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**Student Research Seminar Schedule**

# Preface

Welcome to Purdue University and the 21st Annual Chemical Engineering Graduate Research Symposium! Since its inception in 1992, the ChE Graduate Research Symposium has proven to be an important venue for graduate students to network with professionals from a wide variety of industries while giving those in attendance a flavor of the state-of-the-art research in our department.

The Symposium gives senior Ph.D. students a chance to present their research to industrial representatives and receive feedback from active members of the chemical engineering community. Additionally, the afternoon poster session will showcase the full breadth of the exciting areas of research pursued in the School of Chemical Engineering.

On behalf of the Purdue Chemical Engineering Graduate Student Organization (GSO), I would like to extend my sincere gratitude to the students, faculty, and industrial representatives for their support and participation in this year's Graduate Research Symposium.

I hope you enjoy your visit to Purdue and the activities we have scheduled today!

Nathan Carter
GSO President, 2012-2013

# 2012–2013 GSO Officers

| | |
|---|---|
| Nathan Carter | President |
| Si Chen | Vice President |
| Janie Brennan | Voting Representative |
| Nicole Devlin | First-Year Representative |
| Frank DeVilbiss | Outreach Committee Chairperson |
| Anshu Gupta | Inter-GSO Chairperson |
| Laura Hirshfield | Co-Curricular Activities Chairperson |
| Aniruddha Kelkar | PGSG Representative |
| Atish Parekh | Social Committee Chairperson |
| Caity Schram | Non-Voting Representative |
| Renay Su | Publicity Chairperson |

# 2012 Symposium Coordinators

| | |
|---|---|
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| Si Chen | Treasurer and Website Administrator |
| Caity Schram | Publications Co-Coordinator |
| Renay Su | Publications Co-Coordinator |
| Janie Brennan | Scheduling Coordinator |
| Anshu Gupta | Poster Session Coordinator |
| Nicole Devlin | Judging Coordinator |
| Laura Hirshfield | Industrial Packet Coordinator |
| Frank DeVilbiss | Refreshment & Catering Coordinator |
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| Anuradha Bhat | Industrial Liaison |
| Ranjita Ghose | Industrial Liaison |
| Anshu Gupta | Industrial Liaison |
| Atish Parekh | Industrial Liaison |
| John O’Grady | Industrial Liaison |
| Krishnaraj Sambath | Industrial Liaison |
| Renay Su | Industrial Liaison |
| Anand Venkatesan | Industrial Liaison |

# Schedule of Events

## Wednesday, August 15th, 2012

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|---|---|
| 7:00PM – 10:00PM | **Symposium Mixer**<br>Adelino's Old World Kitchen<br>*112 North 3rd Street, Lafayette, IN 47901* |

## Thursday, August 16th, 2012

| | |
|---|---|
| 7:30AM – 8:30AM | **Breakfast & Welcome**<br>Forney Hall of Chemical Engineering<br>*Henson Atrium* |
| 9:00AM – 10:15AM | **Student Research Seminars**<br>Forney Hall of Chemical Engineering<br>*Session A – Room G124*<br>*Session B – Room B124* |
| 10:15AM – 10:30AM | **Break** |
| 10:30AM – 11:20AM | **Student Research Seminars**<br>Forney Hall of Chemical Engineering<br>*Session A – Room G124*<br>*Session B – Room B124* |
| 11:20AM – 11:30AM | **Break** |

# Schedule of Events

## Thursday, August 16th, 2012 (continued)

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|---|---|
| 11:30AM – 12:30PM | **Keynote Address**<br>**Dr. Karl Jacob**<br>**Research Fellow at Dow Chemical Company**<br>Forney Hall of Chemical Engineering<br>*Room G140* |
| 12:30PM – 2:00PM | **Lunch & Poster Showcase**<br>Forney Hall of Chemical Engineering<br>*Henson Atrium* |
| 2:00PM – 3:15PM | **Student Research Seminars**<br>Forney Hall of Chemical Engineering<br>*Session A – Room G124*<br>*Session B – Room B124* |
| 3:15PM – 3:30PM | **Break** |
| 3:30PM – 4:20PM | **Student Research Seminars**<br>Forney Hall of Chemical Engineering<br>*Session A – Room G124*<br>*Session B – Room B124* |
| 7:00PM – 7:30PM | **Cocktails**<br>Purdue Memorial Union<br>*South Ballroom* |
| 7:30PM – 11:00PM | **Awards Banquet**<br>Purdue Memorial Union<br>*South Ballroom* |

# Student Research Seminar Schedule

## Session A - Morning (FRNY G124)

| | |
|---|---|
| 9:00AM – 9:25AM | **Towards An Examination of Lipid production by *Chlorella protothecoides* Using Compartmentalized Metabolic Flux Analysis**<br>John O'Grady<br>*John A. Morgan* |
| 9:25AM – 9:50AM | **Mechanistic Studies of Chiral Recognition of Solutes by Amylose Tris[(S)-α-methylbenzylcarbamate]**<br>Hung-Wei Tsui<br>*N.-H. Linda Wang and Elias I. Franses* |
| 9:50AM–10:15AM | **Micro-Gap Analysis for Explosives Detection Swabs**<br>Michelle Chaffee-Cipich<br>*Stephen P. Beaudoin* |

—— BREAK ——

| | |
|---|---|
| 10:30AM–10:55AM | **Advanced Sensing and Monitoring of Lithium Ion Batteries**<br>Mark Suchomel<br>*James M. Caruthers and Joseph F. Pekny* |
| 10:55AM–11:20 AM | **Real Time Measurements of the Growth of Selenide Thin-film Photovoltaic Absorbers from Sulfide Nanoparticles**<br>Bryce Walker<br>*Rakesh Agrawal* |

# Student Research Seminar Schedule

## Session B - Morning (FRNY B124)

| | |
|---|---|
| 9:00AM – 9:25AM | **Poly(ethylene oxide) Chains Are Not "Hydrophilic" When They Exist As Polymer Brush Chains**<br>Hoyoung Lee<br>*You-Yeon Won* |
| 9:25AM – 9:50AM | **New Insights into the Effect of Fillers on the Mechanical Behavior of Rubbers**<br>Oluwaseyi (Shay) Ogebule<br>*James M. Caruthers* |
| 9:50AM–10:15AM | **Nonlinear Viscoelastic Behavior of Glassy Polymers in Multi-axial Stress States**<br>Jaewoo Kim<br>*James M. Caruthers* |

—— BREAK ——

| | |
|---|---|
| 10:30AM–10:55AM | **Fission and Fusion of Liquid Drops**<br>Krishnaraj Sambath<br>*Osman A. Basaran* |
| 10:55AM–11:20 AM | **Low Cost Synergistic Desalination Processes**<br>Anand Venkatesan<br>*Phillip C. Wankat* |

# Student Research Seminar Schedule

## Session A - Afternoon (FRNY G124)

| | |
|---|---|
| 2:00PM – 2:25PM | **Probing the Active Redox Sites on Cu/SSZ-13 in the Selective Catalytic Reduction of $NO_x$ by $NH_3$ via *Operando* X-ray Absorption**<br>Shane Bates<br>*Fabio H. Ribeiro and W. Nicholas Delgass* |
| 2:25PM – 2:50PM | **An Integrated Approach for Characterization of Pt Based Aqueous Phase Reforming Catalysts**<br>Paul J. Dietrich<br>*Fabio H. Ribeiro and W. Nicholas Delgass* |
| 2:50PM – 3:15PM | **High Pressure Catalytic Hydrodeoxygenation Reaction Pathways and Kinetics for Dihydroeugenol over $Pt/ZrO_2$ and $Ru/ZrO_2$ catalysts**<br>Sara L. Yohe<br>*W. Nicholas Delgass, Fabio H. Ribeiro, and Rakesh Agrawal* |

—— BREAK ——

| | |
|---|---|
| 3:30PM – 3:55PM | **Tissue Engineering Cues to Direct the Endothelial Differentiation of Mesenchymal Stem Cells**<br>Richard J. Galas Jr.<br>*Julie C. Liu* |
| 3:55PM – 4:20PM | **Effect of DNA Methylation on Chromatin Compaction and Dynamics**<br>Isabel Jimenez-Useche<br>*Chongli Yuan* |

# Student Research Seminar Schedule

## Session B - Afternoon (FRNY B124)

| | |
|---|---|
| 2:00PM – 2:25PM | **Energy Systems Analysis for Sustainable Transportation Fuel**<br>Dharik S. Mallapragada<br>*Rakesh Agrawal, W. Nicholas Delgass, and Fabio H. Ribeiro* |
| 2:25PM – 2:50PM | **Exceptional Event Management Applied to Continuous Pharmaceutical Manufacturing**<br>Anshu Gupta<br>*Gintaras V. Reklaitis* |
| 2:50PM – 3:15PM | **Drug-on-Demand: A Mini-Manufacturing Method of Pharmaceutical Dosage Forms**<br>Laura Hirshfield<br>*Gintaras V. Reklaitis* |
| | —— BREAK —— |
| 3:30PM – 3:55PM | **Introducing Softwares to Facilitate Pharmaceutical Crystallization: *CrystalShape*, *CrystalTomogram*, *CrystalPolar* and *MorphologyDomain***<br>Meenesh Singh<br>*Doraiswami Ramkrishna* |
| 3:55PM – 4:20PM | **Model-based Individualized Treatment for Childhood Leukemia**<br>Jayachandran Deveraj<br>*Doraiswami Ramkrishna* |

# Student Speaker Abstracts

The abstracts for the presentations listed under the Student Research Seminar Schedule appear in the following pages.

Abstracts are listed in order of presentation with simultaneous talks shown on facing pages.

# Towards An Examination of Lipid production by *Chlorella protothecoides* Using Compartmentalized Metabolic Flux Analysis

John O'Grady

*Professor John A. Morgan*

With increasing energy demands, many forms of alternative and sustainable energy production are receiving increased attention. Biodiesel from algae continues to be a promising source of renewable liquid fuel. *C. protothecoides* has demonstrated the highest lipid productivity of any strain of algae when it is grown heterotrophically. However, much still remains to be learned about its primary metabolism. A deeper understanding of the metabolism of this lipid-producing algal strain will set the stage for further improvements in its lipid production, as well as the lipid production of other algal strains with alternate desirable characteristics.

$^{13}$C metabolic flux analysis is a powerful tool to examine the distribution of metabolic rates within a cell. An examination of the labeling patterns in intermediary metabolites makes it possible to determine the flux rates of many key reactions in carbon metabolism. Using subcellular fractionation we will be able to deconvolute the labeling patterns of metabolites located in the plastid and the cytosol, thus separating the fluxes of identical reactions which occur in both of these locations in the cell. We have examined these flux rates using both glucose and glycerol without compartmental analysis and have also adapted the subcellular fractionation technique to be used in on algae for the first time.

# Poly(ethylene oxide) Chains Are Not “Hydrophilic” When They Exist As Polymer Brush Chains

Hoyoung Lee

*Professor You-Yeon Won*

By using a combined experimental and theoretical approach, a model poly(ethylene oxide) (PEO) brush system, prepared by spreading a poly(ethylene oxide)-poly(*n*-butyl acrylate) (PEO-PnBA) amphiphilic diblock copolymer onto an air-water interface, was investigated. The polymer segment density profiles of the PEO brush in the direction normal to the air-water interface under various grafting density conditions were determined from combined X-ray and neutron reflectivity data. In order to achieve a theoretically sound analysis of the reflectivity data, we developed a new data analysis method that uses the self-consistent field theoretical modeling as a tool for predicting expected reflectivity results for comparison with the experimental data. Using this new data analysis method, we discovered that the effective Flory-Huggins interaction parameter of the PEO brush chains is significantly greater than that corresponding to the theta condition, suggesting that contrary to what is more commonly observed for PEO in normal situations, the PEO chains are actually not ``hydrophilic" when they exist as polymer brush chains, because of the many body interactions forced to be effective in the brush situation.

# Mechanistic Studies of Chiral Recognition of Solutes by Amylose Tris[(S)-α-methylbenzylcarbamate]

Hung-Wei Tsui

*Professor N.-H. Linda Wang and Professor Elias I. Franses*

This amylose-based polymeric sorbent has the ability to separate a variety of chiral enantiomers (R and S), such as ethyl lactate, methyl mandelate, pantolactone, and benzoin. These molecules contain OH and C=O functional groups, which may interact with the C=O and NH groups of the sorbent side chains via hydrogen (H-) bonding interactions. From the observed retention factors $k_R$ and $k_S$ and enantioselectivities ($S = k_R / k_S$), as determined with High Performance Liquid Chromatography (HPLC), it was inferred that the molecular recognition mechanisms of these molecules were quite similar. Infrared spectroscopy (IR) data for polymer-solute and Density Functional Theory (DFT) simulations of the interactions of these solutes with the side chains of the polymer led to the following hypothesis for the chiral recognition mechanism. A strong H-bond forms between the solute OH groups and the sorbent C=O groups for both enantiomers as the primary interaction "anchor" point. The strength of this H-bond controls the values of the retention factors. Then a second H-bond forms between the solute C=O groups and the sorbent NH groups only for the R-enantiomers of the above four solutes. The S-enantiomer is prevented sterically from forming such a bond. Molecular Dynamics (MD) simulations were done for a 12-mer polymer model to determine the polymer structure, intrapolymer H-bonding, free functional groups available for binding with the solute, and the geometry of the potentially enantioselective cavities. Monte Carlo (MC) and MD "docking" simulations were done to investigate the interactions of the benzoin enantiomers with the polymer. MD simulations were also done for the other solutes. The simulations are generally consistent with the above hypothesis, and they reveal the specific cavities which may allow enantioselective interactions. The results showed that S is lower as the solute molecular flexibility, as defined from the molecular geometric torsion angles distribution, increases. The results may be useful in predicting how S varies with the solute molecular structure, and in selecting sorbents for specific chiral separations.

9:25AM – 9:50AM SESSION B ROOM B124

# New Insights into the Effect of Fillers on the Mechanical Behavior of Rubbers

Oluwaseyi "Shay" Ogebule

*James. M. Caruthers*

Cross-linked engineering elastomers are rubbery materials capable of deforming upon load application and retracting upon removal. Incorporation of small rigid particulate fillers enhances their mechanical properties (modulus, tensile strength, toughness, tear resistance, etc.) enabling their use in common everyday applications. The automotive, healthcare, construction, adhesives, packaging and consumer products industries are just some of the many commercial areas that employ finished goods containing elastomeric parts.

In their service lifetime, filled elastomers are subjected to a wide range of complex loading conditions. To facilitate efficient rubber design, development of constitutive theories for prediction of their mechanical behavior is vital, forming an area of active research. Despite the various concepts and theories used to explain the mechanical response of filled elastomers to deformation, a complete understanding of stress softening (Mullins), strain dependent dynamic modulus effect (Payne) and other non-linear mechanical properties remains elusive.

In this work, we vary the structure, surface area and surface activity of a particulate filler system and analyzed the resulting changes that occur in the: non-linear properties, including Payne and Mullins effect; and ultimate properties, including tensile strength and tear resistance. In the course of this study, we unexpectedly discovered that certain types of fillers resulted in the material exhibiting necking, an unexpected and novel phenomena for filled elastomers. The implications of this and other findings on the mechanical characteristic features of filled elastomers will be discussed.

# Micro-Gap Analysis for Explosives Detection Swabs

Michelle Chaffee-Cipich

*Professor Stephen P. Beaudoin*

The detection of Improvised Explosive Devices (IEDs) has become increasing important to the Department of Homeland Security (DHS) since the tragic events of September 11, 2001. The ability to detect an IED before it is triggered prevents the loss of countless lives worldwide. A key to effective detection is an efficient means for the collection of trace explosives. Current collection methods can be classified as either contact or non-contact. Contact sampling dislodges explosive particles through physical contact with a swab and collects particles that adhere more strongly to the swab than to the original surface. Non-contact sampling relies on momentum transfer between a moving fluid (typically air) and the explosive residue to dislodge the particles from the surface.

Our research focuses on contact sampling between an explosives detection swab and a variety of surfaces often encountered by airport security. These surfaces included cardboard, plastic, vinyl, and a clear finishing coat for automobiles. There were four unique swabs studied each with different mechanical properties and measured roughnesses. The contact under load between a swab and surface is modeled including the material deformation. From this deformation model, the micro-gaps between the swab and surface are analyzed. This research can then investigate the ability of a swab to interrogate the surface. Low surface interrogation ability indicates that significant areas exist where the swab cannot contact an explosive particle present on the surface, eliminating the possibility of collection. A summary of the surface interrogation ability of each swab with reference to a variety of surface types is presented along with a recommendation for a new explosives detection swab.

# Nonlinear Viscoelastic Behavior of Glassy Polymers in Multi-axial Stress States

Jaewoo Kim

*Professor James M. Caruthers*

Glassy polymers are widely used in a variety of applications including adhesives, coatings, and matrices in fiber-reinforced composites due to their excellent mechanical properties, low density, and chemical resistance. To understand their nonlinear viscoelastic behavior originating from the dependence of the rate of relaxation on deformation and thermal history, yield and post-yield behavior of amorphous polymers in a glassy state have been extensively studied in uniaxial tension and compression. In such geometry, the volume change is known to be relatively small reaching the maximum value of approximately 0.5% at the yield point [1]. Thus, a uniaxial experiment primarily probes the effect of the deviatoric contribution of the strain/stress tensor. From a fundamental standpoint, to study the role of the dilatational contribution, a different geometry is needed. Also, in practical applications, polymers are subject to multi-axial stress states with significant dilatational component, caused by many different kinds of constraints, such as reinforcements and substrate as well as loading conditions.

In this study, longitudinal test is developed and performed in order to observe nonlinear viscoelastic properties including yield and relaxation phenomena in a dilatation-dominated stress state. To confirm that the observed behavior cannot be attributed to damage, multiple loading / unloading cycles are conducted. Then, the pressure-modified von Mises yield criterion is validated using our longitudinal results. Unlike metals where the physics behind the von Mises yield criterion is fairly understood, in case of amorphous glassy polymers exhibiting dependence of yield on the hydrostatic component of stress, the pressure-modified von Mises yield criterion is but a phenomenological assumption. To date, the criterion has been tested empirically with success, but within a limited range of pressures [2]. Using our longitudinal results, we are able to validate the pressure-modified von Mises yield criterion for much wider range of hydrostatic pressures. Another benefit of carrying out the longitudinal test is that, combined with conventional uniaxial test, it will help to de-convolute dilatational and deviatoric contributions to the rate of relaxation, which are present in the constitutive models, for instance, the nonlinear viscoelastic constitutive model by Caruthers, et al [3].

REFERENCES
[1] Powers, J.M.; Caddell, R.M., *Polym. Eng. Sci.* **1972**, 12,432
[2] Quinson, R.; Perez, J., J of Mat. Sci. **1997**, 32, 1371-1379
[3] Caruthers, J.M.; Adolf,D.B.; Chambers, R.S.; Shrikhande, P., Polymer **2004**, 45, 4577-4597

# Advanced Sensing and Monitoring of Lithium Ion Batteries

Mark Suchomel

*Professor James M. Caruthers and Professor Joseph F. Pekny*

Secondary lithium ion battery use is growing with the boom of the smart phone and re-invention of the electric vehicle. Current state of charge (SOC) determination techniques rely on non-stop, accurate current measurements and predictive models tuned from idealized cycling patterns not representative of real world use. Equivalent circuit models are often used to estimate open circuit voltage of a battery under load. Look-up tables and empirical models attempt to correlate fitting parameters with temperature and battery age. Empirical state of health (SOH) and capacity degradation estimations do not acknowledge the system chemistry. Artificial neural networks and Kalman filters are expensive to train and implement.

The goal of this research is to develop and validate new state of charge determination techniques that no longer rely on traditional current measurements. Small voltages, excessive data and limited online integration resolution are technical problems with coulomb counting, resulting in state of charge *estimation* and under utilization of battery materials. Increased SOC accuracy will allow a broader operating window for battery use, decreasing the battery cost – especially for large format electric vehicle packs – and enhancing safety. The new technologies addressed here target mechanical properties of batteries to *directly* measure state of charge. Battery expansion/contraction, mass distribution and material properties are correlated to SOC using acoustic and pressure experiments.

Future work will include development of a new battery model. This proposed model will fill the void between equivalent circuits and full physics models to enhance new state of charge determination techniques. New sensors and a fully automated electric vehicle dynamometer will be used to validate the lumped-parameter model with real-world load cycles. Acknowledging the underlying chemistry without the full physics computational requirements will enhance state of health and capacity fade determination, further increasing the opportunity for battery utilization.

10:30AM – 10:55AM SESSION B ROOM B124

# Fission and Fusion of Liquid Drops

Krishnaraj Sambath

*Professor Osman A. Basaran*

Ranging from raindrops in thunderclouds, to electrosprays in mass spectrometry to printing and coating processes of 5 microns or thinner, the scenario of liquid drops subject to strong electric fields is more common than it is perceived to be. Such drops develop sharp conical tips from which thin jets emanate which subsequently disintegrate into a fine spray of charged droplets. Despite being one of the oldest and most celebrated problems in science, there exist conflicting theories and measurement on the size and charge of these small electrospray droplets. In this work, dynamics of uncharged liquid drops subjected to an electric field is simulated by solving the Navier-Stokes equations augmented with Maxwell's equations using the Galerkin finite element method. Theory and simulations are used here to show that liquid conductivity can be tuned to obtain three distinct scaling regimes for the size and charge of droplets thus formed, a finding that has been missed by previous studies and that bridges the gap between experiments and theory. It is further shown that these charged droplets are Coulombically stable, i.e., they do not explode into finer droplets, irrespective of the size and physical properties of the parent drop, making it the most fundamental law of semi-conducting liquids.

The computational framework developed above for the disintegration of drops was adapted to study the exact opposite problem – collision and coalescence of liquid drops – which has intrigued scientists and engineers for more than a century owing to its ubiquitousness in nature, e.g. raindrop growth, and industries, e.g. breaking (or stabilizing) emulsions in the oil and gas, food and chemical. One of the important indicators for emulsion stability (or its instability) is the time it takes for two drops to drive away the film in between and subsequently coalesce – used to estimate shelf life of bottled products, e.g., mayonnaise, or residence time of coalescer units for water-oil separations. Simulations are used here to calculate this coalescence time and, more generally, elucidate the approach and pre-contact dynamics of drops identifying conditions conducive for coalescence in terms of flow and fluid properties.

# Real Time Measurements of the Growth of Selenide Thin-film Photovoltaic Absorbers from Sulfide Nanoparticles

Bryce Walker

*Professor Rakesh Agrawal*

The feasibility of photovoltaics as a major player in the energy landscape relies heavily on being able to reduce costs through economies of scale. Despite this fact, current production methods are very batch oriented, and hence suffer from poor scalability. Liquid-based deposition methods are a promising technology wherein the processes can be scaled. On particular liquid-based deposition method of interest is through the deposition of an ink of semiconducting nanoparticles suspended in an appropriate solvent.

Nanoparticle based solar cells at Purdue rely on the formation of sulfide nanoparticles that are subsequently reacted in a selenium vapor rich environment that leads to the formation of a densified selenide thin film. With this process, solar cells can be created from both Copper Indium Gallium Selenide (CIGSe) and Copper Zinc Tin Sulfide/Selenide (CZTSSe) with efficiencies greater than 13% and 8% respectively.

With the great capabilities of this process, many questions have been raised with respect to how the films form. To address this issue, we have utilized techniques developed at Helmholtz-Zentrum Berlin (HZB) for the real-time synchrotron-based in-situ energy-dispersive x-ray diffraction (EDXRD). The real-time analysis allows us to probe the basic structure of the film, and watch as the compounds successfully transform from their respective sulfide particles through various intermediates en route to the final selenide film. This insight will allow researchers to greater understand the mechanisms involved, and to create alternative routes for greater device capabilities.

# Low Cost Synergistic Desalination Processes

Anand Venkatesan

*Professor Phillip C. Wankat*

Process synthesis/development, integration and optimization form the triad which is the backbone of any chemical industry. My doctoral research involves synergistic process development and subsequent optimization for techno-economic feasibility.

Water is one the basic substances required for sustenance of life on earth. Unfortunately there is a scarcity of water as an effect of rapid population increase and the associated socio-economic activities. In short, water is one of the grand challenges facing mankind. Desalination of saline waters has emerged as an alternate source of water and Reverse Osmosis (RO), accounts for 96% of desalinated water produced in the U.S. Although RO is the most preferred desalination method, it is plagued by the problem of mineral scaling on membrane. This constrains the operation of RO by reducing the water recovery and increasing the production of brine.

Using principles of process integration and optimization, supported by rigorous Aspen simulations, I developed novel hybrid RO desalination processes involving Ion Exchange (IEX) water softening and heating by direct injection of steam. The hybrid processes developed at the scale of 1 - 96 million US gallons per day for concentrated brackish groundwater of southwest USA and the Colorado River alleviated the problem of mineral scaling and improved the water recovery to as high as 96%. Apart from improvement in recovery, economic benefits were also obtained (US$ 15 million annual savings).

Another critical issue which constrains water recovery, especially in the RO desalination of Produced water is membrane fouling due to hydrocarbons, oil and grease. Produced water is generated from oil and gas (O&G) extraction process. It is the largest volume byproduct stream associated with O&G production, approximately 75 billion barrels (bbls) worldwide annually. The O&G industry in USA produces about 7 bbl of produced water per bbl of oil. Management of produced water has an adverse environmental impact due to its complex composition and disposal costs can be as high as $20/bbl depending on the type of disposal.

A novel hybrid RO/IEX/Adsorption process is proposed for Produced water desalination. This hybrid high recovery process has the potential to reduce the water consumption in O&G extraction (75-225 billion bbls worldwide annually) by improving recyclability. In addition, recovery of hydrocarbons present in produced water can be used as feedstock for downstream operations such as upgradation into valuable chemicals.

# Probing the Active Redox Sites on Cu/SSZ-13 in the Selective Catalytic Reduction of $NO_x$ by $NH_3$ via *Operando* X-ray Absorption

Shane Bates

*Professor Fabio H. Ribeiro and Professor W. Nicholas Delgass*

Stringent regulations for NOx emissions have opened the door for innovation and discovery in deNOx applications. One thriving technology is the selective catalytic reduction of nitric oxide/ nitrogen dioxide ($NO/NO_2$) with ammonia ($NH_3$), which, in the addition of excess oxygen ($O_2$), produces inert nitrogen ($N_2$) and water ($H_2O$). The latest catalyst to be utilized in SCR is Cu/chabazite (CHA) due to its unique ability to perform over a wide range of temperatures in the presence of water without breakdown of the zeolite structure. Since its discovery as an active SCR catalyst, many studies have started to understand its mechanism and, in particular, the role that Cu plays in the mechanistic steps. To look at this, we explored the active Cu environment under standard SCR conditions (no $NO_2$ present) with *operando* X-ray absorption spectroscopy (XAS), which monitored the kinetics of reaction in addition to the x-ray absorption, and compared the experimental results with density functional theory (DFT) calculations.

Work done by our collaborators using DFT suggested the two most stable conformations of Cu under reducing and oxidizing conditions were 2-coordinate Cu(I) and 4-coordinate Cu(II), respectively. These species could exist as a redox couple. *Operando* XAS results for Cu/SSZ-13 showed that Cu existed in a mixed Cu(I)-Cu(II) state under standard SCR, which agreed well with the DFT calculations. To further investigate the possibility of a Cu redox cycle, the oxidizing and reducing half-reactions we expected in the cycle were isolated by switching out a specific gas and watching the changes in Cu via XAS. The mixture of $NO + NH_3$ in the absence of $O_2$ reduced Cu to nearly 75% Cu(I). The mixture of $NH_3 + O_2$ in the absence of NO completely oxidized the Cu to Cu(II). Thus, by cutting off the reducing or oxidizing half reaction of standard SCR, the Cu was driven to an oxidized or reduced state, respectively, showing that a dynamic balance of redox sites existed in the Cu. The implication of this result was that any mechanism suggested for standard SCR over Cu/SSZ-13 should include a redox cycle for Cu between Cu(I) and Cu(II). It is possible that this could be expanded to other Cu exchanged zeolites based on our observation of a mixed Cu state in SAPO-34 and ZSM-5.

Thus, *operando* XAS experiments under SCR and isolated SCR half-reaction conditions have shown that Cu not only exists in a mixed Cu(I)-Cu(II) state, but that a dynamic balance exists in the Cu which can be driven to an oxidized or reduced state when one of the half-reactions is excluded. These results agree with DFT calculations which suggest a Cu(I)-Cu(II) redox couple and should be allowed for in any proposed SCR mechanism.

# Energy Systems Analysis for Sustainable Transportation Fuel

Dharik Sanchan Mallapragada

*Professor Rakesh Agrawal, Professor W. Nicholas Delgass, and Professor Fabio H. Ribeiro*

In a fossil-fuel deprived world, it is likely that all the basic human needs will be met by renewable sources like solar energy. Among them, transportation offers the greatest challenges, owing to its high energy-density fuel requirements, which have traditionally been met by liquid hydrocarbon fuels derived from fossil resources. Here, we use systems analysis tools to develop alternative transportation roadmaps based on the use of renewable carbon sources like biomass, solar $H_2$, heat and electricity, in conjunction with novel processes for producing liquid fuels.

The quantity of liquid fuel produced from biomass is limited by the extent of sustainably available (SA) biomass that can be recovered annually without using additional agricultural land. We outline the systematic synthesis of augmented biomass-to-liquid fuel processes, which maximize biomass carbon conversion to liquid fuel by using supplemental energy derived from sunlight in the form of $H_2$, heat, and electricity. While standalone biomass-to-liquid fuel processes are limited to <50% biomass carbon recovered as liquid fuel, augmented processes overcome this barrier by utilizing biomass as a carbon source combined with supplemental solar energy use. The emphasis is on identifying augmented processes that require the least amount of supplemental solar energy input corresponding to a given biomass carbon recovery. The process synthesis begins with developing a superstructure of all possible process configurations. Subsequently, a mixed-integer nonlinear mathematical framework is formulated and solved via global optimization methods to identify the optimal process configuration for different target carbon recovery levels. The novel features of the process synthesis include: 1) simultaneous process heat, power and mass integration while allowing for co-generation and 2) flexibility to design for different carbon recovery levels to account for solar energy intermittency.

Despite 100% SA biomass carbon conversion to liquid fuel and partial electrification via the use of plug-in hybrid vehicles (PHEV), additional liquid fuel demand could exist, as shown to be possible for the US. For this scenario, systems analysis reveals that extraction of atmospheric $CO_2$ followed by subsequent thermochemical conversion to liquid fuel using $H_2$, heat and electricity is more efficient in utilizing solar energy than any of the currently known photosynthetic routes such as growing dedicated biomass or algae for liquid fuel. Thus, a systematic roadmap outlining the options to supply the fuel for a renewable transportation sector is generated.

# An Integrated Approach for Characterization of Pt Based Aqueous Phase Reforming Catalysts

Paul J. Dietrich

*Professor Fabio H. Ribeiro and Professor W. Nicholas Delgass*

In order to convert biomass to usable fuels and chemicals compatible with current infrastructure, large quantities of hydrogen will be required to reduce the oxygen content of renewable feedstocks. To avoid using hydrogen derived from petroleum or natural gas, catalysts that convert biomass to hydrogen with high rates and selectivity must be developed. Cortright et al[1] have identified aqueous phase reforming (APR) of carbohydrate feedstocks with Pt based catalysts as an effective route for hydrogen production. Addition of a second metal to the Pt system has been demonstrated to increase rates of hydrogen production[2].

In this work, we utilize a characterization approach integrating kinetic experiments, density functional theory (DFT), and spectroscopy, both *operando* (simultaneously measuring kinetics and x-ray absorption spectra) and *ex situ* (measuring spectra in a non-reaction environment), to investigate the active state of the catalyst and determine how the composition, structure, and morphology of bimetallic catalyst particles impact activity and selectivity for hydrogen generation from glycerol. Addition of Co or Mo to a carbon nanotube supported Pt catalyst increased the rate of hydrogen generation by up to a factor of 10. However, Mo promotion decreased hydrogen selectivity, while Co promotion maintained high hydrogen yields.

Using a custom designed *operando* plug flow reactor system allowed for x-ray absorption spectroscopy of the active catalyst during liquid phase reaction at high temperature (230ºC) and pressure (32 bar). *Operando* results indicate that the PtMo particles have a Mo-rich surface and Pt rich core, which form reaction sites that catalyze deoxygenation reactions, reducing yields. By contrast, PtCo particles have a Pt rich surface and Co rich core, which maintains highly selective Pt reaction sites. Density functional theory results indicate that the bimetallic nature of these particles changes the electronic structure, resulting in the observed increase in reaction rates. By coupling characterization results with reaction kinetics, we propose a model for reforming catalysts that may be used to predict better materials.

[1] Cortright, R.D.; Davda, R.R.; Dumesic, J. A. *Nature.* **2002,** *44* (6901), 964
[2] Huber, G.W.; Shabaker, J.W.; Evans, S.T.; Dumesic, J. A. *App. Cat. B: Environ.* **2006,** *62,* 226

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# Exceptional Event Management Applied to Continuous Pharmaceutical Manufacturing

Anshu Gupta

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One of the important challenges in effective real time process management is the implementation of intelligent systems that can assist human operators in making supervisory control decisions, instead of simply sounding an alarm when process variables go out of range. Operator failures to exercise the appropriate mitigation actions often have an adverse effect on product quality, process safety, occupational health and environmental impact. The economic effect of such exceptional events is immense; an estimated $20billion/year loss in petrochemical industry has been reported. The challenges and opportunities for improvements are even larger in the pharmaceutical manufacturing domain because so much of the processing involves particulate and granular systems whose characteristics tends to be more problematic than that of fluids. The development and manufacturing of pharmaceutical products are governed by strict safety regulations but with the advent of Process Analytical Technology (PAT) initiative advanced by the FDA; gives the pharmaceutical industry an opportunity to apply various systems engineering tools. Early detection and diagnosis of process faults while the plant is still operating in a controllable region can help avoid abnormal event progression, production disruptions and productivity losses.

An EEM framework has been developed to deal with fault detection, diagnosis and mitigation of conditions that result from process anomalies. The framework developed uses a combination of Principal Component Analysis (PCA), Signed Digraphs (SDG) and Qualitative Trend Analysis (QTA). PCA has been used for fault detection and SDG/QTA techniques have been used for diagnosis based on faults signature. An ontological database has been created to maintain records of the signatures of a number of exceptional events typical of a dry granulation line and their associated mitigation strategies. Once a fault is diagnosed a respective mitigation strategy is displayed to an operator. The EEM framework has been applied to continuous pharmaceutical product manufacturing line consisting of feeders, blender and roller compacter; and was able to detect and diagnose various commonly occurring exceptional events, either in a given equipment or throughout the whole continuous line, such as; 'No powder entering roll region', 'varying moisture and content uniformity of powder' and 'bridging of powder in feeder'; within few seconds of their inception and to provide mitigation advisories to the operator.

# High Pressure Catalytic Hydrodeoxygenation Reaction Pathways and Kinetics for Dihydroeugenol over Pt/$ZrO_2$ and Ru/$ZrO_2$ catalysts

Sara L. Yohe

*Professor W. Nicholas Delgass, Professor Fabio H. Ribeiro, and Professor Rakesh Agrawal*

The $H_2$Bioil [1] process, involving high pressure biomass fast-hydropyrolysis followed by vapor phase fixed-bed catalytic hydrodeoxygenation (HDO), has been proposed to generate transportation fuels from lignocellulosic biomass. The hundreds of oxygenated vapor compounds generated during the first stage fast-hydropyrolysis complicate the development of new HDO catalysts for the second stage reactor. Therefore, model compound studies are necessary to gain an understanding of how various catalysts perform at removing specific oxygen functional groups.

The lignin-derived compound, dihydroeugenol (2-methoxy-4-propylphenol), was the focus of this study. A comparison of Pt and Ru catalysts supported on $ZrO_2$ was conducted in a vapor-phase fixed-bed reactor at 300$^{o}$C and 24 atm in hydrogen. Weight hourly space velocities were varied from 100-1000 g $hr^{-1}$ g $cat^{-1}$ to provide the kinetic data. For both catalysts, three main reaction pathways were identified: HDO, transalkylation, and hydrogenation of the aromatic ring. The WHSV studies suggest that the oxygen removal pathway occurs via a series reaction, with methoxy group removal occurring first followed by phenol group removal. Transalkylation occurs via methyl attachment to the aromatic ring. Apparent activation energies and reaction orders were measured for products in each reaction pathway. The kinetic results for hydrogenation of dihydroeugenol to 2-methoxy-4-propylcyclohexanol were similar to those for benzene hydrogenation, suggesting that the mechanism of ring hydrogenation for dihydroeugenol is similar to that of other aromatic compounds [2]. Selectivity ratios of the desired deoxygenated products (4-propylphenol, propylbenzene) to their hydrogenated analogs (4-propylcyclohexanol, propylcyclohexane) were compared for the two catalysts. Ru had a higher selectivity towards the HDO versus hydrogenation pathway than Pt. Thus, even though the Pt catalyst had a higher overall rate, Ru was found to be a more favorable catalyst for oxygen removal with minimum hydrogen consumption.

References:

1) R. Agrawal, N. R. Singh, Synergistic Routes to Liquid Fuel for a Petroleum Deprived Future, AIChE Journal,55,7,1898-1905, 2009.

2) S. D. Lin, M. A. Vannice, Hydrogenation of Aromatic Hydrocarbons over Supported Pt Catalysts I. Benzene Hydrogenation, Journal of Catalysis, 143, 539-553, 1993.

# Drug-on-Demand: A Mini-Manufacturing Method of Pharmaceutical Dosage Forms

Laura Hirshfield

*Professor Gintaras V. Reklaitis*

Stimulated by initiatives such as PAT and QbD, the pharmaceutical industry has been focusing on the development of innovative, efficient manufacturing methods. The concept of "mini-manufacturing" of drugs, as opposed to mass production of drugs, has shown promise in this area. "Drug-on-demand" is one such manufacturing method, which uses drop-on-demand printhead technology to deposit active pharmaceutical ingredients (API) onto edible substrates. Besides minimizing a need for mass production of all drugs, this method allows for the layering of different APIs and the creation of individual dosing forms, in which the amount of API can be varied depending on the patient.

This work focuses on the process systems engineering aspects of drug-on-demand, including automation, control and Exceptional Events Management (EEM) strategy. A proper control strategy is necessary so that the system can run at optimal setpoints and adjust in real-time, allowing for an efficient manufacturing process and a precise on-specification drug product. The control strategy for our drug-on-demand setup allows us to execute an automated, optimized, and controlled print cycle while closely monitoring drop size, drug morphology, and drop deposition pattern. The implementation of EEM allows for detection, diagnosis, and mitigation of abnormal events that occur outside of the control space to ensure a more efficient, productive process.

# Tissue Engineering Cues to Direct the Endothelial Differentiation of Mesenchymal Stem Cells

Richard J. Galas Jr.

*Professor Julie C. Liu*

In tissue engineering, there is a growing need for vascularizing tissues *in vitro.* Implants will vascularize *in vivo*, but vascular ingrowth is time-consuming. This slow growth rate is not practical because *in vivo* cell viability is limited to 100-200 microns from the edge of functional vasculature. Pre-vascularization before implantation can increase viability in tissues thicker than this diffusion limit. Recently, it has been shown that mesenchymal stem cells (MSCs) can be differentiated into endothelial cells by treatment with soluble vascular endothelial growth factor (VEGF). The objective of this study is to develop an alternate cue to differentiate MSCs into endothelial cells.

We examined surface-bound VEGF as a cue to direct MSC differentiation into endothelial cells. VEGF was attached to a surface via the bi-functional cross-linker, sulfo-SANPAH. Successful reaction was confirmed by spectrophotometry and ELISA. Surface densities of 1.6 – 31.5 ng/cm$^2$ were obtained. Cells were grown on surface densities of 18.6 or 11.8 ng VEGF/cm$^2$ while treatment with soluble VEGF served as our positive control. Endothelial differentiation was evaluated by protein expression as well as by assessing angiogenic response to ECMatrix and low density lipoprotein (LDL) uptake.

After three weeks on bound VEGF MSCs expressed endothelial proteins and took up LDL. However, cells not treated with VEGF also expressed endothelial proteins and took up LDL, indicating that VEGF is not needed to differentiate MSCs into endothelial cells.

# Introducing Softwares to Facilitate Pharmaceutical Crystallization: *CrystalShape*, *CrystalTomogram*, *CrystalPolar* and *MorphologyDomain* [1]

Meenesh Singh

*Professor Doraiswami Ramkrishna*

Our research focuses on developing tools to understand and control crystallization of Active Pharmaceutical Ingredients (APIs). We have developed a state-of-the-art technique to obtain tomographic images of crystals (or any solid material) using confocal microscopy[1] and process them for crystal shape and shape-related properties using our software "***CrystalTomogram***"[2]. We have also developed a software "***MorphologyDomain***"[3] to predict all possible crystal morphologies (including needles and plates) that may appear during crystallization and a software "***CrystalPolar***"[4] to measure polar plots of growth/dissolution rates of 2D crystals. These softwares can be used together to decide operating conditions (such as solvent, co-solvent, additives, temperature and pressure) to produce suitably grown crystals for efficient formulation of drug in either solid dosage form or injectable products.

**References:**

[1] Singh M.R., Chakraborty J., Nere N., Tung H-H., Bordawekar S. and Ramkrishna D., "Image-Analysis-Based Method for Measurement of 3D Crystal Morphology and Polymorph Identification using Confocal Microscopy," Cryst. Growth Des., 12 (7), 3735-3748, 2012

[2] *CrystalTomogram*: A software to construct crystal morphology from tomographic images, https://engineering.purdue.edu/~drops/softwares/CrystalTomogram.zip

[3] *MorphologyDomain*: A software to visualize accessible crystal morphologies under given operating conditions. https://engineering.purdue.edu/~drops/softwares/MorphologyDomain.zip

[4] *CrystalPolar*: A software to obtain growth/dissolution rates of all crystal faces from the dynamic images of crystals. https://engineering.purdue.edu/~drops/softwares/CrystalPolar.zip

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[1] Please send requests for passwords to access these softwares to Prof. Doraiswami Ramkrishna (ramkrish@ecn.purdue.edu)

# Effect of DNA Methylation on Chromatin Compaction and Dynamics

Isabel Jimenez-useche

*Professor Chongli Yuan*

Epigenetic modification patterns in cells are closely affiliated with human diseases, e.g., cancer and neurological disorders, due to their distinctive role in gene regulation. CpG methylation is the most important epigenetic mark found on DNA and it plays a key role on gene silencing. DNA methylation can affect both chromatin structure and chromatin interaction with other proteins which eventually result in gene activation or silencing. However, the detailed molecular mechanism as to how DNA methylation modulates chromatin structure and function remains unknown. We have studied how the presence of different DNA methylation levels and patterns can affect chromatin features, using state-of-the-art fluorescence spectroscopy techniques. Our results show a dynamic behavior of all nucleosomes i.e. the fundamental chromatin unit, despite of their methylation status or binding to other proteins e.g. linker histone proteins. We also observed that the nucleosome conformation and dynamics can be modulated by a specific DNA methylation pattern depending on the buffer conditions. Finally, DNA methylation does not seem to have a significant impact on linker histone binding. These observations give us molecular insights of regulatory mechanisms driven by DNA methylation. This knowledge can be instrumental in developing new early stage biomarkers of cancer diseases.

# Model-based Individualized Treatment for Childhood Leukemia

Jayachandran Devaraj

*Professor Doraiswami Ramkrishna*

Acute Lymphoblastic Leukemia, commonly known as ALL, is a predominant form of cancer during childhood. With the advent of modern healthcare support, the 5-year survival rate has been impressive in the recent past. However, long-term ALL survivors embattle several treatment-related medical and socio-economic complications due to excessive and inordinate chemotherapy doses received during treatment. In this work, we present a model-based approach to personalize 6-Mercaptopurine (6-MP) treatment for childhood ALL, incorporating the pharmacogenomic variations among patients. Semi-mechanistic mathematical models were developed and validated for i). 6-MP metabolism, ii). red blood cells mean corpuscular volume (MCV) dynamics, a surrogate marker for treatment efficacy, and iii). leukopenia, a major side-effect. With the constraint of getting limited data from clinical settings, a global sensitivity analysis based model reduction technique was employed to reduce the parameter space arising from semi-mechanistic models. The reduced, sensitive parameters were used to individualize the average patient model to a specific patient so as to minimize the model uncertainty with limited clinical data. The model was validated with real patient data obtained from literature and Riley Hospital for Children in Indianapolis. Models fit the data well and mimic diverse behavior observed among patients with minimum parameters. The implementation of the proposed approach in clinical practice is realizable with routinely measured complete blood counts (CBC) and a few additional metabolite measurements. The proposed models and model reduction approach can be utilized to achieve model-based individualized treatment to a specific patient, as opposed to a standard dose for all, and to prescribe an optimal dose for a desired outcome with minimum side-effects.

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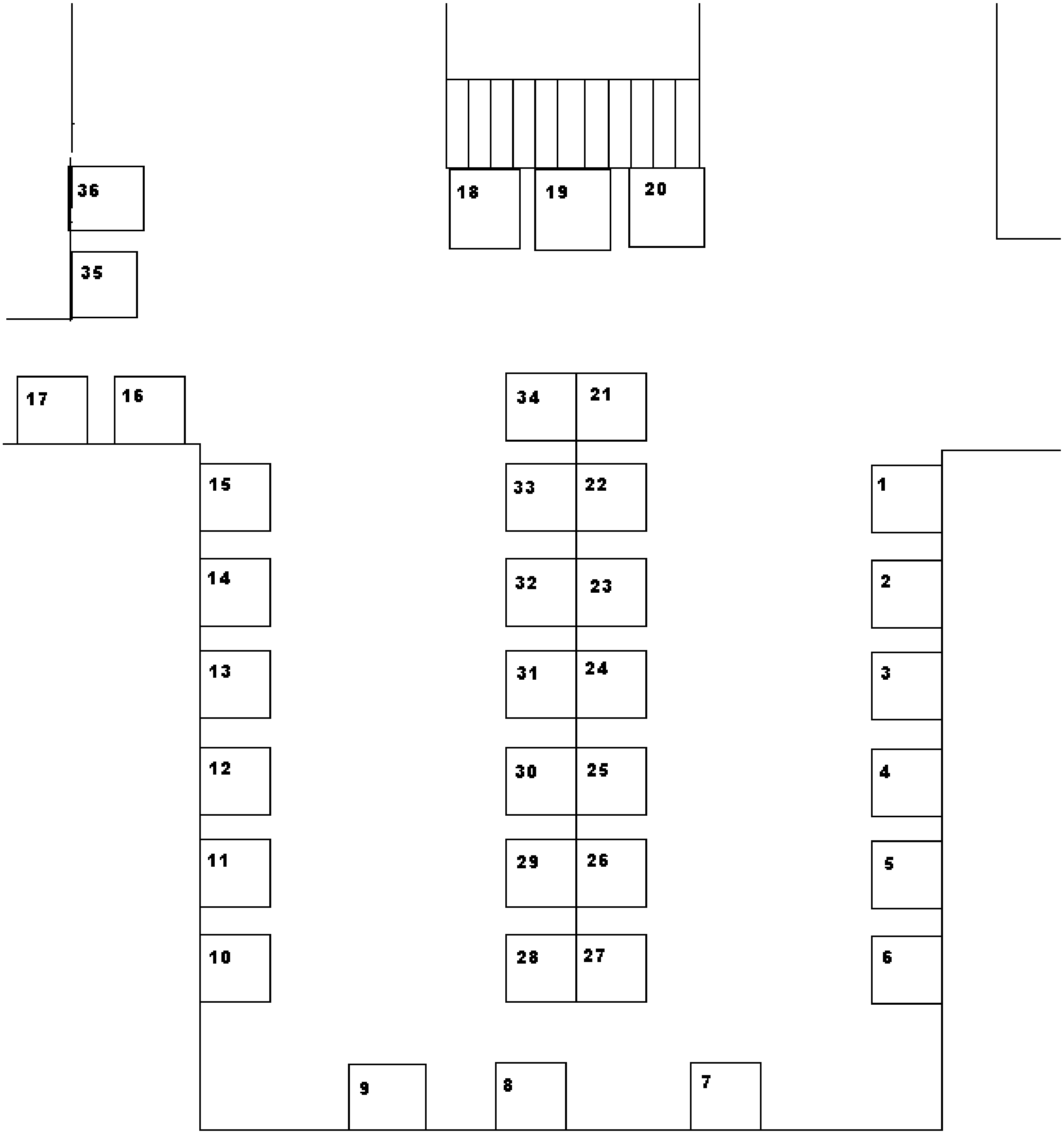

*Forney Hall of Chemical Engineering, Henson Atrium*

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