering and scientific society. Because the pore-scale description is a fundamental approach in hydrodynamics. The most important macroscopic parameters for multiphase flow in porous media, such as capillary pressure and relative permeability, are fundamentally controlled by the pore-scale topology, interfacial tension and contact. This in turn impacts the overall flow behavior. Besides it can be used to obtain macro-scale constitutive equations, to provide multiphase flow properties for large scale models, to predict how these properties may vary with beds type and wettability.
Computational fluid dynamics CFD simulations of the concurrent gas-liquid trickle flow through a trickle bed reactor, at the pore scale, under gas, liquid operations have been performed by using an unsteady phase field method, each of the phase field functions is then used in the conservation equation for each field, this model is implemented by the means of the commercial software COMSOL. The numerical method is developed for efficient modelling of multiphase flow in porous media

with complex interface motion and irregular solid boundaries. The Phase Field interface uses a Cahn-Hilliard equation, including a chemical potential to represent a diffuse interface separating the two phases. The Navier-Stokes equations are used to describe the momentum transport and the conservation of mass.

We present a stable numerical scheme for modelling multiphase flow at the pore scale, one of the important aspects of this problem is the construction of adequate 2D numerical models for modelling multiphase flow in porous media, where the characteristic size of the flow domain is of the order of millimeters. For the simulation of fluid distribution inside pores, the models is based on incompressible Navier-Stockes equations and their extension to diffuse interface using Cahn Hilliard model. The numerical model will take into account the surface tension between each fluids, contact angles with the solid bed, as well as the density and the viscosity of each of the fluids. The phase field method compute the shape of the interface between the two phases and also account for interactions with walls.

In this study, numerical simulations of two-phase flow distribution in a trickle bed are reported, the heat and mass transfer, as well as the chemical reactions, are not considered. The transport properties for two-phase flow patterns at various viscosity ratio and capillary numbers, the numerical performance of diffuse interface model in a specific 2D framework, will be presented and discussed in details. The study parameters were gas and liquid contact angle, flow rates, liquid viscosity, gas density and catalytic bed wettability and geometry (particle shape and size). As the contact angle controls the arrangement of fluids within the pore-space, its experimental evaluation is vital for a holistic understanding of multiphase flow.

F066: Removal of Oil from Wastewater using Colloidal Gas Aphrons

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Abstract.
Oily wastewater affects various ways as it destroy groundwater resources, endangering aquatic life, affects crop production, cause atmospheric pollution, and many more. To prevent the negative impacts of discharging oily wastewater, it is essential to develop an efficient method to remove oil before discharging it to the environment. In this study, the use of flotation using colloidal gas aphrons (CGAs) generated from anionic surfactant sodium dodecyl benzenesulfonate (SDBS) was carried out to remove oil from wastewater. The effect of operating parameters such as initial oil concentration, pH of SDBS solution, pH of oil solution, volume of oil solution, and CGAs temperature were varied. The optimum operating conditions having initial oil concentration 100 mg/L, pH of surfactant solution 5.6, pH of oil solution 3.04, wastewater solution volume 500 mL, and surfactant solution temperature of 50ºC to produce CGAs was best to achieve 91% oil removal. The sonication enhanced the dispersion of oil droplets in the retentate solution and has improved the oil removal from 56% to 66%. For the reuse of the surfactant, graphene was used as an adsorbent to remove oil from the foamate solution. CGAs produced after adsorption was able to remove 84% of oil from wastewater. Thus, flotation, using colloidal gas aphrons proved to be an efficient technique to remove oil from wastewater.

F067: Capturing Impurities from Oil and Gas Using Deep Eutectic Solvents

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Abstract.
In this work, the performance of Deep Eutectic Solvents (DESs) for the

capture of impurities from oil and gas was investigated. The main objective was to propose a novel solution to some industrial challenges in the purification of oil and gas, and in particular, the extraction of mercury, oil desulfurization and CO_2 capture from flue gases. A series of equilibrium experiments was performed to assess workability of the DES for each application from a thermodynamics point of view.

Firstly, DESs were investigated removal of elemental mercury using DESs from oil. Their performance for mercury extraction was assessed experimentally using saturated solutions in *n*- dodecane as the model oil. The effect of the solvent ratios and temperature was studied. An extraction efficiency above 80% was obtained for all four DESs. The efficiency of the DESs together with their low cost made them a great candidates for mercury capture from oil.

Then, desulfurization of oil fuels using DESs was studied in this work. Six DESs based on ammonium salts and polyols have been experimentally investigated for the extraction of sulfur derivatives from two aliphatic hydrocarbons, viz. *n*-hexane and *n*-octane, via liquid-liquid equilibrium (LLE). The objective of this study was to provide insights on: (*i*) the LLE for {*n*-alkane + thiophene + DESs} systems, (*ii*) the effect of type/length of the *n*-alkane, (*iii*) the influences and/or characteristics of the HBAs, such as the different chain length of the alkyl group and the functional group on the ammonium cation, (*iv*) the influences and/or characteristics of the HBDs, particularly the type of the polyol and on the extraction of thiophene from an {*n*-alkane + thiophene} mixture. It was concluded that DESs are promising candidates for extractive desulfurization of fuels.

Finally, the phase behavior of CO_2 with the DESs was measured using a gravimetric magnetic suspension balance operating in the static mode at 293.2 and 298.2 K and pressures up to 2 MPa. The CO_2 solubilities in the studied DES were found to be lower than the benchmark solvents. Nonetheless, DESs are a promising class of absorbents because of their low cost starting materials and preparation, their environmentally friendly character, and their tunability which allows further optimization for CO_2 capture.

P1: Effect of Surface Treatment by Sandblasting on the Quality and Electrochemical Corrosion Properties of a C-1020 Carbon Steel Used by an Algerian Oil Company

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Abstract.
The purpose of the different operations under the term surface preparation is to get a clean surface able to be coated. It is essential to adapt this preparation in terms of the metallurgical nature of the substrate, cleanliness, its shape and roughness. Surface preparations especially the operations of sandblasting, polishing, or grinding prove of capital importance. It allows to modify the superficial properties of these materials, after these treatments the surface becomes very active.
This paper evaluates the mechanical surface treatments effect by sandblasting (Sa 1.5 and Sa 2.5) on the electrochemical corrosion characteristics of C-1020 carbon steel in 3% NaCl solution electrolyte simulating aggressive sea atmosphere. Investigations are conducted using stationary (free potential "E-t, polarization curves "E-i", the Tafel rights and the Rp) and non-stationary electrochemical tools such as electrochemical impedance. The results obtained allowed us to highlight that sandblasted carbon steel degrades with immersion time because of the roughness of the surface. These results were confirmed by the plot of the electrochemical impedance diagrams, confirming that the process governing kinetics is under charge transfer control. Good protection against corrosion cannot be obtained only with a good surface preparation of the adapted steel.

P2: Adsorption of Zn (II) and Cu (II) Ions from Wastewater Using Water Hyacinth (Eichhornia Crassipes)

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Abstract.

The adsorption of zinc and copper from aqueous solutions by dried water hyacinth as a low-cost sorbent was investigated. The influence of pH, contact time, adsorbent dosage and initial concentration was studied using batch adsorption experiments. The equilibrium was analyzed using Langmuir and Freundlich isotherm models. The data were found to have a closer correlation with the Freundlich isotherm for both zinc and copper as evidenced by a higher statistical R^2 coefficient. Results indicate that, under conditions of the experiment, the optimum contact time for removal of Zn (II) using dried water hyacinth was 10 minutes while optimum contact time for the removal of Cu (II) was 60 minutes. The optimum pH and dosage of adsorbent were found to be 4 and 3 g respectively for Zn (II), and 6.5 and 1 g respectively for Cu (II). The maximum removal of Zn (II) was about 71 % at low initial metal ion concentration of 10 ppm and 86% for Cu (II) at initial concentration of

20 ppm. The kinetics data were also subjected to pseudo-first-order and the pseudo-second-order kinetic models. The data could be explained better by using the pseudo-second-order kinetic model for both zinc and copper with R^2=0.9982 for Zn (II) and R^2=1 for Cu (II).

P3: Construction and Synthesis of Carbon Nanostructures via Domestic Microwave Oven

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Abstract.
In this work, a quick and effective method to synthesize carbon nanotubes (CNTs) is presented. Here a 600 W commercial microwave oven operating at 2.45 GHz was utilized to synthesize CNTs from plasma catalytic decomposition of polyethylene. It is shown that the use of carbon source, catalyst, and commercial microwave oven to induce plasma is necessary to carry on this synthesis. The CNTs were synthesized at 750 °C under atmospheric pressure of 0.81 mbar. Field Emission Scanning Electron Microscope (FESEM), Thermogravimetric Analysis (TGA), and Raman spectroscopy were utilized to confirm the presence and quality of produced carbon nanomaterials. Finally a comparison between the use of Polyethylene and Rick Husk as the carbon precursor was also presented.

P4: Formulation and Caracterisation of Controlled Release Ketoprofen Microsponges

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Abstract.
Microsponges are porous, polymeric microspheres drug delivery systems.

They bestow a controlled release of drugs, reduce systemic side effects and enhance stability.

The aim of the present work was:

- To formulate microsponges loaded with Ketoprofen by the quasi emulsion solvent diffusion method employing ethyl cellulose as a polymer and the polyvinyl alcohol (PVA) as an emulsifying agent.
- Study the influence of drug: polymer ratio (Ra), emulsifier concentration (Ec) and stirring rate (Sr) on the production yield (Py) using the design of experiment to identify the key factors and establish a relationship between the choosing response and those factors using analyze of variance (ANOVA)

Results showed that the production yield is affected by polymer ratio (Ra), when the ratio change from 1:1 to 1:5 the production yield change from 40.42% to 81.97%. The stirring rate has no effect and no large change in production yield values as a function of emulsifier.

The linear regression equation is: Py (%) = 61.82+20.152 Ra - 0.093 Sr-3.37 Ec-1.762 Ec*Sr, with R^2(adj) = 99.40% and S=1.17

P5: Simulation modeling for the closed-loop shipping system to transport petrochemical products from a manufacturing plant to international ports

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Abstract.

The geographical location of a petrochemical plant in UAE requires to transport products from a manufacturing plant to other ports for international shipping. For such domestic shipping, several vessels transport products from the port at the manufacturing plant to other international ports, and return to the origin port for another shipping, making a closed-loop system. While the manufacturing company can control all operations at the origin port, it has no control at other ports

because they are managed by other organizations and also used by many other companies. Due to the uncertainties of the terminal availability at the other ports, the unloading at those ports is often delayed so that the travel time of each vessel varies as well. It imposes difficulty on planning vessel schedule at the origin port. As of now, the manufacturing company utilizes ships based on a trivial policy called 'first available first use.' To improve the efficiency of the domestic vessel shipping system, it would be necessary to consider other scheduling policies.

To address aforementioned issues, this study has two objectives. The first one is to develop a scheduling policy to minimize the transportation cost while transporting all produced products. The second is to estimate the required number of vessels with respect to the production volume.

This study develops a reliable simulation model to evaluate the system performance considering all the actual operations in the system including uncertainties. Also, this study proposes two new scheduling policies (i.e., big-vessel use first and reduced returning speed) which are tested by the developed simulation model. The computational tests show that both policies can reduce the transportation cost significantly and using both policies together is preferable. The developed simulation model also determines the required number of vessels for different production volumes caused by facility maintenance or new facility installation.

P6: Integrated management of chemical product manufacturing and maritime inventory routing in the shipping system under various sources of uncertainty

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Abstract.
A maritime inventory routing (MIR) problem is a planning problem where vessel routing and inventory management at maritime transportation legs are simultaneously considered. There exists various sources of uncertainties in MIR problem, yet few studies have been concerned with the uncertainties in MIR problem. This research addresses MIR problem under uncertainty in weather, dock condition, and production plan, and reinforcement learning (RL) is used to deal with the uncertainties in scheduling problems. In the study, two levels of decision-making (strategic planning and tactical planning) are efficiently integrated by combining Markov decision process (MDP) and mathematical programming (MILP). First, strategic level (optimal fleet sizing and mixing problem) of the MIR problem is formulated in MDP, which efficiently capture recurring dynamics dominated by uncertainties, and solved with RL. Then, with the knowledge of uncertainty learned from the RL layer, the tactical level (vessel routing) of the problem is solved by mathematical programming, which can efficiently considers realistic constraints. The effectiveness of the proposed simulation architecture, such as total operation cost and computational time, is compared to a traditional robust approach with a numerical application to a container shipping system of industrial maritime corporation in UAE.

P7: Abrasion wear behavior of A105N steel after heat treatment at different temperatures (500, 600, 700 and 800 °C)

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Abstract.
The aim of this work is the study of the influence of thermal treatments on abrasive wear of A105N steel. After an austenitization treatment for 3 hours at 1100 ° C., the samples are subjected to another treatment at different temperatures 500, 600, 700 and 800 °C. The tribological study was carried out by an abrasion wear machine. The parameters selected for these tests are respectively: the sliding speed of 50 rpm and normal load of 10 N. moreover, all tests were performed without lubrication and weight loss has been measured after a course of 100m. The results showed that the steel treated at 700 °C shows a lowest wear loss indicating a high wear resistance compared to other treatments. Furthermore, the 3D surface topography observed by optical microscope shows the presence of wear particles torn; these black particles were trapped in the surface defects thus forming a third body that protects the surface against degradation.

P8: Structural and tribological behavior of AISI A2 tool steel

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Abstract.
Tool steels constitute a family of carbon steels and alloy steels that are characterized by good wear resistance. These steels are intended for manufacture of tools used for forming, cutting and machining operations of metals and alloys. Among these steels, AISI A2 which is an alloy having a chromium content of 5%, it is used as a cold working steel for cutting and forming applications. The aim of this work is to study the

tribological behavior of AISI A2 steel before and after a hardening treatment at 960 °C. Structural characterization and tribological behavior of steel were investigated using optical microscopy, scanning electron microcopy and wear testing by friction on a pion / disk device. The results obtained show a decrease in coefficient of friction due to improvement of wear resistance of AISI A2 steel by hardening treatment. This improvement is favored by precipitation of very hard particles offering a better resistance to displacement of dislocations.

P9: Hydrogen Recovery by AG2S™ Technology to Improve Hydrofinishing Process in Exhausted Oil Refineries

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Abstract.
Nowadays, the regeneration of used oils and lubricants is an important process for the improvement of sustainability and to decrease the dependence from fossil fuels. The use of lubricants allows to reduce the overall energy demand up to 4.5%. The oil regeneration consists in several process, the most important is the hydrofinishing (HDF). Its scope is to reduce the sulphur content (and in minor part nitrogen and other heterogeneous elements) and increase both the percentage of saturated components and the viscosity index, the main quality specifications for a lubricant base. HDF is a catalytic process that consume important quantity of hydrogen producing as byproduct hydrogen sulphide which must be disposed usually with Claus process. The aim of this work is to evaluate the potentiality application of a new technology (AG2S™) to traditional plant for the recovery of used lubricants. The Acid Gas to Syngas (AG2S™) technology could

improve the environmental impact reducing the CO_2 emissions, and reduce costs. Indeed, AG2S™ consist in a new approach to the reuse of acid gas, like H_2S and CO_2, converting them into syngas. The overall process, resulting from this integration effort, is referred to as Low Environmental Impact Lubricant (LEIL), and involves the three following process integrations: re-use of the H_2S produced by the HDF process as raw material for the AG2S™ technology, usage of the syngas and steam generated by the AG2S™ process as raw materials for the production of hydrogen and its use to decrease the steam reforming load and its costs. Due to its unique and highly integrated layout, LEIL is more sustainable, environmentally friendly and profitable than the original process. In addition, it allows reduction of in the carbon dioxide (CO_2) emissions compared to the standard process due to its new layout (about 0.9%). Actually, with Claus process, hydrogen re-use is not possible since it is converted to water. Standard process takes to significant CO_2 emissions due to the hydrogen carbon footprint. Global Warming Potential of steam methane reforming plant, the most used process for hydrogen production, is estimated around 8-10 kg CO_2-eq per kg H_2. Conversely, the new LEIL process allows to re-use part of the hydrogen consumed in the hydrodesulfurization operation (about 1-1.5%), reducing CO_2 emissions per unit mass of lubricant base produced. Finally, the LEIL process is also more profitable than actual process. In fact, the production of hydrogen is not only associated with a huge carbon footprint but is also expensive since steam methane reforming is an endothermic process and it involves burning a fair amount of fuel. LEIL process allows to recover hydrogen from H_2S and recycle it, decreasing the H_2 consumption per unit mass of lubricants produced (about 0.7-1%). Therefore, it reduces also the production cost per unit mass of lubricant base. This new process was simulated using the process simulation software PRO/II 10.0 by SimSci excluding the AG2S™ section which was simulated with DSMOKE®. DSMOKE® is a software tool for the simulation of a sequence of different reactors (PFR, CSTR, equilibrium…) in series or in parallel eventually coupled with mixer and/or splitter, moreover it uses a detailed kinetic scheme which

consider kinetic of carbon, nitrogen and sulphur. It was coupled with PRO/II using C++ language, the optimization methods and tools used to accomplish this task belong to a well-established numerical library, i.e. BzzMath, developed at Politecnico di Milano over the past 30 years. This configuration allows to include in a commercial software a detailed kinetic scheme and optimize the process with a robust numerical optimizer.

P10: A Study on Second Harmonic Generation Efficiency on Organic Dopant Khp Crystal

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Abstract.
A novel organic nonlinear optical material finds extensive potential application in opto - electronics field in the modernistic world. Single crystals of 2mole percent Benzene 1,3 –diol doped potassium hydrogen phthalate (RKHP) was successfully grown in deionized water with the size up to $11\times9\times2.30mm^3$ at ambient temperature by slow evaporation solution technique. The effect of organic dopant on the growth process, crystalline perfection, vibration patterns, XRD lattice parameter profile and second order NLO properties of RKHP crystal has been systematically investigated. The UV-Vis-NIR spectral analysis signifies that the RKHP crystal is transparent in entire visible and near infrared

region which has a lower cut- off wavelength at 250nm.
The dielectric constant, measured as a function of temperature and frequency showed anomalous behavior and this suggest the existence of ferro electric phase transition in the material. The incorporation of the benzene 1,3 – diol into the crystalline matrix even at very low concentration have been well examined through the vibrational assignments. The Meyer's Index number (1.1) in mechanical hardness study confirm the softness of the crystals. The mechanical parameters such as fracture toughness (Kc), brittleness index (Bi) and yield strength (σy) are calculated from the mechanical study.
The change in intensity pattern in powdered x-ray diffraction profile of dopant specimen reveals the lattice alteration with multiple peaks for highly doped specimen due to the inhomogeneous accommodation of organic molecule into the KHP. They are further supported by the slight variation in the characteristic vibrational frequency in FTIR. Thermal stability and kinetic parameters were evaluated by thermo gravimetric analyzer (TGA) and the decomposition temperature of the crystal has been noted. The photoactive nature of RKHP was confirmed by fluorescence emission spectroscopy. The second harmonic generation efficiency is enhanced at 2mole % of benzene 1,3-diol dopant using Kurtz and Perry technique and their crystalline perfection was improved. The RKHP crystal was also tested for the inhibitory activity against pathogenic microbes using disc diffusion method. Thus a good quality of synthesized transparent RKHP could act as a probable material for transducer, opto electronics and non –volatile memory device applications.

P11: Antidiabetic Activity of Extracts of Pistachia khinjuk on Alloxan monohydrate Induced Diabetic Mice

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Abstract.
Diabetes is spreading all over the world day by day. There are many ways to treat diabetes mellitus which mainly includes synthetic drugs, homeopathic medicine or Unani medicine etc. These Medicines have many side effects. Natural products; which include herbs, shrubs and large plants, cure diabetes mellitus and prove excellent hypoglycemic activity. These herbal medicines have no reported side effects. Many species of family Anacardiaceae show hypoglycemic activity and used from centuries to cure diabetes. Various pistachio species show hypoglycemic activity and have a very long history of herbal remedies. The present study evaluates the hypoglycemic effect of methanolic extract of *Pistachia khinjuk.* Six groups of Swiss albino mice were made for extract (80:20 Methanol: water) of *Pistachia khinjuk* and each group contains six albino mice. All the mice were injected alloxan monohydrate except normal group of wax and extract. Group 1 was treated as normal group and receives no treatment, group 2 receive 5mg/kg of glibenclamide after alloxan monohydrate induction, group 3 receive no treatment after alloxan monohydrate induction, group 4 and 5 receive 500 and 250mg/kg of *Pistachia khinjuk* extract, while group 6 receives 500mg/kg *Pistachia khinjuk* wax after alloxan monohydrate treatment. All the mice for extract (*Pistachia khinjuk*) of group 4, 5 and 6 show hypoglycemic activity and decreases blood glucose level. There may be many factors behind this activity which needs more research on it by isolating and analyzing specific secondary metabolites which causes this effect. The methanolic extract due to phenolic constituents proves to be excellent antidiabetic medicine.

P12: Growth of ZnO:Al by atomic layer deposition: Deconvoluting the contribution of hydrogen interstitials and crystallographic texture on the conductivity

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Abstract.
Aluminium doped ZnO (AZO) is an interesting low cost transparent conducting oxide with further use as inorganic transport layer in multilayer solar cells. Here we present our work on atomic layer deposited (ALD) thin films where with optimised growth conditions we can maintain resistivity of $1x10^{\wedge-3}$ cm even in 50-65 nm thin films grown at low temperatures (530K)We discuss the influence of crystallographic texture for ALD grown films by comparing plain glass, Al_2O_3 c-plane, and Al_2O_3 a-plane substrates. We show that the doping mechanism in ALD grown AZO is more complex than for e.g. sputtered material as a substantial hydrogen interstitial related background doping occurs. We compare results from as grown samples with those briefly annealed at 600K in nitrogen. This process leads to an increased Hall mobility due to improved grain boundary passivation, but reduced carrier concentration due to partial loss of hydrogen interstitials.

P13: Process Simulation and Modelling of Air-Cooled Condenser Using Aspen EDR

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Abstract.
An Air-cooled condenser is a device for rejecting heat from a fluid directly to ambient air. The obvious advantage of an Air-cooled condenser is that it does not require cooling water, which means that plants requiring large cooling capacities need not be located near a supply of cooling water. An air-cooled condenser (ACC) in Natural Gas Liquid (NGL) plant is modelled using Aspen EDR software, an

optimized model is developed by investigating different geometrical parameters of the air-cooled condenser. The developed model is validated using the industrial operation data available before performing the simulations. The outside heat transfer coefficients is enhanced using radiative coating and the enhancement in incorporated with the Aspen EDR software. The fan power is evaluated at different operating conditions (summer /winter) and at different air humidities and air velocities. The results showed favorable outcomes based on the simulation and optimization, the operating cost of the practical process can be reduced by a great extent (up to 40-80%).

P14: Large scale fabrication of $PtSe_2$ thin film by physical method

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Abstract.
Two-dimensional (2D) materials with single or few atomic layers have attracted significant attention from the scientific community due to their potential transport physics and prospects for technological applications. A variety of 2D materials beyond graphene with different bandgaps have been synthesized in recent years. One of them is platinum diselenide (PtSe2) with the bandgap energy of 1.2 eV at one monolayer. However, the low throughput synthesis of high quality 2D thin films has thus far hindered the development of devices. The methods of molecular beam epitaxy (MBE) and chemical vapor deposition (CVD) have been used to achieve large-scale fabrication of high quality PtSe2 films, which were fabricated from Pt thin films with different thickness through selenization process.

Pt films was deposited by using two different techniques. First, Pt films are deposited by sputtering from Pt target in Shamrock system onto

different substrates with 500 nm dry thermal oxide (SiO_2). Secondly, epitaxial Pt thin film were grown onto single crystal substrates (MgO, Al_2O_3) using MBE system. After the fabrication of $PtSe_2$, the electronic and magnetic properties of the interface between two epitaxial grown thin films of platinum diselenide and magnetite have been studied.

This work was supported by the Ministry of Education and Science of Kazakhstan under the research founding MES RK No. AP05135057 financial support.

P15: Investigation of Petro-Physical Properties at Different Scales: Numerial and Experimental Approach

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Abstract.
A clear identification of diverse attributes of flow in porous media is crucial in ever expanding oil and gas field. For example; estimation of Enhanced Oil Recovery (EOR) and sub-surface storage of carbon dioxide cannot be estimated with acceptable accuracy without sound understanding of pore structure, connectivity, wettability and permeability. During last few decades, performance of experiments to estimate hydrodynamic properties have found to take constantly disproportionate amount of time as compared to the technological advances in the field. Digital Rock Physics (DRP) is an evolving field of science which deals with the computational study of flow inside rock pores. With advances in pace of computational processes, DRP has proved to capture hydrodynamic properties quicker than ever.

In this work, a multi-scale imaging, experimental and numerical workflow was developed to determine carbonates hydro dynamic properties using Digital Rock Physics tools. The workflow was initially

applied to a standard carbonate sample (Silurian Dolomite) that exhibited less complex heterogeneities, later applied on Abu Dhabi carbonate reservoirs. The CT scans performed on different size core plugs at different resolution to perform numerical simulations, later results were compared with lab experiments.

Note

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