2018-2019 Research Highlights

Nilesh Ade
PhD CHEN

Moving Towards a Hydrogen Economy through Safer and More Reliable, Design and Operation of Proton Exchange Membrane Fuel Cells

Proton exchange membrane fuel cells (PEMFC) are considered as the best alternative for hydrocarbon-based combustible engines in vehicular applications due to their higher efficiency and cleaner utilization and can serve as a pathway towards implementing a hydrogen economy. However, one of the major hindrance towards their commercialization is the reliability of PEMFC. The deterioration in reliability of PEMFC is caused by the degradation of the polymer electrolyte membrane. More importantly, apart from affecting the performance of the fuel cell, degradation of the membrane can be a contributing cause for an explosion in PEMFC. Therefore, to mitigate the risk associated with explosion in PEMFC and to achieve the required levels of performance, it is essential to study the degradation of this membrane in depth. This study deals with understanding the fundamentals of PEMFC degradation through modeling using computational fluid dynamics (CFD) and minimizing the degradation mechanism by altering design and operating conditions of the PEMFC system. The study will also focus on experimentally determining the rate of degradation for different membrane materials and the membrane material that provides optimized performance and improves the overall safety of the system.

Cassio Ahumada
PhD CHEN

Enhancing the Understanding of Deflagration-to-Detonation Transition (DDT)

There are two main combustion modes in vapor cloud explosions: deflagration and detonation. Deflagrations occur when the flame front travels at subsonic speeds leading to overpressure with the same order of magnitude as the atmospheric pressure. Unlike deflagrations, detonations are characterized by supersonic flame propagation velocities and significant overpressures. Several experimental studies have shown that when proper conditions are met, the flame front may accelerate, reaching the detonation combustion mode. This phenomenon is known as deflagration-to-detonation transition (DDT). However, more recent large-scale tests have demonstrated that intermediate states between laminar deflagrations and CJ detonations are more likely to happen for fuels with low and medium reactivity, such as methane and propane. Therefore, this research project focuses on studying experimentally and numerically intermediate combustion regimes during deflagration-to-detonation transition. The ultimate goal is to understand the effects of layout and fire suppressants on the final flame speed.

Joshiba Ariamuthu Venkidasalapathy
PhD CHEN

A Systematic Approach to Alarm Identification with Application to Tennessee Eastman Problem

Abnormal event management (AEM) of process plants has garnered attention in recent years. It has been estimated that $20 billion are lost due to abnormal situations each year. Efficient monitoring of process variables and timely corrective measure are at the crux of AEM. The most process monitoring techniques in current practice involves the use of alarms to alert the operator, thereby requiring a corrective action to restore normal operation. The ‘alarm identification’ is an important aspect of the alarm system design, which is the focus of this research project. It concerns the selection of a potential subset of process measurements to configure to the alarm system. Most of the previous works on alarm identification involves a qualitative approach. This project aims to develop an alarm identification design technique that incorporates quantitative aspects. The operator-centered approach aims at providing the operator ample time to respond while having fewer active alarms. The proposed approach is implemented on the benchmark industrial case-study: The Tennessee Eastman process control problem.

Pranav Bagaria
PhD CHEN
Effect of Dispersion and Morphology on Dust Explosion Hazard
Dust explosions are a serious and persistent problem for process industries (1 incident per month since 1980 in the United States of America). The threat of dust explosions can be perceived by parameters such as maximum explosion overpressure ($P_{ex, max}$), deflagration index (K_{st}), minimum ignition energy (MIE), minimum explosible concentration (MEC), limiting oxygen concentration (LOC), etc. It is important that these parameters are measured accurately to better understand the risk and take proper safety measures. Parameters such as P_{max}, K_{st}, MEC, MIE and LOC for various dusts are studied using a standard 20-L or 1-m^3 spherical dust explosion vessel in accordance with ISO and ASTM standards. In all these standards, it is assumed that the dust cloud particle size distribution in the air is the same as the particle size distribution of the pre-dispersed dust sample. Recent studies have shown this not to be true. Because dust explosion parameters are significantly dependent on particle size distribution, this general assumption can lead to erroneous results, which can cause severe underestimation/overestimation of dust explosion risk. In addition, the role of particle shape/morphology on these explosion parameters is not understood, but can be very important to understand the combustion mechanism and explosion risk. This research addresses challenges such as: does the formation of dust cloud due to dispersion process changes the particle size distribution? How much shift in size distribution occurs for different materials? What factors affects the shift in size distribution? What is the consequence of this shift on explosion parameters? Can the change in size distribution for different materials be classified and predicted? And what is the role of particle/shape morphology on dust explosion parameters?

Purvali Chaudhari
PhD CHEN
Effect of Partial Inerting on Minimum Ignition Characteristics of Dusts
Dust explosions continue to present a constant hazard to the process industries; thus, mitigation remains an important field of research. Studies have found that the minimum ignition energy (MIE) of a dust is influenced by factors such as temperature, pressure, oxygen concentration, and particle size. Industrially, partial inerting has various advantages over other mitigation techniques and is one of the lesser explored areas in dust explosion mitigation. There is limited understanding of the dust explosion mechanism and less available literature in this area. The objective of the current research is to study the effect of inerting on Minimum Ignition Energy (MIE) for different family of materials. The study also aims to develop a model considering the molecular (bond energies) and macroscopic (limiting oxygen content- LOC) aspects to explain the ignition behavior of dusts under varying conditions.

Harold Escobar
PhD CHEN
Development of a Systemic Approach for Chemical Reactivity Hazards Assessment Applied to Specific Functional Groups
Reactivity tests for identification and understanding of reactive chemical hazards are conducted using different experimental tools of calorimetry. These attempt to predict chemical properties and unsafe process conditions. Moreover, there is often an under prediction of reactivity properties (e.g. over pressure), and experimental techniques face significant challenges for its extensive duration and high costs.

A systemic approach is proposed in order to make a generalized prediction of reactive properties (e.g. Onset Temperature). The main objective of this research is to develop prediction tools based on systematic laboratory testing and molecular models techniques. This will expedite reactive hazard assessment, thus reducing the related costs in industry. Functional groups will be chosen based on different criteria including incident history. Therefore by using molecular properties and kinetic parameters obtained from experimental testing, reactivity descriptors will be developed and verified with existing data.

Tatiana Flechas
PhD CHEN
CFD Modeling of Liquefied Gases Discharging Through a Pipeline Full Bore Rupture
Large amounts of substances are transported in pipelines worldwide. This activity represents a hazard that needs to be quantitatively assessed through discharge models that are capable of accurately predicting the outflow when a pipeline ruptures. When a pipeline transporting a pressurized liquefied gas ruptures (*e.g.*, CO_2, LPG pipelines), the expansion generates a phase transition which results in a two-phase release. Numerous researchers have developed one-dimensional models to describe the discharge of liquefied gases when a pipeline full bore rupture occurs. However, a systematic study on how the accuracy of different equations of state affects the depressurization prediction is lacking for this case. The main objective of this research is to propose a two-dimensional discharge model using Computational Fluid Dynamic (CFD) tools in order to predict the pressure and temperature profiles along the pipeline, as well as the discharge rate and phase transition; while investigating the effect of different equations of state on the predictions for the full bore rupture scenario. In order to validate the 2-D discharge model, full bore rupture experiments with dense-phase CO_2 pipelines are used. The validation step evaluates the assumptions to model the transient phenomenon. Once the full bore rupture study is completed, the subsequent step will be to propose a three-dimensional model to predict the behavior of liquefied gases discharging through punctures. The previous scenario will complete the picture for predicting the discharge of flashing liquids when a pipelines ruptures.

Christopher Gordon
PhD CHEN
Maintenance Planning Using Machine Learning and Multi-Objective Stochastic Optimization
Maintenance planning and process operations in chemical manufacturing plants are subject to several sources of uncertainty ranging from volatile feedstock prices to uncertainty in equipment failure times. In the context of assuring the mechanical integrity of assets in ageing plants, the present research employs process systems engineering principles to develop novel optimization algorithms for preventive and predictive maintenance planning in the presence of uncertainty. The research spans different approaches to plant maintenance and consists of three aspects: (1) predictive maintenance using deep neural networks and support vector machines, (2) scheduling of turnaround activities subject to resource constraints using global event-based continuous-time optimization, and (3) preventive maintenance planning using multi-objective multi-stage stochastic programming with integer recourse. The results of the research can be used to prioritize maintenance actions, to improve overall equipment availability, and to maximize plant productivity.

Hallie Graham
PhD CHEN
Comprehensive Testing Hierarchy for Reactive Chemical Identification
Reactive chemicals are a major hazard affecting the processing, storage, and handling of chemicals that can lead to serious consequences such as fires, explosions, and toxic gas releases. In the Chemical Safety Board's Reactive Hazard Investigation of 167 serious accidents, over 40 classes of chemicals were identified with no clear dominating class and most were not rated as reactive chemicals. While most research focuses on classes already in use, this research plans to address the issue of how to identify a reactive chemical by developing a hierarchy of testing procedures through experiments and molecular modeling. The goal of this research is to produce a testing procedure for the vast majority of reactive chemicals that can be used by industry to identify potential risk before production.

Richard Gustafson
PhD MSEN
Effects of Hydrogen on the Strength and Fracture Characteristics of Multigrain Metals

The presence of atomic hydrogen in metals plays an important part in metals in the process industries; Metal grain structure also plays an important role in determining the strength and mechanical properties of metals. The generation, migration, and diffusion of hydrogen is difficult to experimentally study. Hydrogen's interaction in multi-grain systems is less-well understood. By developing a hydrogen multi-grain model and mapping changes in properties to failure through a model system of palladium-hydrogen, insight is developed into the hydrogen concentration and grain-size effects on properties of metals exposed to hydrogen.

Zohra Halim
PhD CHEN

Cumulative Risk Assessment Model to Analyze Increased Risk Due to Impaired Barriers in Offshore Oil and Gas Facilities

The Deepwater Horizon incident, as well as many other large-scale disasters, reminds us that multiple factors can contribute to a catastrophe, and these factors can be technical, operational, human or organizational in nature. Even though we carry out investigations to learn from these incidents, incidents keep happening as we fail to incorporate those learnings into risk assessment models. There is a need to carry out better risk assessments that will incorporate learning from the past, consider how the various factors are deviating from their safe state and predict the cumulative risk arising from the deviations. Existing risk assessment methods use expert opinion to consider the contribution of human and organizational factors to risk and rely on generic data that cannot capture the deviation of various factors. This research focuses on bridging the gap for a better cumulative risk assessment that will remove complete reliance on expert opinion. It uses learnings from past incidents and current plant data to update the information about how various technical and non-technical factors are deviating in a facility so that their influence on the failure probabilities of barriers can be better understood and managed.

Ahmed Harhara
PhD CHEN

CFD Analysis of a Tube Rupture Scenario

Shell and tube exchangers are commonly used in the oil and gas, chemical, and nuclear industries. One fault that may occur with heat exchangers is a tube rupture- an overpressure scenario in which high pressure fluid flows into the low pressure region. This overpressure event may compromise the mechanical integrity of the exchanger and can lead to the equipment's failure. To protect against such scenarios, overpressure protection measures such as relief devices are installed on the low pressure side of the exchanger. To determine the size of the relief device that must be installed, API 521 recommends a dynamic analysis to be performed when there are large differences in pressure between the shell and tube side. Using ANSYS Fluent, the peak pressures from a 2D model are compared against a dynamic analysis. Finally, both results are then compared against known experimental data.

Prerna Jain
PhD CHEN

Resilience Analysis Framework for Process Design and Operations

Increasing process safety and risk management challenges in the process industries and change in the public perception of hazards and risk globally have necessitated exploring tools for efficient risk management. The application of the resilience engineering perspective is gradually being explored as an approach for considering the dynamics of socio-technical aspects based on systems theory. The resilience methodology emphasizes non-linear dynamics, new types of threats, uncertainty, and recovery from upset or catastrophic situations. The main focus of this research is to propose a holistic method to integrate both technical (process parameters variations) and social (policy/regulations, human and organizational) factors including prediction, survival, and recovery analysis for process facilities. The framework developed in this research is called Process Resilience Analysis Framework (PRAF) comprising of four aspects: early detection, error tolerant design, plasticity, and recoverability. PRAF would be applicable to both onshore and offshore installations, primarily focusing on early detection of unsafe zones, assessment of aggregate risks and prioritization of safety barriers during abnormal situations, and reduction in response time resulting in enhanced recovery and mitigation of consequences.

Chenxi Ji
MS SENG

Facility Safety Study of LNG Offshore System

The motivation of this research is to establish a general offshore operation system to involve both marine transportation process and chemical safety process. The purpose of this research is to apply chemical process safety methodology to shipping and offshore industry, trying to support decision-makers facing LNG-FSRU siting problems and to arouse public concern of nearshore/offshore safety. GIS-based multi-attribute decision analysis (MADA) was adopted as the main logic of this research, and the evaluation framework was constituted by four layers (objective layer, process layer, hazard layer and attribute layer) by considering the data availability. Furthermore, three consecutive processes were determined for the whole system. For navigational process and berthing process, the operation process was realized by statistic tools and ship simulators. For LNG transferring process, the simulation runs were carried out by chemical consequence software. The whole evaluation framework was structured by the identified hazards and attributes. Based on the value of final LNG offshore system, the preferred alternative can be determined accordingly.

Zeren Jiao
MS CHEN

Optimize Ventilation Systems in Confined and Unconfined Workplaces Using Computational Fluid Dynamics (CFD)

Ventilation is the most common method to control toxic and explosive airborne materials in confined and unconfined spaces. The purpose of ventilation is to dilute or remove toxic and explosive vapors with air to prevent potential poisoning or explosion. In this study, Computational Fluid Dynamics (CFD) tools will be utilized to better understand the efficiency and mechanisms of ventilation systems. The objective of this work is to evaluate the optimized ventilation systems in both confined and unconfined workplaces, by considering the installation location and exhaust air flow rate. The results of the CFD simulation can serve as reference to maximize ventilation efficiency and minimize the energy cost.

Pratik Krishnan
PhD CHEN

Modeling of High Expansion Foam for LNG Vapor Risk Mitigation

The consumption of natural gas is expected to increase by over 70 percent over the next few decades, as it is a cleaner source of energy compared to oil or coal. Liquefaction of natural gas can be an effective way of storage and transport because its volume is around 600 times lower in liquid form. However, a leak of liquefied natural gas (LNG) can result in a catastrophic scenario. It may form a vapor cloud, which can migrate downwind near ground level due to its dense gas behavior and potentially ignite. The NFPA recommends the use of high expansion foam to mitigate LNG release vapor risk. The objective of this research is to understand the mechanisms of heat transfer involved between foam and LNG, and create a model for high expansion foam in order to estimate how much is needed and the optimal method of application.

Pritishma Lakhe
PhD CHEN

Process Safety in Nanomaterials

The large-scale production of nanomaterials is of increasing commercial and academic interest due to its immense potential in diverse applications. As nanomaterials are gaining prominence, it is important to investigate its potential process safety hazards. One of such nanomaterials is graphene. Graphene is desirable for energy storage and for composite filler applications among others. There is no economically viable method to produce graphene in large quantities and therefore, graphene oxide (GO) route is predominantly used. This method involves oxidation of graphite to GO and its subsequent reduction to a produced graphene-like material called reduced graphene oxide (rGO). The GO route has shown potential for bulk production at high yield. However, prior studies have shown that GO can undergo explosive decomposition under certain conditions and its synthesizing steps involve producing unstable oxides. This research will study (1) thermal stability of GO for safer storage and handling conditions; (2) hazards during GO synthesis to recommend safer operating conditions.

Guanyang Liu
PhD CHEN
Mitigation of Thermal Runaway Risk for Polymerization Process
Thermal runaway has been a major threat to the process industry for decades. In light of numerous failure modes that lead to runaway and its catastrophic consequences, it is necessary to develop methods to mitigate thermal runaway risk. Reports show that the polymerization process is where thermal runaway occurs most often. The unique kinetic and flow behavior of polymerization escalates the difficulty of preventing thermal runaway. The present research focuses on the development of a polymerization reaction inhibition system (PRIS) and thermal runaway early detection techniques. By deep understanding of kinetic-transport interactions in the polymerization process, theoretical insights are expected to guide industrial applications of mitigation methods.

Edna Mendez
PhD CHEN
Effects of Flow Conditions on the Performance of Corrosion Inhibitors in Pipes
Major process safety incidents have been caused by corrosion all over the world. These incidents are usually linked to leakage of highly flammable liquids or gases, causing severe damage to the environment, affecting people, and ultimately resulting in monetary losses. Despite the increasing knowledge of corrosion, efforts are still needed to understand different damage mechanisms and their control methods. One of the most common active corrosion mitigation techniques in refineries is the use of corrosion inhibitors. Film-forming corrosion inhibitors create a protective layer that can be influenced by different flow characteristics and flow regimes. These changes in hydrodynamic conditions have an effect on the performance of corrosion inhibitors. This work focuses on the fundamental understanding of the hydrodynamics of the system coupled with analysis of the corrosion behavior using electrochemical techniques. The objective of this research is to study the influence of different flow parameters on the efficiency of corrosion inhibitors under corrosive environments such as CO_2.

Shayan Sean Niknezhad
PhD ITDE
Energy Policy and Security
The energy demand is increasing as the population of the world is snowballing. Albeit developed countries will have less energy consumption growth in comparison to the underdeveloped countries such as India and China in the next 25 years. Securing the energy supplies along with more energy diversification is crucial in the United States of America in order to export energy, maintain positive GDP, being less dependent on the middle east crude oil, dominate the energy prices in the world, and enhance energy and environmental sustainability. Lifting the ban on the U.S oil exports, revolutions in crude oil extraction, U.S. LNG exports, and smart grids are few game changers in the next coming decades. This research aims at optimizing the current energy systems including production, distribution and consumption, and evaluating the infrastructures that are required to guarantee the domestic energy security, mitigate the environmental externalities, and give the U.S. energy power to avoid financial crisis and inflations due to energy price or shortages.

Sunhwa Park
PhD CHEN
With DAHAZID, Prevention and Mitigation of Potential Incidents Related to LNG Process
This research aims at three main goals to contribute on the prevention/mitigation of potential incidents at an LNG facility: 1) application of the new Hazard Identification tool, semi-automatic hazard identification (DAHAZID) to review previous incidents and analyze their common aspects with regard to LNG facilities. This analysis will suggest how to prevent and mitigate potential incidents at LNG processes (e.g., safer process design, conditions and safeguards and mitigation methods). 2) Consequence modeling for LNG, LNG + expansion foam or water curtain to check the given mitigation methods, and 3) actual experiments to ascertain the mitigation methods at the possible LNG incidents.

Trent Parker
PhD CHEN
Risk-Based Optimization of Alarm Systems Used in Industrial Applications
Alarm systems serve a critical role in the safe operation and control of plants by alerting operations staff of possible process deviations from normal operation. However, even with alarm systems installed, up to 90% of process incidents are attributable to human error. Thus, user-friendly alarm systems are crucial to ensure effective operator responses and thus safe plant operation. Alarms may fall into the categories of process alarms or critical safety alarms. However, there often exist a large number of alarms that fall in the range between these two categories. At times, the role of alarm management for operations staff can become unclear, particularly when multiple alarms occur simultaneously. This research aims to provide a framework to determine the optimum combination of audible and visual signals so as to prioritize operator response time to safety issues and process upsets based on relative risk and minimize the likelihood of alarm flooding.

Susmitha Purnima Kotu
PhD CHEN
Integration of Electron Impedance Spectroscopy and Microfluidics for Investigating Microbially Influenced Corrosion Using Co-Culture Biofilms
Microorganisms can carry out corrosion reactions on metal surfaces resulting in microbiologically influenced corrosion (MIC). MIC is a significant problem in the oil and gas, water pipelines and tanks and costed about $460 billion globally in 2013. MIC has been extensively studied using batch reactors or large scale circulating loops. Both suffer from nutrient limitation and do not correctly represent the MIC environment. Thus, a small-scale continuous flow system that better represents flowing conditions for studying MIC is desirable.

A microfluidics-based flow system, consisting of microscale flow channels in a manner similar to pipelines where MIC is a major concern, is an attractive alternative. We developed a microfluidic flow cell by coating a pair of metal electrodes on glass. A microfluidic channel placed on this electrode pair allows corrosive microbes to be cultured on metal. This configuration allows MIC to be directly monitored using electrochemical impedance between the two electrodes while visualizing microbial community growth using confocal microscopy. Thus, this microfluidic MIC model enables integration of microbe-driven corrosion mechanisms along with microbial community growth at the metal surface.

Ankit Saini
MS Seng
Comparative Study of Nano-Powder Synthesis Methods for Process Performance and Exposure Hazards
Nanomaterials exhibit unique physical and chemical properties that impart specific characteristics essential in making engineered materials, but little is known about what effect these properties may have on human health. Research has shown that the physicochemical characteristics of particles can influence their effects in biological systems. These characteristics include particle size, shape, surface area, charge, chemical properties, solubility, oxidant generation potential, and degree of agglomeration. Nanomaterial-enabled products such as

nanocomposites, surface-coated materials, and materials comprised of nanostructures are unlikely to pose a risk of exposure during their handling and use as materials of non-inhalable size. However, some of the processes used in their production (e.g., formulating and applying nanoscale coatings) may lead to exposure to nanomaterials, and the cutting or grinding of such products could release respirable-sized nanoparticles. This research will focus on comparative analysis of nano-powder synthesis methods for the performance and potential hazards of engineered nanoparticles with the aim to identify measures that can be taken to minimize workplace exposures.

Sankhadeep Sarkar
MS SENG
Process Safety in Garment Industry
Garment industry is characterized by fiber to yarn & yarn to fabric production, pretreatment, dyeing, printing and finishing treatments. These complex systems entail presence of wide variety of processes, raw materials, machines, transport systems and storage sites, which are prone to hazards. This research is intended to identify the process hazards in the existing garment industries, correlating them with the earlier incidents, suggesting an efficient predictive/preventive program and validating its practicality with a cost-benefit analysis.

Jyoti Sharma
MS SENG
Study of Adiabatic Calorimeter Variability
Adiabatic calorimetry is a reliable technique to obtain both thermodynamic and kinetic parameters of a reactive chemical. The APTAC and ARC are popular types of adiabatic calorimeters for evaluating these parameters. Consistent and reliable thermal hazard assessment is critical for the design and control of industrial processes, which contain thermal hazards from reactive chemicals. However, there is often variability between the values reported in literature for various calorimeters and between laboratories. Often this was believed to be due to age, contamination, improper reagent preparation, passivation, incorrect thermocouple calibration, or non-adiabatic conditions and heat loss. This research study will examine the potential differences between the results reported for various calorimeters.

Yueqi Shen
PhD CHEN
Thermal Stability Analysis of Benzoyl Peroxide
This research is a comprehensive study of the runaway behavior of a benzoyl peroxide (BPO) hybrid system using isothermal and adiabatic calorimeters. The aim of this research is the advancement of understanding of thermal decomposition of BPO under various conditions. More specifically, this research will systematically study and develop thermodynamic and kinetic parameters related to BPO, and further the use of this particular knowledge to mitigate the risks in storage, transportation and manufacturing process.

Yang-Denis Su-Feher
PhD CHEN
Quantifying Ease of Control for Inherently Safer Design
The most cost-effective approach to prevent incidents is to add process design features to prevent hazardous situations, rather than having to rely on mitigative or emergency response measures to deal with process upsets once they occur. This is the fundamental principle behind inherent safety. However, process control systems are ubiquitous and necessary to maintain control over the process once it is put into operation. Furthermore, it is known that the ability of the process control system to maintain control over the design depends on the design itself. A more accurate assessment of safety can be obtained in the early design stages by integrating inherently safer process design with an understanding of the ease by which the design can be controlled, also known as its “ease of control”. This research seeks to create an index that will quantify the inherent safety of the process

design and its ease of control. This index will be used to compare the inherent safety of different chemical processes, and how changes to the design can impair or improve the ease of control.

Yue Sun
PhD CHEN
Process Hazards Evaluation and Safer Design for Oxidation of Secondary Alcohol to Ketone Using Hydrogen Peroxide
Ketones are produced on massive scale in industry as solvents, polymer precursors, and pharmaceuticals. Current ways of producing ketone through alcohol dehydrogenation are energy intensive and usually expensive, hazardous and toxic due to employing strong oxidizing agents. In 1997, Kazuhiko Sato, et al., found a way of producing ketones via 30% hydrogen peroxide oxidation of alcohol, which is considered as 'green chemistry' since it is organic solvent and halide-free. A great deal of laboratory work was subsequently done focusing on different catalysts and experimental conditions as well as their effects on yields of different ketones. However, there are safety concerns for scale-up regarding this reaction system because of its runaway potential. Thus, the purpose of this work is to conduct a comprehensive study of thermal and kinetic behavior of this reaction system. Calorimeters, such as DSC, Phi-TEC and RC1e, are used to help study, experimentally and theoretically, these reactions under normal operating and runaway conditions. The findings will be further used to propose measures for safer design and scale-up of this reaction process in order to avert a potential runaway.

Nafiz Tamim
PhD CHEN
Developing Leading Indicators Framework for Predicting and Preventing Offshore Blowouts
Leading indicators are effective organizational tools that can identify vulnerabilities in a system. Offshore drilling operations and well activities have always been very challenging due to technological and operational complexities and it is quite difficult to develop well specified risk indicators for these high risk operations. This research work aims to develop leading risk indicators-based probabilistic models for offshore drilling and other well operations (e.g., workover) to predict gas kicks and possible blowout scenarios. This work proposes a cause-based approach to develop sets of leading indicators for different categories and organizational levels. Probabilistic models are developed for evaluating the relative importance of different leading indicators and for assessing their impacts on the key causal factors of well control barrier failure. This work continues to build comprehensive risk models combining real-time indicators with operational and organizational factors to predict and prevent blowout incidents.

Yuhe Tian
PhD CHEN
Integrated Framework for Process Intensification with Safety, Control and Operability
Process intensification technologies are promising tools to create the next generation of modular, intensified, and innovative manufacturing technologies and processes. Despite the increasing interests in the field of process intensification from both industry and academia, the development of a systematic approach for intensified designs is still in its incipient stage. Challenges include the large set of feasible process intensification options, proper criteria to evaluate the controllability and reliability of a novel process technology, and accurate risk assessment with lack of precedent. With the aid of modeling and simulation tools, this research aims to promote an integrated framework for process intensification incorporating safety, control and operability.

Jingyao Wang
PhD CHEN
Inherently Safer Reactor Design
One of the common root causes for thermal runaway batch incidents is lack of understanding on the reactive chemical hazards and insufficient cooling/pressure relief systems. The objective of this research is to apply both experimental and computational approach to design the inherently safer reactor as well as identify safer

operating conditions. Experimentally, response surface methodology is applied to determine the relationship between operating input variables such as different catalyst amounts/dosing rates/temperatures with process output response such as product yield and reactor pressure in isothermal calorimetry RC1e. Computationally, a kinetics model is developed based on experimental data. Parametric sensitivity analysis is performed to investigate the critical operation parameters affecting the reactor safety and efficiency. Furthermore, the developed kinetics model is applied to design inherently safer continuous reactor. Quantitative risk assessment and techno-economic analysis are finally used to compare the continuous/batch flowsheet.

Mengxi Yu
PhD CHEN

Weak Signal Detection Using Data Mining Techniques

Data mining is a process used to explore patterns and extract useful information from big databases. It has been widely used in business and marketing for many years, and it is becoming even more widely used in the field of engineering. In contrast to some data giants, such as Amazon and Google, who treat data as high-value assets, process industries collect massive operation data from sensors, but this data is seldom explored deeply or is only analyzed after incidents occur. However, incidents do have an incubation period during which events develop and accumulate without being detected. Some of the events are called weak signals since they are difficult to recognize, but they are early indications for incidents. Thus, the goal of the research is to apply data mining techniques in process industry to detect weak signals, so that corrective actions can be taken and prevent incidents.

Shuai Yuan
PhD CHEN

Aerosol Combustion and Explosion Study

Liquids can be ignited below their flash point if they are in the form of aerosol, which has attracted more attention recently because many incidents involve the explosion of aerosol. The other reason aerosol attracts more attention is the explosion of aerosol has the so called air fuel bomb effect, which results in a more dangerous situation. However, there is no established standard study procedure for aerosol explosion and combustion. Based on the similarity between a dust explosion and an aerosol explosion, we adopted the procedure of studying a dust explosion to investigate an aerosol explosion. This research involves the modification of 36-L dust explosion apparatus to 36-L aerosol explosion apparatus. The consequence quantification parameters, such as Pman and deflagration index, also have been adopted to quantify the consequence of aerosol explosion. The characteristics of the aerosol cloud are characterized through the droplets size distribution, measured through a Malvern laser, and the overall equivalence ratio within 36-L vessel. The second phase of this study is applies the CFD software, Ansys Fluent, to simulate the three processes within the experiments; droplets dispersion, ignition of the droplets, and the explosion process.

Lin Zhao
PhD CHEN

Thermal Hazard Assessment of Styrene System during Polymerization and Storage

Polymerization reactions are highly exothermic in nature, and are one of the industrial processes that are most frequently involved in thermal runaway incidents. Polymerization runaway reaction can take place in reactors, process tanks, and storage vessels. Once initiated, the reaction termination rate will decrease dramatically due to the increase of system viscosity and immobility of the polymer chain ends. As a result, for most polymerization processes, the runaway reaction auto-accelerates and generates a huge amount of heat, leading to loss of containment, fire, and explosion.

In order to prevent polymerization runaway incidents, contributing factors to uncontrolled reactions and their relative importance need to be carefully analyzed in a systematic way. This study focuses on identifying and evaluating thermal stability and runaway behavior of crucial components (monomer, initiator, inhibitor, and contaminant) and their combinations in styrene polymerization process using calorimetry. Various calorimetry results will be integrated with kinetic models to determine the safe operating envelope of the styrene system during reaction, transportation, and storage.

Jiayong Zhu
PhD CHEN
Sour Gas Dispersion Modeling
Heavy gases, such as hydrogen sulfide and chlorine, are hazardous materials that maximize the dangerous effects on nearby people and the ecosystem, because the gases tend to travel near the ground, where wind speed decreases and gases dilute slowly. Heavy gas dispersion models are crucial to provide decision makers with quick assessment of potential impacts as well as land use planning. Many heavy gas models are available, but some of them may not be fully validated against experimental data in complex situations. DEnse GAs DISpersion (DEGADIS) and CFD models are widely used in current industries. However, they both have their limitations: the DEGADIS model cannot consider different wind directions and varying wind speeds while CFD models generally take a large amount of time for one scenario simulation. More importantly, the near-field (within 100 meters) results obtained from the DEGADIS model are conservative, with predictions being two to five times larger than the experimental data, whereas CFD models sometimes underestimate the results. We need to overcome the disadvantages of current models. The objective of this research is to develop a semi-empirical mathematics equation to estimate hydrogen sulfide gas concentration profile in the near field. The proposed model will consider obstacles, varying wind speed and humidity.

Wen Zhu
PhD CHEN
Thermal Risk Analysis of Nitro Aromatic Compounds in the Presence of other Chemicals
Mononitrotoluene (MNT) is a typical nitro aromatic compound used in the production of dyes, rubber chemicals, flexible foams and agricultural chemicals. However, incident history demonstrates inadequate recognition and evaluation of reactive hazards of nitro aromatic compounds. Advance reactive system screening tool (ARSST) and automatic pressure tracking adiabatic calorimeter (APTAC) have been used to experimentally study this reaction in order to better understand the mechanisms that result in the explosion of MNT. Key parameters such as “onset” temperature, “onset” pressure, self-heat rate and pressure rate are reported. The effect of certain additives has been screened and kinetics of the reaction has been developed. All of the related hazard-information in this study helps to determine safer operation conditions for handling, storage and transportation of MNT in the chemical process industry.

Zhuoran Zhang
MS SENG
Development of a Hazard Identification Method to Determine Safe Distance of Chemical Fire for the Preparedness of First Responders
The first emergency responders, whether it is a fire department of a city or a fire brigade of an industrial facility, are directly in harm’s way. They are trained to run to a fire while everyone else is running away. But clearly, there are times when even the emergency responders should not approach a fire. A couple of recent tragedies are a stark reminder of this, such as the West, TX fertilizer plant fire and explosion and the Tianjin port explosion. In this study, several process hazard analysis and consequence modeling software (e.g. Phast by DNV GL and ALOHA® by EPA) will be utilized to better understand the characters of hazard material, the effective range of a chemical fire or explosion, and the time window to safely put out the fire. The objective of this work is to develop a hazard identification method to pre-determine a safe distance to fight a chemical fire.

<u>Faculty Fellows Program</u>

Ahmed Al-Douri
PhD CHEN
A Framework for Reliability, Availability, Maintainability Optimization in Chemical Plant
The problem of integrating RAM assessment and optimization into the conceptual design phase and techno-economic analysis reports is examined in this work. Integrating RAM analysis into process design has a management side and an engineering side (Grievink et al. 1993). The management side is concerned with introducing changes and affecting a transition in an organization in order to use RAM tools in design. Moen (2000) explored the challenges a major oil company dealt with when it incorporated reliability goals into the project development phase.

As for the engineering side, it is concerned with the development of reliability engineering tools to improve system effectiveness. Goel (2003) developed a framework for integrating RAM attributes into the conceptual design stage to obtain qualitative RAM targets. Thus, this work is distinguished from other existing works in that it presents a framework that can be used to determine an economically optimum level of reliability for a system/subsystem based on its costs and benefits. Reliability costs include capital and labor costs associated with improved reliability, while benefits include minimizing downtime and thus increasing revenue. Also, this work is not solely concerned with the reliability assessment of a system/subsystem, but allows for design modifications which can be utilized in process synthesis to optimize RAM. Finally, this work will introduce a modified return on investment metric incorporating RAM aspects that can be utilized in the optimization of design modification options.

Ali Azhar
PhD CHEN
Nanowires for Thermoelectric Applications
Nanowires are one-dimensional nanostructures with diameters less than one hundred nanometers and a length-to-width ratio greater than one thousand. Nanowires can be used in a wide variety of applications, including thermoelectric power generation, which involves applying a temperature gradient across a thermoelectric material to produce current. Thermoelectric generators can be a viable source of clean energy and bolster the nation’s energy security amid dwindling reserves of conventional fossil fuels. A major advantage of using thermoelectric generators is that they have no moving parts, making them silent, robust, and reliable. However, these generators currently operate at very low efficiencies. Nanowires are promising for thermoelectric electricity generation as they have been shown to improve the efficiency of thermoelectric generators over bulk materials. An increase in the efficiency of thermoelectric generators will lead to an increase in the economic feasibility of processes such as waste heat harvesting in aircraft and cars, resulting in accelerated commercialization of the generators. Innovation in the production of thermoelectric generators is especially important in space related research, as these devices can be used to reliably power probes in deep space, where photovoltaic cells are ineffective. In fact, radioisotope thermoelectric generators currently power NASA’s Voyager and Cassini spacecraft. Thus, nanowires produced from novel materials have the potential to increase the efficiencies of thermoelectric generators and pave the way for widespread use of these generators in both terrestrial and space applications. Currently, research is being performed to synthesize and characterize nanowires composed of magnesium silicide and pseudo-binary alloys of magnesium silicide and magnesium stannide. These materials are attractive candidates for thermoelectric power generation due to their low toxicity, low density, and high relative abundance.

Yixi Chen
PhD CHEN
A Novel Approach of Large-Scale Synthesis and Assembly of Nanostructured Materials
Large-scale synthesis and assembly of nanomaterials, *e.g.*, nanowires, is one of the major challenges of commercial applications of nanotechnology. For instance, zinc phosphide (Zn3P2) nanowires, which are

synthesized on a zinc foil and manually scraped from the substrate, contain an appreciable amount of bulk zinc metal when they are assembled into a pellet form by hydraulic press. This results in loss in quantity of Zn3P2 nanowires and reduction in performance of the device. Herein, a simple approach to synthesizing a bulk-scale assembly of Zn3P2 nanowires is developed. In this method, a zinc pellet with sacrificial salt is directly converted to a Zn3P2 nanowire pellet. This technology can be applied to other types of nanomaterials and allows the assembly of nanostructured materials into bulk form without introducing any byproduct.

Pankaj Goel
PhD EEN
Decision Support System for Abnormal Situation Management
Modern industrial plants have thousands of sensors deployed in the field connected to the control system units such as Distributed Control Systems (DCS), Programmable Logic Controllers (PLC), and Emergency Shutdown Systems (ESD) for routine operations. In addition, due to the ease in configuring alarms in control systems in the past few decades, the number of alarms in plants has increased significantly. This has resulted in decreased system performance and additional workload on operators, which worsens during an abnormal situation. In this research, it is assumed that the alarm rationalization process has been completed by the organization and that the number of alarms during normal operations is under manageable conditions. However, the alarm flood condition still occurs during an abnormal or upset state. This research is focused on making a decision support system for the operators using data-driven methodologies. Such a system will improve early detection, prediction of abnormal situation and provide assistance in decision making for the operators during abnormal operations. The process includes data acquisition, data mining and analysis, generating information from the available datasets and creation of a smart dashboard to provide details to the operator. The resultant proactive system would ensure safer, reliable, and productive operations.

Yimin He
PhD I/O PSYC
Counterfactual Thinking and Safety Behavior
Workplace safety has been receiving increasing attention by both researchers and organizations, as it is a source of substantial costs to organizations. Incidents may result in bodily injuries and property damage. One individual factor that may be responsible for incidents is safety behavior. Little is known about how individual mental models influence safety behaviors and the mechanism of such relationships. The current study aims to examine the impact of one kind of mental thought, counterfactual thinking, on safety behavior and several important predictors of safety behavior (*e.g.,* safety knowledge and safety motivation) proposed as explanatory mechanisms for this association. This study will provide important evidence regarding the underlying mechanisms explaining why counterfactual thinking promotes safety behavior.

Pallavi Kumari
PhD CHEN
Study of Dependence of Control Layers for Rare Events and its Application to Dynamic Risk Assessment
Process variable upsets in a process operation is caused by different sources, such as variation in feed specifications, wrong settings, control system malfunctions and operator error. These upsets lead to unprofitable process operation due to production of sub-quality products and increased energy usage resulting from a deviated process variable, and subsequently to near miss or incidents if not stopped by control layers and safety system in place. The near misses or incidents are the outliers originating from the failure of control layers. This project first aims to identify the significant process variable associated with an incident, and then study the dependence of control layers for the identified process variable upset in outlying region and predict the frequency and probability of near misses based on that.

Changwon Son
PhD ISEN

Identifying and Enhancing Resilience of an Incident Management Team

Disasters have long been a persistent threat to social systems including organization, community, and government. Uncertainty and complexity of the disasters, either being natural or technical, gave rise to resilience in incident management during disasters. Resilience is generally defined as a system's capacity to adjust the system's performance and to meet both routine and non-routine work demands from a disaster.

To identify and enhance resilience of an Incident Management Team (IMT), the research conducts various methods including naturalistic observation, interview, and experimental study. As an initial attempt to understand the IMT's actual operations and identify resilient performance, a naturalistic observation was conducted and analyzed. This analysis will help identify challenges to coping strategies and success patterns and develop technical work process and training supports to enhance resilient performance of the IMT, which will be examined via experimental study.

Lecheng Zhang
PhD CHEN

Biodegradable Low-Temperature Oil Herder

When oil is spilled offshore, the harsh conditions at the remote location may make the oil spill response challenging. The weathering effect and evaporation of oil can also slow down the cleaning process. In the open water region, the spilled oil could spread much quicker due to gravity, wind, current and wave effects, which would hinder the mitigation process. The countermeasures of open-water oil spillage generally include mechanical recovery, oil herders combining in-situ burning, and dispersant biodegradation. Among those methods, oil herder is more applicable at remote location with limited resources, i.e. arctic area.

We are developing a biodegradable herder formula based on Konjac powder to increase the crude oil clean up ratio. The herder/cosurfactant formula is easily applicable in terms of effectiveness, cost, and nontoxic nature. Comparing to other products in the market, the Konjac based oil herder has a better oil herding performance at low temperature.

<u>MKOPSC-Qatar</u>

Moustafa Ali
MS CHEN

Subsea Gas Release Consequence Modeling

Subsea gas releases can result from different causes including blowouts from oil and gas wells, drilling operations, leakage from transport pipelines, or malfunction of subsea processing equipment. Subsea releases will result in the dispersion of the hydrocarbon as it rises to the sea surface leading to potentially catastrophic impacts on human life, the environment and offshore installations. Consequence analysis provides quantitative information on the risk and potential hazards that could be caused by these events. Although many models have been developed for subsea releases, these models present limitations for representing underwater plume turbulences, gas dissolution and high flowrates environment. In addition, phenomena like hydrates formation, bubble size distributions and releases containing toxic gases like hydrogen sulfide (H_2S) have not received much attention. The objective of this research is to develop a comprehensive CFD-based model for subsea gas releases.

Ibrahim Lokmane Daoudi
MS CHEN

Modeling of a Gas Release from Underground pipeline

Buried pipelines are commonly used for transporting natural gas. Any failure due to corrosion or breakage of the pipe, might lead to a gas leak, which can cause significant human and physical damage. Many models are available for gas dispersion into the atmosphere, but not as many are available for underground gas leak. The modeling of such cases heavily depends on the flow mechanism of the gas through the soil. Thus, it is important to understand and model different types of flow mechanisms, in order to effectively design for prevention and mitigation, as well as to prepare for emergency response. The objective of this research is to model gas releases from underground pipelines by focusing on the gas release rates on soil displacement, and the effect of the orifice orientation of the leak.

Jack Altwal
PhD CHEN
Influence of Particle Size and Humidity on Sulfur Dust Explosion Properties
Dust Explosions are a widely occurring phenomenon that negatively impact several industries, including the sulfur industry. There is very little information available in literature on sulfur dust explosion properties. This research aims to perform an experimental investigation of sulfur dust explosion properties; specifically, the minimum explosible concentration (MEC), maximum explosion overpressure (P_{max}), and dust deflagration index (K_{st}). A particular emphasis of this research is to determine the effect of particle size and humidity on the explosion properties. This research also aims to develop a theoretical model that predicts the impact of particle size and humidity on the dust explosion properties that will assist to improve the management of sulfur dust explosion risks.

Jasir Jawad
MS CHEN
Dynamic Simulations of the Impact of Depressurization of a Vessel on Interconnected Vessels
Thermal runaway may occur due to an uncontrolled exothermic reaction in reactors or storage vessels. An inadvertent pressurization of a vessel following a thermal runaway may pose an explosion hazard. Emergency Relief Systems (ERS) are commonly used for risk reduction measures to protect the reactor or vessel from the consequences of a runaway reaction. ERSs can be connected to effluent handling systems that may include the use of catch tanks. Sizing of the ERSs requires the understanding of the reaction kinetics, thermodynamics, and fluid dynamics of the reactive system before and during venting. Such phenomena are quite complex and yet to be fully understood. The aim of this research is to develop a model to perform dynamic simulation of the depressurization of a vessel to a catch tank, and to validate the simulator using experimental data.