



# 11<sup>th</sup> Annual AIChE Midwest Regional Conference

March 18-19, 2019 University of Illinois at Chicago (UIC)

Organized by the AIChE Chicago Local Section







Monday March 18th, Morning						
7:45	8:30	8:45	9:45	10	:00	11:30
	Breakfast & R	egistration			Registration	
		Morning Keynote	Coffee Break	Track 1 Session 1	Track 2 Session 1	Lunch with
Opening	Introduction	Erin Kane, President & CEO (AdvanSix)	(Outside Cardinal)	Process Safety	Refining & Petrochemicals	Students (Illinois A&B)
	Cardir	nal Room		White Oak	Illinois C	
		Monday	v March 18th, Afte	rnoon		
12:30	1:30 1:40		3:20	3:30		
			Registration			
Afternoon Keynote		Track 1 Session 2	Track 2 Session 2		Track 1 Session 3	Track 2 Session 3
Dr. Huimin Zhao, Chemical Engineering Professor (UIUC)	Coffee Break (Outside Cardinal)	Energy & Sustainability	Process Simulation, Optimization & Control	Coffee Break (Outside Cardinal)	Bio-Medical & Nano- Engineering	Purification of Petrochemical Streams
Cardinal Room		White Oak	Illinois C		White Oak	Illinois C

Monday March 18th, Evening				
5:00	5:15 6:30			
	Registration			
	Poster Session	Local Section Meeting		
Break	Poster Viewing & Networking	Dr. Markita Landry, Chemical & Biomolecular Engineering Professor (UC Berkeley)		
	East Terrace	Cardinal Room		

Tuesday March 19th, Morning						
7:45	8:30	8:45	9:45	10	:00	11:30
	Breakfast & R	egistration		Registration		
		Morning		Track 1	Track 2	
		Keynote		Session 1	Session 1	
	Chairman's	Dr. Asha	Coffee Break		Process and	Lunch with
Opening	Introduction	Oroskar,		Solutions to	System	Students
Opening	Introduction	President &	(Outside	CO2 Brobloms	Modeling of	
		CEO of	Cardinal)	COZ Problems	Hydrocarbon	(Illinois A&B)
		Orochem			Systems	
	Cardinal Room			White Oak	Illinois C	
		Tuesday	y March 19th, Afte	rnoon		
12:30	1:15	1:30		3:10	3:20	
	Registration					
		Track 1	Track 2		Track 1	Track 2
Arternoon Keynote		Session 2	Session 2		Session 3	Session 3
Dr. Randy Snurr, John	Coffee	Modeling and		Coffee Break		
G. Searle Professor	вгеак	Simulation for	Young		Water &	Bio-Medical &
and Department	(Outside	Chemical and	Professionals	(Outside	Wastewater	Material
Chair, Northwestern	(Outside	Bio-Pharma	session	Cardinal)	Systems	Engineering
University	Cardinal)	Industry			-	
Cardinal Room		White Oak	Illinois C		White Oak	Illinois C

Tuesday March 19th, Evening		
5:00	5:30	
	Young Proffesionals Social	
Brook	Network & Relax	
ыеак	La Taberna Tapas 1301 S. Halsted St Chicago, II	
	Chicago, IL	

Track 1 {White Oak} Monday March 18 <sup>th</sup>			
Session 1: Process Safety		Chair:	
[10:00-11:30]		Peter Herena (Baker Risk)	
10:00 Common Hazards Identified During Dust Hazard Analysis (DHA)			
	Adam Connor. Baker Risk		
10:22	Correct Use of Pressure Relief Sy	stems as Independent Protection Layers	
	Todd W. Drennen, P.E., Baker Rist	k	
10:44	<b>Building Siting Evaluations: Who</b>	put that there?	
	Jessica M. Morris, Ph.D., Exponen	nt	
11:08	Balancing Protective Safety and S Peter G. Herena, Baker Risk	Spurious Trips on Safety Instrumented Systems	
Session 2:	Energy & Sustainability	Chair:	
[1:40-3:20	]	Hakim Iddir (Argonne National Laboratory)	
1.40	Safaty and Thormal Managamon	t Challongos for Li ion Battorios in Autonomous	
1.40	Vehicles Annlications	t Chanenges for Li-for Batteries in Autonomous	
	Said Al-Hallai . AllCell Technologie	es. LLC	
2:05	Techno-Economic Analysis of Li-ion Battery Manufacturing to Reduce Cost and		
	Energy		
	Naresh Suserla & Shabdir Ahmed, Argonne National Laboratory		
2:30	2:30 Facet dependent cation segregation in layered lithium transition-metal oxide		
	cathode MATERIALS		
	Juan C. Garcia, Javier Bareño, Guoying Chen, Jason R. Croy, Hakim Iddir, Argonne		
	National Laboratory		
2:55	Enabling High-Energy Lithium- ar	nd Manganese-Rich Cathodes	
	Arturo Gutierrez, Devika Choudhu	ury, Soroosh Sharifi-Asl, Reza Shahbazian-Yassar,	
	Anil Mane, Jason Croy, Argonne	National Laboratory	
Session 3:	Bio-Medical & Nano-Engineering	Chair:	
[3:30-5:00	]	Seok Hoon Hong (IIT)	
3:30	Improving colicin production via	optimizing cell-free protein synthesis	
	Xing Jin, IIT		
4:00	A new platform for nonivasively	of the differentiation stage of indiviual living	
	Isamar pastrana-Otero, UIUC		
4:30	Soft Lithography based on photo Yang Lin, UIC	lithography & two-photon polymerization	

	Track 2 {Illinois C} Monday March 18 <sup>th</sup>		
Session 1: Refining & Petrochemicals		Chair:	
[10:00-11:30]		Hadjira Iddir (UOP)	
10:00	10:00 Reduce your stack emissions for a better environment		
	Rich Johnson, UOP		
10:30	On-Purpose Propylene from Prop	pane	
11.00	Complex-wide Perspectives on F	nhanced Naphtha Upgrading	
	Bryon Egolf, UOP		
Session 2:	Process Simulation,	Chairs:	
Optimizat	ion & Control	Ha Dinh (UOP)	
[1:40-3:20	9]	Norah Ghazinoor (UOP)	
1:40 Mathematical Optimization of Membrane-free Desalination Systems that Utilize Low-grade Heat.			
2:05	2:05 Performance Assessment and Modification of an Adaptive Learning Model Predictive Control.		
2:30	2:30 How to make money in dynamic energy markets: uncertainty modeling and optimization frameworks		
2:55	2:55 Ontimizing novel membrane systems and materials discovery: mathematical		
	frameworks Elvis Eugene & William A. Phillip & Alexander W. Dowling, UND		
Session 3: Purification of Petrochemical StreamsChairs: Jay Gorawara (UOP)[3:30-5:00]Stephen Caskey (UOP)		<i>Chairs:</i> Jay Gorawara (UOP) Stephen Caskey (UOP)	
3:30	Purification of Olefinic Streams	Part I - Adsorbent Selection Criteria and	
	Fundamentals		
	Stephen Caskey, UOP		
4:00	Purification of Olefinic Streams	Part II - Applications and Process Flow Schemes	
	Stephen Caskey, UOP		
4:30	4:30 Options for CS2 removal for Naphtha fed Ethylene Crackers		
Jay Gorawara, UOP			

	Track 1 {White Oak} Tuesday March 19 <sup>th</sup>			
Session 1: Solutions to CO2 Problems		Chair:		
[10:00-11:30]		David Bahr (Carbon Clean Solutions USA, INC.)		
10:00	D:00 Reduce Operating Costs in Biogas Upgrading to Renewable Natural Gas David Bahr, Carbon Clean Solutions USA, INC.			
10:30	No Carbon Left Behind			
	Matt Hagen, LanzaTech			
11:00	Integration of CO2 Capture Into	an Existing Power Plant		
	Danielle Koren, Sargent and Lund	y LLC		
Session 2:	Modeling and Simulation for	Chair:		
Chemical and Bio-Pharma Industry Jaydeep Kulkarni (ANSYS) [1:30-3:10]		Jaydeep Kulkarni (ANSYS)		
1:30	Advanced Residue Fluid Catalytic Lev Davydov, Azita Ahmadzadeh,	c Cracking (RFCC) Regenerator Analysis Reza Mostofi, UOP		
1:55	Simulation-based digital twins to improve asset operation and maintenance management			
2:20	Lyophilizer/freeze-dryer equipment qualification using computational fluid dynamics			
2:45	2:45 A 4-Phase Model and Simulation of Methane Production from a Gas Hydrate Reservoir			
	Deniz Hinz, Hamid Arastoopour a	nd Javad Abbasian, IIT		
Session 3: Water & Wastewater SystemsChairs:[3:20-5:00]Jarad ChampionTat Ebihara (Jacobs Consultancy)		<i>Chairs:</i> Jarad Champion Tat Ebihara (Jacobs Consultancy)		
3:20	Evaluation of water treatment te	echnologies for scale reduction		
	Elliot Lewis & Mike Hickey, P.E., Geosyntec consultant			
3:40	Industrial Wastewater Treatability Studies – The Importance of Designing the Right System			
4.00	IVIIKE HICKEY, GEOSYNTEC CONSUltants			
4.00	UU Stormwater and Process wastewater Treatment Technology Selection for a			
	Tat Ebihara & Aruna Vadel, Jacob	s Consultancy		
4:20	Boiler Feedwater Treatment Tec	hnology Selection for an Industrial Complex		
	Tat Ebihara & Ken Martins & Stev	e Alt, Jacobs Consultancy		
4:40	Engineers Without Borders - El Savador Drinking Water Project Lianne Estrella, Donohue & Associates			

	Track 2 {Illinois C} Tuesday March 19 <sup>th</sup>		
Session 1:	Session 1: Process and System Modeling of Chair:		
[10:00-11:30]			
10:00 <b>Prediction of temperature profile of Sensative material during transportation</b>			
during extreme weather			
	Klaus R. Menschig, Stepan		
10:30	Gas-Solid Fluidized Bed Stripper	- A Review	
	Allan Issangya & R. Cocco & B. Fre	eireich & SB Reddy Karri, <i>PSRI</i>	
11:00	Dampening Regeneration Peak P Xiaoming Wen, UOP	Profiles of Temperature Swing Adsorption	
Session 2:	YP session	Chairs:	
[1:30-3:10	]	Larry Avtzis	
		Kim Douglas (Abbott)	
1:30	1:30 Job search for chemical Engineers		
	Robert Anderson, <i>IIT</i>		
2:20	Intro to Partcicle Technolgy		
	Ben Freireich, <i>PSRI</i>		
Section 2.	Pia Madical & Matarial	Chaira	
Enginoorin		Chuirs. Moonoch Singh (LIIC)	
[3·20-5·00	'8 1	Satish I. Parulekar (IIT)	
[3.20-3.00	J		
3:20	Synergistic effect of fatty acids a	nd nisin on inhibiting biofilm and persister	
	formation of Listeria monocytog	enes	
	Jiacheng Zhou, IIT		
3:40	A new platform for nonivasively	of the differentiation stage of indiviual living	
	Quantum Capacitance Based Am	plified Graphene Phononics for Studying	
	Neurodegenerative Diseases		
	Bijentimala Keisham, UIC		
4:00	Probiotic Leuconostoc mesenter	oides inhibits biofilm formation of Listeria	
	monocytogenes		
4.20	Kulli Fang, III	h to identify substants are stitute of subst	
4:20	A bottom-up proteomic approac	n to identify substrate specificity of outer	
	Sarah Wood Northwostern Univ	Pgie	
1.10	Sub Diffraction Limit Tomperature	cisily no Manning in Hotorogonacus Matarial	
4.40	Systems	ויפ ואמצטווא ווו הפנפוטצפוופטעג ואמנפרומו	
	Dova Vasaei Evnonent		
	r uya Tasaci, Lxpullelit		

Posters {East Terrace} Monday March 18 <sup>th</sup>			
[5:15-6:30] Chair: Adam Kanyuh (UOP)			
Inhibiting biofilm formation of pathogens using novel plant- derived chemicals	Riya Narjari & Kaixi Wu & Xing Jin & Won Keun Oh & Seok Hoon Hong		
Experimental enhancement of food waste hydrothermal liquefaction with combined effects of biochemical composition and reaction conditions	Aersi Aierzhati		
Computationally-efficient high-throughput screening of nanoporous materials for hydrogen storage	N. Scott Bobbitt & Benjamin Bucior & Arun Gopalan & Neda Bagheri & Randall Snurr		
Revealing governing mechanism of directed self-assembly of sub 10 nm particles into textured substrates	Zhen Luo		
Increased Electron Transport Inside Microbial Fuel Cell Through Interfacing Graphene with Geobacter	Sheldon Cotts & Bijentimala Keisham & Vikas Berry		
The Mechanisms of Bacteria Inactivation and Attachment on the Conductive Electrodes with Applying Low Voltages	Meng-Hsuan (Irene) Lin		
WS2-induced enhanced optical absorption and efficiency in graphene/silicon heterojunction photovoltaic cells	Rousan Debbarma & Sanjay Kumar Behura & Yu Wen & Sonwei Che & Vikas Berry		
Random Sampling of Ionic Radii and Discrete Distributions for Structural Stability and Formability of Titanium-Based Perovskites	Hisham Maddah & Vikas Berry & Sanjay Behura		
Electrochemical synthesis of ammonia as a means of energy storage by the reduction of nitrogen over copper in alkaline medium.	Nishithan C. Kani & Aditya Prajapati & Meenesh Singh		
Asphaltene aggregation and deposition on solid surfaces during EOR gas flooding	Mohammed H. Khalaf & G.Ali Mansoori		
Electrochemical Oxidation of Methane over Transition Metals and Bi-metallic Catalysts	Aditya Prajapati & Meenesh R. Singh		
Novel Carbon-Ti4O7 composites reactive electrochemical membranes for water treatment	Soroush Almassi & Brian P. Chaplin		
Optimization of an electrical discharge plasma spinning disc reactor	Joshua Luoma & Chase Nau-Hix & Selma Mededovic Thagard		
Topical Treatment for Abnormal Scars Using Spherical Nucleic Acids	Adam Ponedal & Adam Ponedal & Shengshuang Zhu & Anthony J. Sprangers & Xiao-Qi Wang & David C. Yeo & Daniel C. S. Lio& Mengjia Zheng & Suguna P. Narayan & Matt Capek & Amy S. Paller & Chenjie Xu & Chad A. Mirkin		

Engineering a Light-Responsive DNA Polymerase for Data Encoding	Joshua Saltzberg & Alec Castinado & Keith Tyo
Data-Driven Methods to Accelerate the Design of Metal-Organic Frameworks	Benjamin Bucior & N. Scott Bobbitt & Nathaniel Tracy- Amoroso & Arun Gopalan & Randall Q. Snurr
A Novel Anion Exchange Membranes with Excellent Performance in Vanadium Redox Flow Batteries	Allison Nordvall & Tongshuai Wang & Chulsung Bae & Sangil Kim
A novel ion selective membrane for Lithium Polysulfide Redox Flow Batteries	Yuechen Gao & Tongshuai Wang & Chulsung Bae & Sangil Kim
High efficient ion selective membrane separator for room temperature sodium polysulfide redox flow batteries	Xueyang Wang & Aazadeh Amiri & Tongshuai Wang & Chulsung Bae & Sangil Kim

2019 AIChE Midwest Regional Conference Volunteers				
MRC 11 Chairs	Conference Chair: Dennis O'Brien			
	Academia Programming Chair: Satish J. Parulekar			
	Industrial Programming Chair: Patrick Shannon			
MRC 11	Adam J Kanyuh	Ellen Arnold	Rachel Brenc	
Organizing	Azita Ahmadzadeh	Janet Werner	Reza Mostofi	
Commitee	Betul Bilgin	Jeffrey Zalc	Robert Tsai	
	Connor Wegner	Kimberly Douglas	Shahineze Saada	
	Don Chmielewski	Larry Avtzis	Shannon Brown	



	Keynote Speakers {Cardinal}
	Monday March 18 <sup>th</sup> , 8:45 am
	Erin Kane
	President and CEO, AdvanSix Inc.
	"AdvanSix Spin: Challenges and Opportunities for our 90 yr old "New"
	Company
	Monday March 18 <sup>th</sup> , 12:30 pm
1000	Huimin Zhao
4-51	Professor, University of Illinois at Urbana-Champaign
	"Biosystems Design by Directed Evolution"
	Monday March 18 <sup>th</sup> , 5:15 pm
	[Chicago Section Monthy meeting]
(-> P	Markita Landry
	Assistant Professor LIC-Berkeley
	"Nanomaterials Engineering to Probe and Control Living Systems"
1	Tuesday March 19 <sup>th</sup> , 8:45 am
ad,	
	Asha Oroskar
	President and CEO, Orochem Technologies Inc.
	"Natural vs Synthetic molecules for Health & wellbeing: Why does
	Nature always win in the end??"
	T
Der Contraction	Tuesday March 19 <sup>th</sup> , 12:30 pm
1364	Pandy Snurr
	Professor and Department Chair, Northwestern University
	"Metal-Organic Frameworks at Tunable Diattforms for Gas Storage
	Chemical Separations and Catalysis"

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Oak Brook Pointe 700 Commerce Drive, Suite 200 Oak Brook, IL 60523-1702 630.756.7000 | contactus@middough.com www.middough.com <u>Process Safety</u> Monday, March 18<sup>th</sup> Session 1, Track 1 Chair: Peter Hereña

### Common Hazards Identified During Dust Hazard Analysis (DHA)

Adam Connor, *Baker Risk* Abstract Forthcoming

### Correct Use of Pressure Relief Systems as Independent Protection Layers

Todd W. Drennen, P.E., Baker Risk

For Layers of Protection Analysis (LOPA) scenarios involving overpressure of equipment, pressure relief systems are often given significant Independent Protection Layer (IPL) credit, and in most cases this is appropriate. However, LOPA teams need to be aware of the many factors of design, installation, and maintenance of these systems that must be properly addressed in order for this IPL credit to be valid. These factors are represented in the context of generic IPL criteria of Independence, Functionality, Integrity, Reliability, and Management of Change. Auditability, Additionally, appropriate IPL credit for multiple relief devices and the use of rupture disks in combination with pressure relief valves is defined, and best practices are presented for developing recommendations that most effectively address identified LOPA gaps.

### Building Siting Evaluations: Who put that there?

#### Jessica M. Morris, Ph.D., Exponent

There is no "one-size-fits-all" blueprint for designing the infrastructure and layout for a process plant. All process plants and facilities are laid out according to their own unique constraints. Property boundaries, chemical inventories, buildings, personnel, and other factors can all have a significant effect on the facility layout through building siting. Recommended practices for building siting are discussed, as described in API RP 752. The two generalized approaches for building siting are (1) prescriptive and (2) risk-based. The prescriptive approach utilizes "spacing tables" or index methods relying on experience-based rules. The risk-based approach applies consequence analysis for maximum credible events that may affect each building. These two approaches to building siting are explored in this presentation, and the pros and cons of each method will be presented using an example propane facility.

#### Balancing Protective Safety and Spurious Trips on Safety Instrumented Systems

Peter G. Hereña, Baker Risk

This presentation will describe methods by which operating companies can optimize Safety Instrumented System (SIS) design and test methods to achieve specific safety or financial goals. Doing so requires understanding of traditional SIS performance metrics like probability of failure on demand (PFD), combined with economic metrics of installed cost, maintenance cost, and cost due to spurious trip. Using principles of reliability theory and a cost prediction model, it is possible to optimize for lowest lifecycle cost, lowest installed cost, highest onstream time, maximum safety within a specific cost constraint, or other objectives.

#### Energy and Sustainability

Monday, March 18<sup>th</sup> Session 1, Track 2 Chair: Hakim Iddir

#### Safety and Thermal Management Challenges for Li-ion Batteries in Autonomous Vehicles Applications

#### Said Al-Hallaj , AllCell Technologies. LLC

The presentation will provide an overview of safety and thermal management challenges of Li-ion batteries in electric mobility and autonomous vehicles applications. Li-ion batteries are the energy storage technology of choice for electric mobility, autonomous vehicles and smart grid applications due to its high energy density, higher power, long cycle life, and cost. However, major concerns of its safety were highlighted in recent high profile fire events which unless addressed properly will hinder further development and market growth. Successful attempts to prevent thermal runaway propagation in Li-ion batteries has been reported in the literature and will be discussed in this presentation.

#### Techno-Economic Analysis of Li-ion Battery Manufacturing to Reduce Cost and Energy

Naresh Suserla & Shabdir Ahmed, Argonne National Laboratory

Lithium ion batteries are becoming increasingly popular for their use in hybrid and battery electric vehicles. The drive towards large-scale commercialization of electric or hybrid electric automobiles is challenged by high battery prices. The U.S. Department of Energy (U.S. DOE) has sponsored programs in support of the U.S. Advanced Battery Consortium (USABC) [1] goals to develop battery packs for battery electric vehicles (BEV) with selling price of \$100 per kWh. Argonne National Laboratory has developed, BatPaC [2], a comprehensive spreadsheet tool for estimating the cost of Lithium Ion Batteries (LIB). BatPaC enables the design of automotive lithium ion batteries, using specifications such as the energy storage capacity, the electrode chemistry combination, and a host of other parameters and constraints. The model then estimates the cost of this battery when produced in large volume, typically 100,000 packs per year. In this work, each cost contributing component, ranging from materials costs to the cost of unit operations, is studied in detail to identify methods and the extent of reduction possible to minimize the overall battery cost. Detailed process and economic models are developed to estimate the cost and energy required in the manufacturing of lithium ion batteries. As the cost of materials is a major contributor to the overall battery cost, the primary focus of this work is to identify production routes to reduce material costs. Techno-economic models are developed to estimate the cost and

energy required to produce a variety of battery materials including cathode materials such as nickel-cobalt-manganese oxide (NCM) [3] and lithium manganese oxide (LMO) and electrolytes materials such as lithium hexafluorophosphate (LiPF6) [4]. In this presentation, a collage of results will be presented highlighting the key learnings and outcomes from the aforementioned studies. The results will show the impact of various process, operating, and economic parameters on the overall battery cost. Also, the pathways to minimize the battery manufacturing cost will be outlined.

# Facet dependent cation segregation in layered lithium transition-metal oxide cathode materials

Juan C. Garcia, Javier Bareño, Guoying Chen, Jason R. Croy, Hakim Iddir, Argonne National Laboratory

Abstract Forthcoming

### Enabling High-Energy Lithium- and Manganese-Rich Cathodes

Arturo Gutierrez, Devika Choudhury, Soroosh Sharifi-Asl, Reza Shahbazian-Yassar, Anil Mane, Jason Croy, Argonne National Laboratory

Lithium- and manganese-rich (LMR) composite materials are attractive due to the inherent safety and relative low cost of manganese based cathodes when compared to compositions where nickel or cobalt comprise  $\geq$  50% of the transition metal content. Moreover, LMR composites exhibit high initial specific energy densities (800 - 1000 Wh/kgoxide) due to their high reversible capacities (250 – 300 mAh g-1). Yet, there are a couple of major challenges that need to be addressed for wide scale adoption of LMR composite materials. First, irreversible structural changes (i.e. surface reconstruction, oxygen loss, migration of metals and dissolution) are initiated during 1st cycle activation, which lead to energy fade of the system upon extended cycling. Second, the LMR cathode experiences high area-specific-impedance (ASI) when the cathode material is at states-of-charge

 $(SOC) \le 50\%$ , which will also negatively affect the electrochemical performance. Therefore, new strategies to mitigate surface reconstruction and high specific impedance must be developed and understood in order to facilitate greater use of LMR composite materials in electric vehicle applications. This presentation will provide an overview of some of the strategies being developed with this end in mind.

#### **Bio-medical & Nano-Engineering**

Monday, March 18<sup>th</sup> Track 1, Session 3 Chair: Seok Hoon Hong

## Improving colicin production via optimizing cell-free protein synthesis

#### Xing Jin, IIT

Colicins are antimicrobial proteins produced by Escherichia coli and have a great potential to be developed as a viable alternative of antibiotics. Cell-free protein synthesis (CFPS) is an excellent platform to produce toxic proteins as it eliminates cell viability concern which is a frequent problem in cell-based protein production. Previously, we demonstrated that colicins produced by CFPS are active in eradicating antibiotic-tolerant bacteria known as persisters, but some colicins exhibited poor solubility or cell-killing activity. In this study, we improved solubility of colicin M from 16% to nearly 100% by supplementing chaperoneenriched E. coli extracts. Cytotoxicity of colicin E3 was increased by adding or co-producing the E3 immunity protein during CFPS reaction, implying that the E3 immunity protein is necessary to enhance the colicin E3 activity in addition to protecting the host strain. We also identified that the colicins are synthesized rapidly; colicin E1 within three hours of incubation was produced to the similar level of activity and solubility compared to the colicin incubated up to 20 hours. Taken together, colicin production could be easily optimized using CFPS platform for improving the solubility and activity of colicins.

A New Platform for Noninvasively Identifying of the Differentiation Stages of Individual,

#### Living Hematopoietic Stem Cells in Response to Extrinsic Cues Using Raman Micro-

#### Spectroscopy and Multivariate Analysis

#### Isamar pastrana-Otero, UIUC

Blood cancers result from anomalies during hematopoiesis, which is the process of producing the blood and immune cells in the body via hematopoietic stem cell (HSC) differentiation. Bone marrow transplantation is used to replace the mutated HSCs in the cancer patient with healthy HSCs from a living donor. To enable expanding HSCs outside the body for transplantation, the effects of extrinsic cues on HSC fate decisions to self-renew or differentiate must be determined. Microscale platforms have been developed to minimize the number of rare HSCs needed to screen the effects of various extrinsic cues on HSC fate decisions. However, conventional techniques cannot accurately and noninvasively identify differentiation stages on the single cell level. To address this obstacle, we have shown that partial least square-discriminant analysis (PLS-DA) of single cell Raman spectra can accurately identify the lineages of fully differentiated cells from laboratory lines, and the differentiation stages of individual, chemically fixed cells from distinct hematopoietic cells populations. To enable using this approach to screen the fate decisions of individual, living HSCs and their progeny within microscale screening platforms, an artificial bone marrow niche that is compatible with Raman microspectrsocopy analysis of living cells must be developed. Towards this aim, Raman-compatible substrates have been fabricated, and hydrogels functionalized with extracellular matrix protein found in the bone marrow niche were synthesized on their surfaces. The ability to identify the differentiation stages of primary hematopoietic stem and progenitor cells harvested from mice using single cell Raman microspectroscopy and PLS-DA was evaluated. Future work will aim to incorporate cytokines and bone marrow niche cells into the platform and optimize the Raman microspectroscopy and PLS-DA approach. Successful development of this microscale screening platform will facilitate efforts to identify the effects of matrix stiffness, cytokines,

ligands, and niche cells on early HSC fate decisions and may accelerate progress towards the ultimate goal of in-vitro HSC expansion.

### Soft Lithography based on photolithography & two-photon polymerization

Yang Lin, UIC

Over the past decades, soft lithography has greatly facilitated the development of microfluidics due to its simplicity and cost-effectiveness. Numerous fabrication techniques such as multi-layer photolithography, stereolithography and other methods have been developed nowadays to fabricate master moulds with complex 3D structures. But these methods are usually subjected to low resolution or sophisticated fabrication procedures. Besides, high-resolution methods such as two-photon lithography, electron-beam lithography, and focused ion beam are often restricted by fabrication speed and total fabricated volume. Given the fact that the region of interest in typical microfluidic devices is usually very small while the rest of the structure does not require complex 3D fabrication methods, conventional photolithography and two-photon polymerization are combined for the first time to form hybrid approach in fabricating master moulds. It not only benefits from convenience of photolithography, but also gives rise to complex 3D structures with high resolution based on twophoton polymerization. Finally, a 3D passive micromixer was created as the demonstration along with studies of the key parameters during fabrication to further prove the concept.

#### Refining and Petrochemicals

Monday, March 18<sup>th</sup> Track 2, Session 1 Chair: Hadjira Iddir (UOP)

### Reduce your stack emissions for a better environment

#### Rich Johnson, UOP

The oil refining industry produces many products for the world to use. During the refining process energy is used and the combustion products are sent to the atmosphere. This discussion is focused on the fluid catalytic cracking unit (FCC) which generates a large amount of combustion gases during the catalyst regeneration process. Due to the nature of the FCC feed, the stack gas will include various amounts of sulfur oxides (SOx), nitric oxides (NOx) along with catalyst particulate matter (PM). These are considered the main pollutants that could be emitted into the atmosphere and can be detrimental to the environment. There are regulations around the world that limit the quantities emitted. Thus, pollution control devices are added to the FCC flue gas, upstream of the stack, to reduce the amount of the SOx, NOx, and PM. Each component requires a specific method for removal. In this presentation, we will discuss these technologies and the levels of reduction possible. By reducing these pollutants, the surrounding environment is better

protected.

#### **On-Purpose Propylene from Propane** Mike Vetter, *UOP*

Honeywell UOP's Oleflex technology uses catalytic dehydrogenation to convert propane to propylene and isobutane to isobutylene. Honeywell UOP's Oleflex technology is proven to have the lowest cash cost of production and the highest return on investment compared with competing technologies. Its low energy consumption, low emissions and fully recyclable, platinumaluminabased catalyst system minimizes its impact on the environment. Independent reaction and regeneration systems are in place that allow continuous use of catalysts for steady state operation. The unique process design maximizes operating flexibility and on-stream reliability.

In addition to the C3 Oleflex process, Honeywell UOP also licenses C4 Oleflex technology, which converts isobutane to isobutylene, the primary ingredient for making high-octane fuel and synthetic rubber. Honeywell UOP is a leading international supplier and licensor of process technology, catalysts, adsorbents, equipment, and consulting services to the petroleum refining, petrochemical, and gas processing industries. Honeywell UOP is part of Honeywell's Performance Materials and Technologies strategic business group, which also includes Honeywell Process Solutions, a pioneer in automation control, instrumentation and services for the oil and gas, refining, petrochemical, chemical and other industries.

### Complex-wide Perspectives on Enhanced Naphtha Upgrading

#### Bryon Egolf, UOP

Catalytic naphtha reforming is a key process technology within the refining and petrochemicals industry. The process is best known for providing high octane gasoline and hydrogen; however, is also a primary source for para-xylene and benzene used in the production of plastics. Honeywell-UOP has provided a long history of innovations into the industry since first inventing the catalytic reforming process in the late 1940's. This presentation will introduce the process, and discuss the business drivers shaping how the process is integrated with other process units in a modern refining & petrochemical complex.

#### Process Simulation, Optimization, and Control

Monday, March 18<sup>th</sup> Track 2, Session 2 Chairs: Ha Dinh (UOP) and Norah Ghazinoor (UOP)

#### Mathematical Optimization of Membranefree Desalination Systems that Utilize Lowgrade Heat.

Alejandro Garciadiego, UND

Access to clean, fresh water is an ever-growing concern for modern society: water is critical to ensure human health, to protect threatened ecosystems, and to promote economic growth and prosperity. Modern seawater desalination technologies remain energy intensive; they required three to four times the theoretical minimum energy for separation. This underscores the critical need for energy efficient and renewable driven desalination technologies to address these expanding needs for clean water. Directional solvent extraction is a promising new desalination technology. It relies on liquid-liquid extraction with a thermoresponsive solvent that can be regenerated using low-grade heat. Previous work has relied on experimental testing and insights from molecular simulations to explore new thermoresponsive solvents.

In this work, we propose the first mathematical optimization framework for the DSE process with the ultimate goal of systematically guiding molecular discovery of new thermoresponsive solvents. Additionally, we discuss the importance of predictive thermodynamic models for our framework. Preliminary results show that with the use of high efficiency heat recovery DSE could be a competitive renewable membrane-free desalination technology.

#### Performance Assessment and Modification of an Adaptive Learning Model Predictive Control.

#### Iman Hajizadeh, IIT

Control of chemical processes with time-varying parameters and nonlinear dynamics is challenging. The presence of stochastic disturbances, random measurement noises and unknown time-varying delays can make the problem more complex. A time-invariant model cannot describe the dynamic behavior of these processes accurately and an offline-tuned controller cannot perform satisfactorily when the process is subjected to major disturbances1,2.

In this work, we propose a data-driven recursive subspace identification approach and an adaptive learning model predictive control (ALMPC) with a comprehensive controller performance assessment system (CPAS). To obtain an accurate and reliable time-varying model of the process, we extended the optimized version of the recursive predictor-based subspace identification method to better handle stochastic disturbances, measurement noises, and variable delays3-5. This is done by incorporation of constraints on the fidelity and accuracy of the identified models, correctness of the sign of the input-to-output gains, and the integration of heuristics to ensure stability of the recursively identified models. Then, an ALMPC is designed using this recursively

updated model to handle constraints on the manipulated variables and outputs as well as any safety limits of the process6. To make the controller more efficient for mitigating the effects of unknown disturbances, the controller parameters are modified using information from a feature extraction method that can detect significant changes based on the rate and shape of variations in the outputs in real-time.

Furthermore, a CPAS is developed to analyze the closed-loop behavior and modify the parameters of the control system. To this end, various performance indices are defined to quantitatively evaluate the controller efficacy in real-time. The controller assessment and modification module also incorporates on-line learning from historical data to anticipate impending disturbances and proactively counteract their effects.

Using a multivariable simulation platform for type 1 diabetes mellitus (T1DM), the CPAS is applied to the problem of regulating blood glucose concentrations (BGC) in people with T1DM by means of controlled insulin delivery with artificial pancreas (AP) systems, and the results demonstrate the improvement in controller performance using the assessment module. The results based on new developed techniques show an excellent performance in increasing the average percentage of time spent in the target range (BGC  $\in$  [70, 180] mg/dL) by 38 % and reducing the mean and standard deviation of BGC by 43 and 13 mg/dL, respectively. The average maximum value of BGC was reduced by 52 mg/dL without any significant change in the average minimum value of BGC (a decrease of 4 mg/dL). These outcomes demonstrate a significant improvement in the AP system and their potential to be used in developing a fully automated AP that can function without any manual information and accommodate major disturbances to the BGC.

#### How to make money in dynamic energy markets: uncertainty modeling and optimization frameworks

#### Xian Gao, UND

The electricity markets under the smart grid paradigm provide the diverse energy resources many lucrative opportunities. We compare two frameworks, self-schedule and bidding via offering curves, for participating in both day-ahead market (DAM) and fifteen-minute market (FMM), using historical data from California. We show how to combine probabilistic price forecasts and twostage stochastic programming to maximize realized revenues from energy market participation while managing risk.

#### Optimizing novel membrane systems and materials discovery: mathematical frameworks

#### Elvis Eugene, UND

Membrane systems are superior to current separations processes because of lower footprints (compactness) and lower mass transfer limitations (rapidity) and are therefore an exciting field of research for sustainable technology. However, there exists a critical need to systematically identify the most promising applications for novel membrane materials and identify the gaps in scientific knowledge that most inhibit their translation to scalable technologies.

In the first example, at the materials (nano-) scale, we explore the feasibility of triblock polymers for residential water purification systems to remove heavy metal contaminants. We develop a systemsscale mathematical model for an arbitrary adsorption based separations process and perform sensitivity analysis to set nanomaterial performance targets. For the water purification case study, we find that we already have the materials needed to efficiently remove heavy metal contaminants at home. However, the cyclic nature of the adsorption process would necessitate the development of new infrastructure to regenerate depleted membranes yearly, which is one of the future directions we will be exploring in this project.

the second example, In we propose а superstructure optimization framework to elucidate novel configurations of staged membrane processes in a continuous diafiltration cascade. In continuous diafiltration processes, dialysate is strategically added to offset concentration effects and achieve recovery of high

purity and high-value products. Although common for niche separations in industry, few studies have systematically analyzed multi-stage diafiltration processes. In an illustrative case study, we show how combining novel recycle strategies with modest improvements in membrane materials could enable new lithium and cobalt separation technologies for battery recycling.

Finally, we conclude with some remarks on future opportunities for systems engineering to guide material discovery and ultimately realize integrated engineering frameworks that span molecular to infrastructure scales.

#### **Purification of Petrochemical Streams**

Monday, March 18<sup>th</sup>

Track 2, Session 3

Chairs: Jay Gorawara (UOP) and Stephen Caskey (UOP)

#### Purification of Olefinic Streams Part I -Adsorbent Selection Criteria and Fundamentals

#### Stephen Caskey, UOP

Adsorbents play a key role in the safe, efficient production of olefins for the petrochemical industry. Adsorbents are used for the removal of contaminants allowing hydrocarbon products to meet key specifications and protecting expensive downstream catalysts from deactivation. There are several classes of adsorbents used in olefinic service: 1) physical adsorbents such as UOP MOLSIVTM adsorbents, aluminas, and hybrid alumina/zeolite and 2) reactive adsorbents such as UOP GB products based on metal oxides and sulfides. The fundamentals of adsorbents will be discussed.

The appropriate selection of adsorbents depends on a multitude of factors beginning with the type and concentration of the contaminant to be removed. Furthermore, feedstock compositions and operating conditions are key concerns. An additional, often overlooked, factor in the selection of an adsorbent for purification of olefinic streams is the minimization undesirable side reactions of the feed olefins such as isomerization, oligo/polymerization, and hydrogenation. These reactions are exothermic and can lead to safety concerns. Furthermore, undesirable reactions can lead to coking on the adsorbent and shorten adsorbent life. The key criteria for adsorbent selection will be presented.

#### Purification of Olefinic Streams Part II -Applications and Process Flow Schemes Stephen Caskey, UOP

Adsorbents have long been used in the processing of olefinic streams from steam crackers in the production of high purity olefin products. The rise of refinery-petrochemical integration has only increased the demands on adsorption units as refinery derived feedstocks are generally considered to have higher level of harder to remove contaminants. Two general classes of adsorbents are used - regenerable and nonregenerable adsorbents. The process unit for a non-regenerable adsorbent is a simple flowthrough unit where an adsorbent is used for a given period of time and then replaced as needed. On the other hand, additional considerations are necessary in the implementation of a regenerable adsorbent. Three types of regenerations are possible including thermal, pressure, and concentration swing processes. A combination of these approaches is often used to optimize the working capacity of an adsorbent. Examples of key adsorption units using UOP adsorbents in petrochemical production will be discussed.

#### Options for CS2 removal for Naphtha fed Ethylene Crackers

#### Jay Gorawara, UOP

Ethylene Producers have linked carbon disulfide (CS2) in petrochemical grade naphtha to corrosion in locations downstream of the cracker as well as to deterioration of pygas hydrogenation catalyst activity. This has led some producers to implement very low specifications (ppm levels) of CS2 in petrochemical grade naphtha. Consequently, high CS2 containing petrochemical grade naphtha has resulted in it being discounted, and limits its pool

#### of potential customers.

To help meet this growing need to reduce CS2 content of petrochemical naphtha, UOP has developed a new adsorbent, MOLSIV<sup>™</sup> CS2-100, for CS2 removal. Extensive pilot plant testing with a variety of commercial feeds has been conducted to demonstrate the technical and economic viability of an adsorptive solution. In addition, UOP is leading the efforts to commercialize an adsorbent to remove CS2 from pygas. An adsorptive solution for CS2 removal in this stream will allow ethylene producers the flexibility to choose the most cost effective naphtha feedstock without the associated disadvantages of processing CS2 containing naphtha.

#### Solutions to CO<sub>2</sub> Problems

Tuesday, March 19<sup>th</sup> Track 1, Session 1 Chair: David Barr (Carbon Clean Solutions USA, INC.)

### Reduce Operating Costs in Biogas Upgrading to Renewable Natural Gas

David Bahr, Carbon Clean Solutions USA, INC. Abstract Forthcoming

#### No Carbon Left Behind

Matt Hagen, LanzaTech

As a global community, we today face an increasing challenge and responsibility to drastically reduce greenhouse gas emissions (GHG) in the transport and chemicals supply chain. Over the years, the global refining industry has stepped up its efforts to produce cleaner burning transport fuels primarily from a SOx, NOx and PM standpoint. Renewable fuels legislation has also been adopted in most geographies to address GHG emissions from the ground transport sector. To produce the volumes needed to support decarbonization of the transport sector, however, we must look at a broader pool of options, including technologies

that can produce low carbon fuels for blending, with no impact on land or food resources.

LanzaTech has developed a gas fermentation technology that converts recycled carbon rich industrial off gases from many industries including the metals processing and oil refining industries into fuels and chemicals. This technology has now been demonstrated at commercial scale and represents a novel biological pathway for low carbon fuel and chemical production, while adding value to industrial waste streams. This approach embodies the circular economy as it takes waste streams to make new products with reduced environmental impact.

### Integration of CO2 Capture Into an Existing Power Plant

Danielle Koren, Sargent and Lundy LLC Abstract Forthcoming

<u>Modeling and Simulation for Chemical</u> <u>and Bio-Pharma Industry</u> *Tuesday, March 19<sup>th</sup> Track 1, Session 2 Chair: Jaydeep Kulkarni (ANSYS)* 

### Advanced Residue Fluid Catalytic Cracking (RFCC) Regenerator Analysis

Lev Davydov, Azita Ahmadzadeh, Reza Mostofi, *UOP* 

A Residue Fluid Catalytic Cracking (RFCC) regenerator typically consists of two consecutive bubbling beds combusting coke on deactivated catalyst under partial burn (below stoichiometric) conditions. The RFCC regenerator may well be the largest piece of equipment in a refinery, so improvement in coke combustion efficiency in such a vessel can make it smaller and shorter and thus reduce capital investment for a new RFCC unit.

CFD analysis was employed to understand the flow patterns inside the regenerator and develop a more efficient design. A two-fluid model for gas and solids, coupled with the kinetic theory, and employing the EMMS drag force correlation were used to simulate the flow of air and particles and their respective residence time distribution in the regenerator. The new regenerator design features a compartmentalized second stage with individual air distributors supplying air to each compartment. Because of different air flow rates through these air distributors, the EMMS drag model was tuned differently for the flow in the inner and outer compartment to match the commercial observations from similar systems.

CFD results shows the radial pressure decreases at the bed interface from the regen center to the chamber wall. Residence time distributions of air showed a typical bubbling bed behavior corresponding to four CSTRs in series per compartment, while those of catalyst followed a two-CSTR behavior. Compartmentalization led to a more efficient use of oxygen in the regenerator which now required smaller fluidized bed volumes to sufficiently regenerate catalyst. The latter directly translates into the capital costs of the vessel.

## Simulation-based digital twins to improve asset operation and maintenance management

Anchal Jatale and Jaydeep Kulkarni, ANSYS, Inc.

Abstract Forthcoming

#### Lyophilizer/freeze-dryer equipment qualification using computational fluid dynamics

Tong Zhu, AbbVie

Abstract Forthcoming

#### A 4-Phase Model and Simulation of Methane Production from a Gas Hydrate Reservoir

Deniz Hinz, Hamid Arastoopour and Javad Abbasian, IIT

Abstract Forthcoming

#### Water and Wastewater Systems

Tuesday, March 19<sup>th</sup> Track 1, Session 3 Chair: Tat Ebihara (Jacobs)

### Evaluation of water treatment technologies for scale reduction

Elliot Lewis, Geosyntec consultant

Geosyntec was retained by a process engineering firm to conduct a water softening technology evaluation in support of an overall plant expansion design for their client, a chemical manufacturer in the greater Chicago region. The client has historically experienced scaling issues within their boilers, cooling towers, and utility piping due to excessive hardness of the source water. The plant uses groundwater sourced from a well on-site to provide utility, process, and drinking water. Sodium zeolite ion exchangers are used to treat boiler feedwater, otherwise no additional treatment is provided for utility water at the facility.

To address these issues, current and projected facility water usage was reviewed to develop an overall water balance. Based upon usage patterns and raw water chemistry, strategies for hardness removal focused on centralized and decentralized water softening, treated water storage, boiler feed water polishing, and waste management. Several alternatives for water softening were evaluated, including cold lime softening via a solids contact clarifier, lime pellet softening, ion exchange, and reverse osmosis. Cost and non-cost factors were used to compare each alternative and to develop a final recommendation for the system.

#### Industrial Wastewater Treatability Studies – The Importance of Designing the Right System

#### Mike Hickey, Geosyntec Consultants

Treatability studies are an important step in the process design of industrial wastewater treatment systems. The complex waste composition and variable concentrations often seen in industrial wastewater create an additional layer of risk in the design process. Treatability studies can reduce risk and save clients time and money spent pursuing a design of the wrong system. This presentation will present two case studies, where treatability studies identified potential issues with conceptual treatment methods prior to system design.

Case Study 1 - Geosyntec performed a treatability study to determine the feasibility of using a sequencing batch reactor (SBR) to provide secondary treatment of wastewater produced from the cleaning process during the production of airplanes at a future facility in Zhoushan, China. The main objectives of the testing were to prove the SBR technology could sufficiently remove the BOD to below the discharge limit of the new facility as well as to determine the kinetics of the reaction to assist in the design of a full-scale system. During the testing, the growth of poor settling bacteria was observed, indicating the need for additional operation controls for the full-scale design.

Case Study 2 - Geosyntec performed a treatability study to determine the feasibility of chemical precipitation to remove discrete solids from a pharmaceutical company wastewater stream. The main objective of the testing was to determine the chemical dose rates and sludge volume produced to appropriately design the full-scale system. Testing showed the necessary chemical addition rates and subsequent sludge volume would be impractical for full-scale application.

#### Stormwater and Process Wastewater Treatment Technology Selection for a Fuel Terminal Facility

#### Tat Ebihara, Jacobs Consultancy

The process evaluation and design basis for a wastewater treatment facility is presented for a fuel terminal in Australia. A treatment system was needed to meet anticipated water discharge requirements for both process wastewater and stormwater. Several alternative treatment technologies considered were gravity separation, dissolved gas flotation, granular activated carbon (GAC) polishing beds, and constructed wetlands.

The equipment configuration and expected operating and performance ranges for these unit processes are presented. The primary technologies selected for further process development was coalescing plate oil-water separation and GAC treatment. The design basis for both process wastewater and stormwater was developed as part of this project. This process evaluation included effectiveness in meeting final water quality objectives, costs, operability, reliability, maintainability, and regulatory requirements. The final process configuration selected to be the most cost-effective and lowest risk treatment for this application was an interceptor pit, coalescing plate separator, bag filtration, and GAC polishing beds prior to final discharge to surface water. Management procedures for solids generated by the treatment system were also developed. The final portion of this process evaluation included sizing criteria for each major component, reflecting best industry practice, as well as the predicted effluent criteria and design targets for the overall treatment process.

## Boiler Feedwater Treatment Technology Selection for an Industrial Complex

#### Tat Ebihara, Jacobs Consultancy

"Early phase process evaluation and decision analysis for a 7,800 gallon per minute boiler feedwater treatment process is presented for a major Midwestern U.S. industrial complex to improve steam system reliability. Four water sources were considered for the new steam system: Great Lakes water, local groundwater, groundwater under the lake bed, and recovered cooling water. The Great Lakes water source presented the lowest total dissolved solids and lowest risks for pre-treatment reliability. Several pretreatment alternative concepts were considered for solids and turbidity removal including media filters, microfiltration, and gravity clarification. Treating maximum seasonal turbidity using chemical coagulation and clarification upstream of ultrafiltration was considered to be the most cost-effective and lowest risk technology for this application. Demineralization technology

alternatives were a combination of six reverse osmosis and/or ion-exchange configurations:

1- Two-Pass Reverse Osmosis and Electrodeionization polishing

2- Two-Pass Reverse Osmosis with Decarbonation, and Electrodeionization polishing

3- Single Pass Reverse Osmosis with Decarbonation and Mixed-Bed Ion Exchange polishing

4- Two-Pass Reverse Osmosis

5- Two-Bed Ion Exchange with Decarbonator and Mixed-Bed Ion Exchange polishing

6- Two-Bed Ion Exchange with Decarbonator and Cation Ion Exchange polishing

The six alternative demineralization processes were evaluated through a multi-objective decision analysis (MODA) that includes consideration of ability to meet water quality target objectives, costs, operability, robustness, maintainability, technology risks, environmental impacts, and permitting requirements. The costs for each of the treatment process configuration were considered for a system capable of delivering a sustained peak flow of 7,800 gallons per minute of finished water. Results of the MODA analysis and cost analysis resulted in the final selection of two-bed ion exchange, with decarbonator, and mixed-bed ion exchange polishing process.

Engineers Without Borders - El Savador Drinking Water Project

Lianne Estrella, Donohue & Associates Abstract Forthcoming

Process and System Modeling of Hydrocarbon Systems

Tuesday, March 19<sup>th</sup>

Track 2, Session 1

Chair: Adam Kanyuh (UOP)

Prediction of temperature profile of Sensative material during transportation during extreme weather

Klaus R. Menschig, Stepan

Shipping temperature sensitive material requires provisions during times of extreme weather. A simple heat loss model was developed based on the open source CFD platform, OpenFOAM, and its laplace solver for heat transfer. The presentation covers the mesh and solver development, resulting solutions, comparison to experimental values, and parameters to consider.

#### Gas-Solid Fluidized Bed Stripper - A Review

Allan Issangya, PSRI

A hydrodynamics review of fluidized bed strippers as influenced by types of internals and operating conditions.

### Dampening Regeneration Peak Profiles of Temperature Swing Adsorption

Xiaoming Wen, UOP

Temperature Swing Adsorption (TSA) processes have been widely used for natural gas processing for removing water, sulfur, CO2, heavy hydrocarbons, etc. In a TSA process, a feed gas first enters an adsorber to adsorb the contaminants. The adsorber is regenerated by raising the temperature of the adsorbent typically by purging the bed with a preheated gas. The hot regeneration effluent gas, after cooling, is further processed to remove the contaminants before this spent regeneration gas can be reused, recycled or disposed. Due to the dynamic nature of a TSA process, the compositions in the effluent regeneration stream tend to vary with time, generating a peak concentration, several orders of magnitude higher than its average. The downstream unit to process the spent regeneration gas needs to be sized based on the peak, which results in a significant increase of the equipment size. The fluctuation of stream compositions can also result in unstable operation for the downstream units, especially if combustion or oxidation is involved in these downstream processing units. In this presentation, we will show that if the spent regeneration gas is to be processed in a downstream unit which is sensitive to the concentration peak or fluctuation of the spent regeneration gas, a fixed-bed adsorberadsorptive capacitor can be used to dampen the peak concentration profile. The benefit of this solution will be demonstrated using an example from a Middle East natural gas complex, where UOP's Amine GuardTM FS, Molecular Sieve, and SelexoITM processes are used for pretreatment. A simulation tool has also been developed for dynamic modeling and design of an adsorptive capacitor. Model results have been compared with pilot plant data.

#### Young Professionals Session

Tuesday, March 19<sup>th</sup> Track 2, Session 2 Chairs: Larry Avtzis, Kim Douglas (Abbott)

#### Job search for chemical Engineers

#### Robert Anderson, IIT

Based on the author's long career in industrial management including twenty years as a campus recruiter and extensive work with students seeking jobs, this workshop will share best practices suitable for undergraduate and graduate students as well as AIChE members from the Chicago area. The job market is changing and company expectations are expanding. A strong technical background may be necessary but is not nearly sufficient in today's market. Consider that a half hour campus interview will open or close doors for you. Your campaign to persuade the recruiter to allow you past the first hurdle should be viewed as a \$5,000,000 marketing campaign when you consider expected salary over a work life of 50 years. That should provide perspective as to why prepare vou must an excellent story.

After an overview of the job search process, do's and don'ts will be discussed. Participants are encouraged to bring their questions and be prepared to participate.

Intro to Partcicle Technolgy Ben Freireich, *PSRI* 

#### Abstract Forthcoming

<u>Bio-medical and Material Engineering</u> *Tuesday, March 19<sup>th</sup> Track 2, Session 3 Chairs: Meenesh Singh (UIC), Satish J. Parulekar (IIT)* 

# Synergistic effect of fatty acids and nisin on inhibiting biofilm and persister formation of Listeria monocytogenes

#### Jiacheng Zhou, IIT

A foodborne pathogen, Listeria monocytogenes, causes a life-threatening disease listeriosis and threatens the food safety. The FDA-approved antimicrobial peptide nisin has been used to prevent contamination of food product from Gram-positive pathogens including L. monocytogenes. However, the formation of biofilms and persisters (i.e., metabolically dormant bacterial population) has resulted in the failure of nisin treatment. Fatty acids, which have been known to exhibit antimicrobial activities, are widely used for therapeutics, food preservation, and agriculture. From the screening of fatty acid library, we found that two fatty acid compounds are effective in inhibiting biofilms and persister formation of Gram-negative pathogens. In this study, we investigated whether the fatty acid treatment in combination with nisin promotes inactivation of L. monocytogenes, especially biofilms and persisters. The fatty acid only treatment reduced the level of biofilms and persisters, while nisin only treatment resulted in the development of resistant population of L. monocytogenes ATCC19115 strain. However, the co-treatment of the fatty acid and nisin synergistically enhanced the killing of L. monocytogenes by decreasing the number of survived cells and inhibiting Listeria biofilms. These results are particularly important in improving food safety in that the food-grade fatty acids can be applied to repress the occurrence of resistant mechanisms of foodborne pathogens by inhibiting biofilm and persister cell formation.

#### A new platform for nonivasively of the differentiation stage of indiviual living Quantum Capacitance Based Amplified Graphene Phononics for Studying Neurodegenerative Diseases Bijentimala Keisham, UIC

Blood cancers result from anomalies during hematopoiesis, which is the process of producing the blood and immune cells in the body via hematopoietic stem cell (HSC) differentiation. Bone marrow transplantation is used to replace the mutated HSCs in the cancer patient with healthy HSCs from a living donor. To enable expanding HSCs outside the body for transplantation, the effects of extrinsic cues on HSC fate decisions to self-renew or differentiate must be determined. Microscale platforms have been developed to minimize the number of rare HSCs needed to screen the effects of various extrinsic cues on HSC fate decisions. However, conventional techniques cannot accurately and noninvasively identify differentiation stages on the single cell level. To address this obstacle, we have shown that partial least square-discriminant analysis (PLS-DA) of single cell Raman spectra can accurately identify the lineages of fully differentiated cells from laboratory lines, and the differentiation stages of individual, chemically fixed cells from distinct hematopoietic cells populations. To enable using this approach to screen the fate decisions of individual, living HSCs and their progeny within microscale screening platforms, an artificial bone marrow niche that is compatible with Raman microspectrsocopy analysis of living cells must be developed. Towards this aim, Raman-compatible substrates have been fabricated, and hydrogels functionalized with extracellular matrix protein found in the bone marrow niche were synthesized on their surfaces. The ability to identify the differentiation stages of primary hematopoietic stem and progenitor cells harvested from mice using single cell Raman microspectroscopy and PLS-DA was evaluated. Future work will aim to incorporate cytokines and

bone marrow niche cells into the platform and optimize the Raman microspectroscopy and PLS-DA approach. Successful development of this microscale screening platform will facilitate efforts to identify the effects of matrix stiffness, cytokines, ligands, and niche cells on early HSC fate decisions and may accelerate progress towards the ultimate goal of in-vitro HSC expansion.

#### **Probiotic Leuconostoc mesenteroides inhibits biofilm formation of Listeria monocytogenes** Kuili Fang, IIT

A food-borne pathogen Listeria monocytogenes causes listeriosis, which is considered as lethal illness among immunocompromised patients. Biofilm formation of L. monocytogenes poses resistance and toughness toward sanitation methods such as traditional antibiotics. This study investigated the efficacy of six probiotic strains in controlling L. monocytogenes biofilms. Three probiotic strains of Leuconostoc mesenteroides showed the inhibitory effects toward Listeria biofilms assessed by 96-well based crystal violet assay, colony counting method, and confocal microscopy observation. Biofilm populations of two Listeria strains (serotype 1/2a ATCC15313 and serotype 4b ATCC19115) in dual culture with each probiotic strain were decreased by 4 to 44-fold compared with single species Listeria biofilms in BHI medium. Among the three probiotics, W51 strain resulted in the highest Listeria biofilm inhibition without affecting the growth of L. monocytogenes. Further Listeria biofilm study in the cell-free supernatant of W51 culture with different molecular weight revealed that large protein molecules (> 30 kDa) secreted by the W51 probiotic may be responsible for inhibiting Listeria biofilms. Therefore, our investigation suggests that the probiotics can be used to repress the biofilm development of L. monocytogenes.

#### A bottom-up proteomic approach to identify substrate specificity of outer membrane proteases OmpT and PgtE

#### Sarah Wood, Northwestern University

Identifying peptide substrates that are efficiently cleaved by proteases can give insights into the substrate recognition and specificity, guide the development of inhibitors and improve the sensitivity of assays. Self-assembled monolayers for matrix-assisted laser desorption-ionization mass spectrometry (SAMDI-MS) and peptide arrays were used to identify peptide substrates for bacterial outer membrane proteases in the omptin family, including OmpT and PgtE. In one example, peptide arrays were used to identify a tetrapeptide substrate for OmpT, and analysis of protease activity for the preferred residues at the cleavage site (P1, P1') and nearest neighbor positions (P2, P2') and their positional interdependence revealed FRRV as the optimal peptide with the highest OmpT activity. Substituting FRRV into a fragment of LL37, a natural substrate of OmpT, led to a >400 fold improvement in OmpT's catalytic efficiency with a kcat/Km value of 6.1 x 106 M-1 s-1. In another example, the same methods were used to identify the preferred peptide substrate for PgtE, leading to the discovery of distinctive substrate specificities of OmpT and PgtE, two proteases within the same family that share similar cleavage sites but little is known about their absolute substrate specificities and substrate preferences.

### Sub-Diffraction-Limit Temperature Mapping in Heterogeneous Material Systems

#### Poya Yasaei, Exponent

Structural defects and heterogeneities are essential to achieve desired structures to harvest novel functionalities and/or improved performances in many applications such as electrochemical catalytic systems, thermoelectric energy conversion devices, and electronics. However, heterogeneities with nanoscale features can adversely affect the operation limits, reliability, and safety of the systems by modifying the electrical and thermal transport characteristics and power dissipation patterns. Mapping temperature with high spatial resolution is crucial in identifying localized hot-spots due to the presence of various defects and interfaces, and to establish structure-property-processing correlations in the aforementioned applications. This talk will discuss recent advances and applications of scanning thermal microscopy (SThM) as a practical temperature mapping sub-diffraction-limit technique with spatial resolution and sub-50-mK temperature resolution which is complementary to other conventional thermography techniques such as infrared (IR) microscopy. Particularly, examples will the presented on applying SThM to different material systems including massproduced titanium carbide atomic layers (Ti 3 C 2 T x where T stands for surface terminations) which is part of the MXene family (2D transition metal carbides and nitrides). Another example on characterization of power dissipation in lateral interfaces of chemical vapor deposited (CVD) transition metal dichalcogenides (TMDs) will also be presented.