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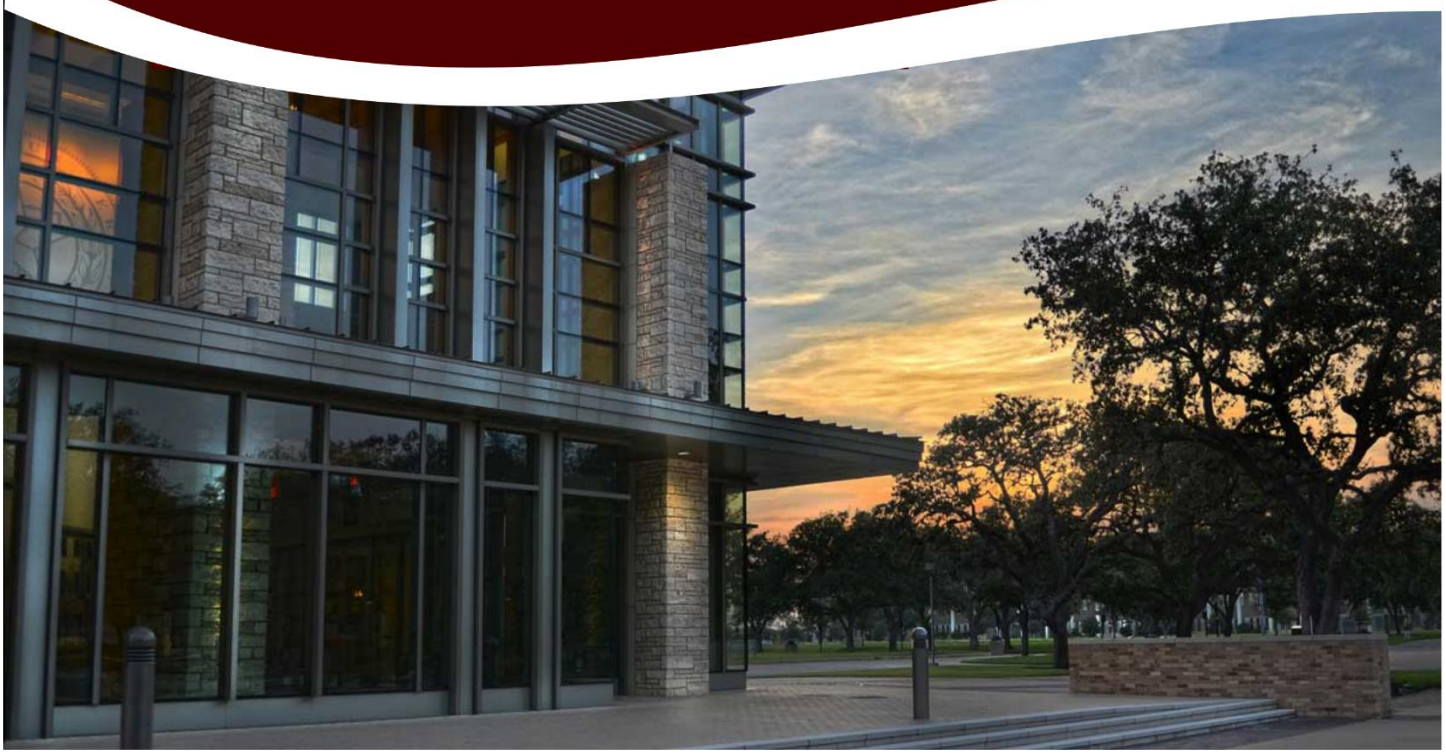
Artie McFerrin Department of
CHEMICAL ENGINEERING
TEXAS A&M UNIVERSITY

4th Chemical Engineering Graduate Student Association
ANNUAL RESEARCH SYMPOSIUM

Friday, March 10, 2017 | 8:00 am - 5:30 pm | MSC, Texas A&M University



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Dr. Jim Harris

BASF We create chemistry

WELCOME

On behalf of the organizing committee we extend you a warm welcome to College Station and the 4th Annual Research Symposium. The purpose of the symposium is to showcase the research conducted in the department and provide students with an opportunity to present their research to industrial representatives. We gratefully acknowledge the sponsorship provided by Ascend Performance materials, Shell, Dow, Texas A&M Division of Research, The Kaneka Foundation, Dr. Jim Harris, BASF and Texas A&M Student Engineering Council. This symposium represents the ideal environment for the exchange of ideas to aid in the advancement of science and technology. We wish all the participants a productive and enjoyable event.

ADVISORY COMMITTEE

DR. ARUL JAYARAMAN	DR. M. SAM MANNAN	DR. HOMA KHOSRAVIAN	DR. MICAH GREEN

ORGANIZING COMMITTEE

Pritishma Lakhe	**Monica Hwang**	**Behnaz Rahmani**
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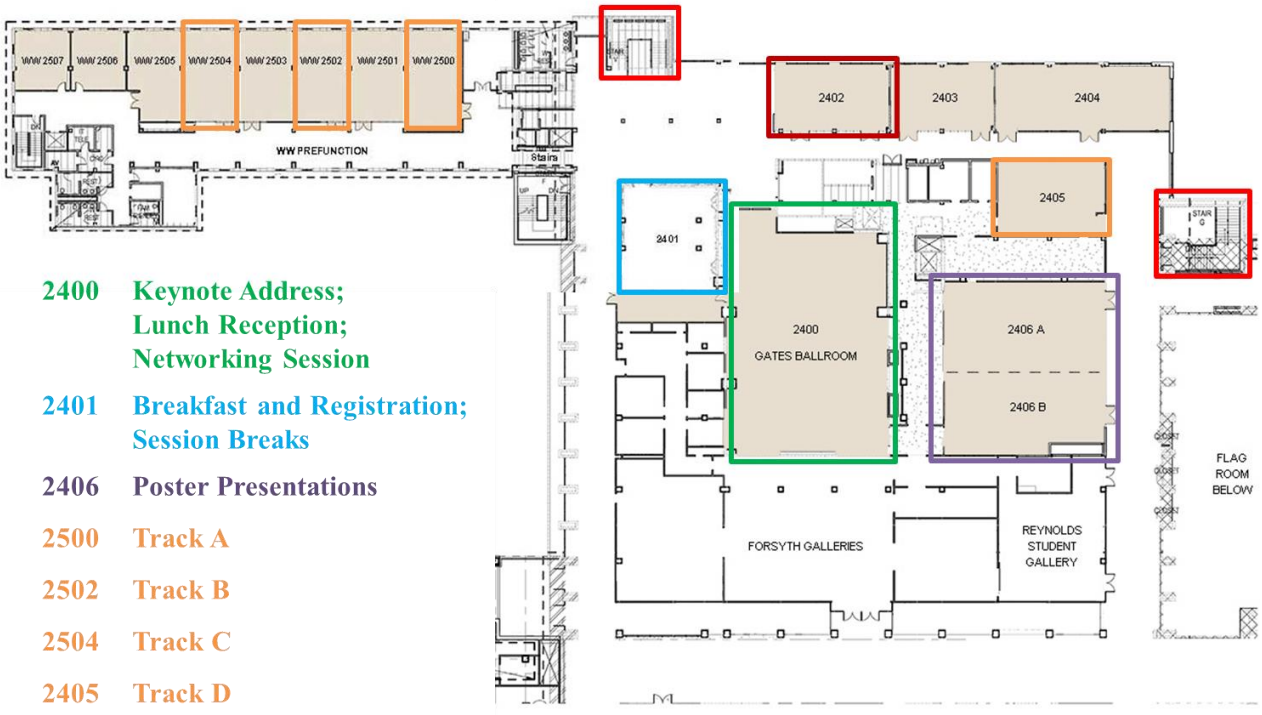
SCHEDULE

Time	Event			
8:00 – 9:00	Breakfast and Registration			
9:00 – 9:15	Opening Remarks by Pritishma Lakhe and Dr. Nazmul Karim			
9:15 – 9:45	Keynote Address by Dr. Angela Summers			
9:45 – 10:00	Break			
	Track A- MSC 2500	**Track B- MSC 2502**	**Track C- MSC 2504**	**Track D- MSC 2405**
10:00 – 10:20	Nirup Nagabandi	Pilar Suarez-Martinez	Melis Onel	Shachit Iyer
10:20 – 10:40	Yixuan Song	Susmitha Kotu	Ishan Bajaj	Utkarsh Shah
10:40 – 11:00	Tianyu Yuan	Hyosung An	Chiranjivi Botre	Priya Balasubramanian
11:00 – 12:15	Poster Session I			
12:15 – 1:30	**Lunch**			
1:30 – 2:45	Poster Session II			
2:45 – 3:15	Dr. Carl Willis	Dr. Cesar Granda	Dr. Leo Chiang	
3:15 – 3:30	**Break**			
3:30 – 3:50	Lubna Ahmed	Ravi Chawla	Prerna Jain	Kevin Topolski
3:50 – 4:10	Bharatvaaj Ravi	Lecheng Zhang	Syeda Zohra Halim	Gerald Oguremem
4:10 – 5:10	**Networking Session**			
5:10 – 5:20	Closing Remarks and Awards by Monica Hwang			

Research Focus

- Advanced Materials
- Safety Engineering
- Bioengineering
- Process Systems Engineering

BUILDING LAYOUT



2400 Keynote Address; Lunch Reception; Networking Session

2401 Breakfast and Registration; Session Breaks

2406 Poster Presentations

2500 Track A

2502 Track B

2504 Track C

2405 Track D

2402 Quiet Room

Emergency exits are marked

KEYNOTE ADDRESS - Dr. Angela Summers

Dr. Angela Summers, Ph.D.
President, SIS-TECH Solution, LP

From Sci-fi Nerd to Engineer to Vintner – a chemical engineer's journey

Dr. Angela Summers started SIS-TECH over 15 years ago with $1,000 and a desire to stop process safety incidents. With over 100 employees and contractors, SIS-TECH has become a respected and trusted provider of services and systems for process safety and critical control applications of automation systems. She has over 30 years of experience in instrumentation and controls, process design, and environmental pollution controls. Dr. Summers holds a PhD in chemical engineering. She was named an Engineering Fellow of the University of Alabama and a Centennial Fellow of its chemical engineering department (top 100 graduates in 1st 100 years of the program).

INDUSTRIAL SPEAKER – Dr. Cesar Granda

Dr. Cesar Granda, Ph.D.
CTO, Earth Energy Renewables

Being Pragmatic About Caring for the Environment through Chemical Engineering

Certain scientific topics can be the subject of endless political controversy despite the fact that scientists and engineers should be above politics. Caring for the environment happens to be one of such topics, where the government can take very different approaches depending on who is in charge. As chemical engineers, we have the opportunity to deliver pragmatism to the debate by offering profitable solutions to the problem, rather than approaches that many times can be a burden on the economy and are not sustainable in the long run.

Earth Energy Renewables is developing a technology, which can sustainably attain a profitable outcome while solving environmental problems and caring for the environment. This technology, which has its roots at the Texas A&M University Chemical Engineering Department, employs Biotechnology and conventional Chemical Engineering. The process uses a mixed consortium of naturally occurring microorganisms to ferment or digest any biodegradable material, such as organic wastes (e.g., organic garbage, wastewater, organic effluents, and agricultural residues) or crops (e.g., corn, sorghum, grass) and produce valuable chemical products. These chemical products, which are organic acids (e.g., acetic, propionic, butyric acids) are recovered from the fermentation effluent and purified. As such, these acids can be commercialized into a well-established market allowing the company to become profitable and self-sufficient. These acids are also well-established intermediates to produce other valuable chemical products, such as ketones, esters, primary and secondary alcohols, and even biofuels, such as gasoline and jet fuel, which represent a good opportunity for substantial growth and sustainability as well as for a significant positive impact on the environment.

INDUSTRIAL SPEAKER – Dr. Carl Willis

Dr. Carl Willis, Ph.D.
Research Fellow, Kraton Polymers

Ion Containing Block Copolymers

In 2010, Kraton Polymers started producing a grade line of ion containing, styrenic block copolymers under the tradename of Nexar® Polymers. The polymers are made by a 3 step process. In the first step, a 5 block copolymer is prepared by a living anionic polymerization technology; the living anionic polymerization method affords block copolymer segments that are nearly monodispersed in molecular weight. In the second step, the polymer is selectively hydrogenated to remove C=C unsaturation. In the final step, the pentablock copolymer is selectively sulfonated in the polystyrene block (center segment).

The sulfonated polystyrene segment in these polymers gives the material unique structure and unusual performance features. Solutions of these polymers tend to be structured which gives rise to the interesting rheological properties observed for the solutions.

The Nexar Polymer solutions have been cast into membranes which have found utility in energy recovery ventilation applications.

Additionally, the Nexar Polymer solutions have also been printed onto fabrics and the resulting coated fabrics made into garments that provide an improved micro-climate for the wearer. This technology provides a mechanism for cooling the person wearing the garment when working in a hot climate.

This presentation will focus on the science that supports these technologies.

INDUSTRIAL SPEAKER – Dr. Leo H. Chiang

Dr. Leo H. Chiang, Ph.D.
Associate Technology Director, The Dow Chemical Company

Advances in Big Data Analytics at The Dow Chemical Company

In the Big Data era, Dow is collecting large volume of data (in the order of terabytes each day) of various kinds such as process data, experimental lab data, business transaction data, image data, and text data. While these data present a unique opportunity to improve process understanding and bring value to Dow, it is often challenging to use the right data and right tools to make the right decisions in real-time. This talk highlights recent advancements in the big data analytics journey at Dow in the areas of Enterprise Manufacturing Intelligence, multivariate analysis, on-line fault detection, inferential sensors, and batch data analytics.

NOTES

Oral Presentations

Track A – MSC 2500

Track	Morning	Presentation
A1	**10:00 – 10:20**	**SILVER METAL-ORGANIC-INORGANIC COMPOSITES AS THERMAL INTERFACE MATERIALS** *Nirup Nagabandi, Cengiz Yegin, Jun Kyun Oh and Mustafa Akbulut*
A2	**10:20 – 10:40**	**HIGH OXYGEN GAS BARRIER IN MULTILAYER THIN FILMS THROUGH PH MANIPULATION OF MONTMORILLONITE CLAY NANOPLATELETS** *Yixuan Song, David A. Hagen and Jaime C. Grunlan*
A3	**10:40 – 11:00**	**VERSATILE THERMOCHROMIC SUPRAMOLECULAR MATERIALS BASED ON CHARGE TRANSFER INTERACTIONS** *Tianyu Yuan, Mariela Vazquez, Mark A. Olson and Lei Fang*

Track	Afternoon	Presentation
Industry	**2:45 – 3:15**	**ION CONTAINING BLOCK COPOLYMERS** *Dr. Carl Willis, Research Fellow, Kraton Polymers*
A4	**3:30 – 3:50**	**FLAMMABILITY STUDIES BY CONE CALORIMETER ANALYSIS OF SILICA CROSS-LINKED POLY (METHYL METHACRYLATE)** *Lubna Ahmed, Ruiqing Shen, Logan Hatanaka, Bin Zhang, Sam Mannan, Zhengdong Cheng and Qingsheng Wang*
A5	**3:50 – 4:10**	**STUDY OF FACTORS THAT AFFECT DUST EXPLOSION CHARACTERISTICS OF FIBROUS DUST MATERIALS** *Bharatvaaj Ravi, M. Sam Mannan and Chad Mashuga*

Track B – MSC 2502

Track	Morning	Presentation
B1	**10:00 – 10:20**	**SPRAY-ON POLYMER-CLAY MULTILAYERS AS A SUPERIOR ANTICORROSION METAL PRETREATMENT** *Pilar C. Suarez-Martinez, Jerome Robinson, Hyosung An, Robert C. Nahas, Douglas Cinoman and Jodie L. Lutkenhaus*
B2	**10:20 – 10:40**	**MODIFIED MICROFLUIDIC FLOW SYSTEM FOR ASSESSMENT OF MICROBIOLOGICALLY INFLUENCED CORROSION** *Susmitha Purnima Kotu, Sam Mannan and Arul Jayaraman*
B3	**10:40 – 11:00**	**CONDUCTING BLOCK COPOLYMER BATTERY ELECTRODE BINDERS COMPARED AGAINST THEIR HOMOPOLYMER BLEND ANALOGS** *Hyosung An, Xiaoyi Li, Cody Chalker, Maria Stracke, Rafael Verduzco and Jodie L. Lutkenhaus*

Track	Afternoon	Presentation
Industry	**2:45 – 3:15**	**BEING PRAGMATIC ABOUT CARING FOR THE ENVIRONMENT THROUGH CHEMICAL ENGINEERING** *Dr. Cesar Granda, CTO, Earth Energy Renewables*
B4	**3:30 – 3:50**	**TORQUE-DEPENDENT MOTOR REMODELING AND MECHANOSENSING IN E. COLI** *Ravi Chawla, Katie M. Ford and Pushkar P. Lele*
B5	**3:50 – 4:10**	**NOVEL JANUS NANOPLATELETS FOR ENHANCED OIL RECOVERY** *Lecheng Zhang, Mingxiang Zeng and Zhengdong Cheng*

Track C – MSC 2504

Track	Morning	Presentation
C1	**10:00 – 10:20**	**BIG DATA APPROACH TO FAULT DETECTION AND DIAGNOSIS IN BATCH PROCESSES USING NONLINEAR SVM-BASED FEATURE SELECTION** *Melis Onel, Chris A. Kieslich, Yannis A. Guzman Christodoulos A. Floudas and Efstratios N. Pistikopoulos*
C2	**10:20 – 10:40**	**NOVEL METHOD FOR DERIVATIVE-FREE OPTIMIZATION BASED ON PARAMETRIC APPROACH** *Ishan Bajaj and M. M. Faruque Hasan*
C3	**10:40 – 11:00**	**PROCESS MONITORING OF NONLINEAR INDUSTRIAL PROCESSES USING MULTISCALE REPRESENTATION OF IMPROVED KERNEL PARTIAL LEAST SQUARE (KPLS) TECHNIQUE** *Chiranjivi Botre, Majdi Mansouri, Mohamed N. Nounou, Hazem N. Nounou and M. Nazmul Karim*

Track	Afternoon	Presentation
Industry	**2:45 – 3:15**	**ADVANCES IN BIG DATA ANALYTICS AT THE DOW CHEMICAL COMPANY** *Dr. Leo H. Chiang, Associate Technology Director, Dow*
C4	**3:30 – 3:50**	**RESILIENCE-BASED LOSS OF CONTAINMENT (LOC) EVENTS PREDICTION ANALYSIS FOR POLY VINYL CHLORIDE PROCESS SYSTEM: UNCERTAINTY QUANTIFICATION** *Prerna Jain and M. Sam Mannan*
C5	**3:50 – 4:10**	**CUMULATIVE RISK ASSESSMENT MODEL TO DETERMINE INCREASED RISK DUE TO IMPAIRED BARRIERS** *S. Zohra Halim and M. Sam Mannan*

Track D – MSC 2405

Track	Morning	Presentation
D1	**10:00 – 10:20**	**DESIGN AND OPTIMIZATION OF MODULAR TECHNOLOGY FOR INTEGRATED CARBON CAPTURE & CONVERSION OF CO2 USING METHANE SOURCES** *Shachit S. Iyer, Ishan Bajaj, Priyadarshini Balasubramanian and M. M. Faruque Hasan*
D2	**10:20 – 10:40**	**AN IMPROVED APPROACH FOR ROBUST SCHEDULING UNDER UNCERTAINTY** *Utkarsh D. Shah, Yannis A. Guzman, Logan R. Matthews and Christodoulos A. Floudas*
D3	**10:40 – 11:00**	**CO2 CAPTURE AND CONVERSION TO CHEMICALS VIA SYNGAS: SUPERSTRUCTURE-BASED PROCESS SYNTHESIS, MODELING, AND OPTIMIZATION** *Priyadarshini Balasubramanian, Ishan Bajaj and M. M. Faruque Hasan*

Track	Afternoon	Presentation
D4	**3:30 – 3:50**	**ANCHOR-TENANT MODELS FOR THE SYNTHESIS OF ECO-INDUSTRIAL PARKS THROUGH CARBON-HYDROGEN-OXYGEN SYMBIOSIS NETWORKS** *Kevin Topolski, Mohamed Noureldin, and Mahmoud El-Halwagi*
D5	**3:50 – 4:10**	**DYNAMIC MODELING AND OPTIMIZATION OF RENEWABLE HIGH-PRESSURE PEM HYDROGEN PRODUCTION AND STORAGE** *Gerald S. Ogumerem and Efstratios N. Pistikopoulos*

Poster Session I

MSC 2406

11:00 A.M. – 12:15 P.M.

Advanced Materials

P.1 **Aramid Nanofiber/Graphene/Carbon Nanotube Composite Electrodes for Structural Energy and Power**
Anish Patel, John Harris and Jodie L. Lutkenhaus

P.2 **Solid-state Synthesis and Thermoelectric Properties of Magnesium Silicide**
Azhar Ali, Venkata Vasiraju, Yixi Chen and Sreeram Vaddiraju

P.3 **Electric Field Induced Birefringence in Isotropic Suspensions of Nanoplates**
Carlos Mejia, Abhijeet Shinde, Ivan Dozov, Padetha Tin, Patrick Davidson and Zhengdong Cheng

P.4 **Biodegradable 3D Printed Oil Absorbents with Tunable Capillary Architectures**
Duanduan Han and Victor Ugaz

P.5 **Electrolyte Structure and Behavior of Polysulfide species in Lithium-Sulfur Batteries**
Ethan P. Kamphaus and Perla B. Balbuena

P.6 **Rapid Microwave-assisted Synthesis of Hybrid Zeolitic-Imidazolate Frameworks with Mixed Metals and Mixed Linkers**
Febrian Hillman, John Zimmerman, Seung-Min Paek, Mohamad R. A. Hamid, Woo T. Lim and Hae-Kwon Jeong

P.7 **Liquid Surfactants for Processing Boron Nitride Nanosheets (BNNSs)**
Touseef Habib, Dinesh Sundaravadivelu Devarajan, Fardin Khabaz, Dorsa Parviz, Thomas C. Achee, Rajesh Khare and Micah J. Green

Process Systems Engineering

P.8 **Model order reduction of parabolic PDE systems based on temporally-local Dynamic mode decomposition with control**
Abhinav Narasingam and Joseph Sang-Il Kwon

P.9 **Global Optimization of Constrained Grey-Box Models for Well Injection and Production**
Burcu Beykal, Fani Boukouvala, Nadav Sorek, Hardikkumar Zalavadia, Eduardo Gildin, Christodoulos A. Floudas and Efstratios N. Pistikopoulos

P.10 **Improved Data-Driven Mathematical Modeling and Global Optimization Framework: An Application in Refinery Planning Operations**
C. Doga Demirhan, Fani Boukouvala Kyungwon, Kim Hyeju Song, Efstratios N. Pistikopoulos and Christodoulos A. Floudas

P.11 **Simultaneous Process Network Synthesis and Process Intensification Using Grid Superstructure**
Jianping Li, Salih Emre Demirel and M. M. Faruque Hasan

Pharmaceuticals and Bioengineering

P.12 **Binding of Cholera toxin subunit B with heterogeneous glycolipids on cell mimicking surfaces**
Pratik Krishnan, Akshi Singla, Chin-An Lee, Joshua D. Weatherston, Nolan C. Worstell and Hung-Jen Wu

Poster Session II

MSC 2406

1:30 P.M. – 2:45 P.M.

Advanced Materials

P.22 **Synthesis and Characterization of CdIF-1: A Cadmium Version of ZIF-8**
Jingze Sun, Liya Semenchenko, and Hae-Kwon Jeong

P.23 **Computational Study of the Adsorption of a Phenanthrene Derivative over a Model Zeolite**
Monica M. Garnica-Mantilla, Ana E. Torres-Hernández, Luis E. Camacho-Forero , Carlos M. Celis-Cornejo, Gustavo E. Ramírez-Caballero and Perla B. Balbuena

P.24 **PIL-Derived Carbon**
Rui Sun, Kelly M. Meek and Yossef A. Elabd

P.25 **Water-Based Assembly of Polymer-Metal Organic Framework (MOF) Functional Coatings**
Souvik De, Manjula I. Nandasiri, Herbert T. Schaef, Benard Peter McGrail, Satish K. Nune and Jodie L. Lutkenhaus

P.26 **Porous nanomaterials with high performance energy storage**
Wanmei Sun and Micah Green

P.27 **The Effect of Water on the Thermal Transition Observed in Poly(allylamine hydrochloride)-Poly(acrylic acid) Complexes**
Yanpu Zhang, Ran Zhang, Maria Sammalkorpi and Jodie L. Lutkenhaus

Process Systems Engineering

P.28 **Simultaneous Design and Control of a Binary Distillation Column**
Baris Burnak, Justin Katz, Nikolaos A. Diangelakis and Efstratios N. Pistikopoulos

P.29 **Modeling of hydraulic fracturing and design of online optimal pumping schedule to achieve uniform proppant concentration**
Prashanth Siddhamshetty and Joseph Sangil Kwon

P.30 **Systematic Process Intensification Using Building Blocks**
Salih Emre Demirel, Jianping Li and M. M. Faruque Hasan

P.31 **Systematic Analysis and Optimization of Energy-Water Nexus**
Spyridon D. Tsolas, M. Nazmul Karim and M. M. Faruque Hasan

P.32 **Natural Gas to Liquid Transportation Fuels Utilizing Chemical Looping Technologies for Syngas Generation: Process Synthesis and Global Optimization**
William W. Tso, Alexander M. Niziolek, Onur Onel and Christodoulos A. Floudas

P.33 **Monetization of Stranded Gas through Ammonia and Urea Production**
Zehao Gou, Debalina Sengupta, Mike Dou and M.M. El-Halwagi

Safety Engineering

P.34 **The Integration of Design, Control, and Safety**
Denis Su-Feher, Yogesh Koirala, Efstratios Pistikopoulos and M. Sam Mannan

P.35 **A systematic approach to alarm design with application to Tennessee Eastman Problem**
Joshiba Ariamuthu Venkidasalapathy, Costas Kravaris and M. Sam Mannan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Research at Texas A&M

Solving real-world challenges

Ranking among the world's leading research institutions with more than $892.7 million in research expenditures (FY2016), Texas A&M is at the forefront in making significant contributions to scholarship and discovery, including that of science and technology.

Texas A&M ranked in the top 20 of the National Science Foundation's Higher Education Research and Development survey (2015), based on expenditures of more than $866.6 million in fiscal year 2015. Texas A&M is one of only a few institutions in the nation to hold triple designation as a land-, sea-, and space-grant university and is one of only 62 members of the prestigious Association of American Universities.

Texas A&M's Division of Research is committed to a truly comprehensive university where students, researchers, and inventors bring scholarship and innovation to bear for the benefit of the community, the state, and the nation.

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ARTIE MCFERRIN DEPARTMENT OF CHEMICAL ENGINEERING
TEXAS A&M UNIVERSITY

2016 Department Fact Sheet

The Artie McFerrin Department of Chemical Engineering at Texas A&M University is one of the top rated chemical engineering departments in the world. It is also one of the largest, fully accredited chemical engineering programs in the country. The department has become a prolific chemical engineering research hub, with the faculty producing more than 200 refereed journal publications in 2016.

Located in the 205,000 square-foot, Jack E. Brown Chemical Engineering Building, the department provides its students and faculty members access to the latest resources, including 88 research and teaching facilities, six general classrooms, 13 conference rooms, and four computer laboratories.

Research

The Artie McFerrin Department of Chemical Engineering at Texas A&M University has faculty engaged in a wide breadth of studies ranging from highly applied research in the areas of biomass utilization, process safety and hydrocarbon processing to very fundamental research in nanotechnology, life sciences, process systems engineering and molecular simulation. The ultimate goal of the work is to positively impact society by providing new knowledge.

Department Research Areas

- Biomedicine | Biomolecules
- Biofuels | Biotechnology
- Catalysis
- Complex Fluids | Microfluidics | Soft Matter
- Computational Chemical Engineering
- Energy
- Environmental | Sustainability
- Materials | Microelectronics
- Multiscale Systems Engineering
- Nanotechnology
- Process Safety | Process Systems Engineering
- Reaction Engineering
- Thermodynamics

Department Head

M.Nazmul Karim | Professor | T. Michael O'Connor Chair II
nazkarim@tamu.edu

Enrollment

Total Enrollment	**969**
Undergraduate	714
Graduate	255
Master's	117
Ph.D.	138

Faculty

Total Faculty	**36**
Professors	15
Endowed Professors	8
Chair Holders	4
Associate Professors	8
Assistant Professors	6
Research Assistant Professors	1
Lecturers/Senior Lecturers	5
Professors Of Practice	2
Emeritus Faculty	5
Referred Journal Publications	203

Gender Diversity

Female	37%
Male	63%