



# MARY KAY O'CONNOR PROCESS SAFETY CENTER

TEXAS A&M ENGINEERING EXPERIMENT STATION

## 2013-2014 RESEARCH HIGHLIGHTS



### ***"Making Safety Second Nature"***

The Mary Kay O'Connor Process Safety Center was established in 1995 in memory of Mary Kay O'Connor, an operations superintendent killed in an explosion on October 23, 1989. The center's mission is to promote safety as second nature in industry around the world with goals to prevent future accidents. In addition, the center develops safer processes, equipment, procedures and management strategies to minimize losses within the processing industry. However, the center realizes that it is necessary to advance process safety technologies in order to keep the industry competitive. Other functions of the center include that it serves all stakeholders, provides a common forum, and develops programs and activities that will forever change the paradigm of process safety. The funding for the center comes from a combination of the endowment, consortium funding and contract projects.

## Note from the Director

Without a doubt, one of the most rewarding aspects of my job as director of the Mary Kay O'Connor Process Safety Center is working to educate and prepare the next generation of engineers. Towards this goal, the center continues to play a pivotal role in engineering education at Texas A&M University, helping produce exemplary professionals with a strong commitment to safety in the workplace and at large.

The students working with the Mary Kay O'Connor Process Safety Center are talented, dedicated and ambitious, as evidenced by the wide breadth of research areas in which they are involved. From important studies on safety climate to critical research on liquefied natural gas hazards and dust explosions, our students are applying sound science to real-world issues vital to the process industries.

I invite you to peruse this publication and learn more about the center and our students who truly are "making safety second nature." As always, feel free to contact me with feedback or questions at 979.845.3489 or via email at [mannan@tamu.edu](mailto:mannan@tamu.edu).



**Dr. M. Sam Mannan**

Director, Mary Kay O'Connor Process Safety Center  
Regents Professor, Chemical Engineering  
Holder of the T. Michael O'Connor Chair I

A handwritten signature in black ink, appearing to read "M. Sam Mannan", with a long, sweeping horizontal line extending to the right.



## Industry Research Activities

Chemicals play a key role in today's high-tech world. The modern chemical industry is linked to every technologically advanced industry. Only a handful of the goods and services we enjoy on a daily basis would exist without essential chemical products.

Safe use of chemicals creates a healthier economy and a higher standard of living, but unsafe use threatens lives, businesses and ultimately our world.

To that end, our programs and research activities enhance safety in the process industries. Our educational activities are aimed at making safety second nature to everyone in the industry. In addition, we develop safer processes, equipment, procedures and management strategies to minimize losses.

Center personnel conduct studies pertaining to general issues of process safety as well as specific interests of the center's consortium members. Overall research goals are to develop:

- Systematic identification and evaluation risk, based on severity of consequences and probability of occurrence, to prioritize projects related to certain processes; types of process, storage and transportation systems; and various chemicals
- Projects to most effectively address the risks identified
- Inherently safer process schemes for the most common and most hazardous processes
- Technology and methods to develop engineering design concepts and implement such processes
- Devices, systems, and other means for improving safety of chemical operations, storage, transportation, and use by prevention or mitigation
- Improved prediction and analysis of behavior of hazardous chemicals and the systems associated with them





## Expertise

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Dr. Sam Mannan, center director, is an internationally recognized expert on process safety and risk assessment. In addition to his many professional honors and achievements, Dr. Mannan has served as a consultant to numerous entities in both the academic and private sectors. He also has testified before the U.S. Congress on multiple occasions, lending his expertise on matters of national security as it relates to chemical safety and infrastructure.

Other center researchers include leaders in the fields of process safety management; liquefied gas safety; ammonia and fertilizer plant safety; refinery and chemical plant safety engineering; and risk assessment for the process industries.

Center personnel are active in technical committees of professional societies such as the American Institute of Chemical Engineers, the American Society of Mechanical Engineers, the American Society of Safety Engineers, the Systems Safety Society and the National Society of Professional Engineers.

In addition, the center Steering Committee provides guidance to the operational activities of the center, while the Technical Advisory Committee reviews and refines the research agenda.



## Service

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The Mary Kay O'Connor Process Safety Center provides a neutral forum to discuss difficult issues related to process safety. Towards that goal, the Chemical Safety Program Assessment Project is a significant effort that brings together a diverse group of stakeholders. Objectives include identifying national chemical safety goals; identifying and implementing activities necessary to accomplish these goals; and establishing a measurement system to help gauge progress toward these goals.

In addition, the center serves as an information resource base for process safety, acting as a library and software laboratory. It provides consultation services for small and medium enterprises, government agencies, institutions, local emergency planning committees and others agencies. Independent accident analysis services are also available to industry and government agencies, particularly for accidents suggesting new or complex phenomena.



## Resources

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The Reactive Chemicals Laboratory is equipped with several calorimeters for studying thermal behavior of reactive systems. With this experimental capability, the thermal behavior of wide ranges of reactive systems and systems of questionable chemical compatibility can be investigated. The Aerosol Laboratory can be used to study the behavior of fluid aerosols leaking from manufacturing processes. Additionally, the center is linked to tremendous resources throughout The Texas A&M University System, including:

- Texas A&M University experts in chemical engineering, chemistry, industrial psychology and other departments
- The Hazard Reduction and Recovery Center, the largest research center in the world for studying the effects of natural and technological hazards
- The Department of Aerospace Engineering's Low Speed Wind Tunnel, a self-contained research facility capable of conducting a wide variety of tests for industry, governmental agencies, educational institutions and private individuals
- The state-of-the-art Brayton Fire Training Field, which includes full-scale buildings, towers, tanks and industrial plant structures for training simulations for career and volunteer firefighters and fire marshals

## “Designing a synergistic flame retardant system and gaining fundamental understanding of the synergistic effect through kinetic modeling”



Lubna Ahmed

Fire retardancy of plastics is becoming increasingly important in term of their wide spread application in our day to day life and subsequent fire hazard associated with it. Most polymers burn by producing gas phase fuels which combine with air and sustain the fire until the entire polymer is burnt. Recently flame retardant nanocomposites have gained popularity since they do not pose health or environmental threats

as opposed to traditional flame retardant additives. Flame retardant nanofillers like clays, metal oxide nanoparticles, carbon nanotubes when added to the polymers, operate typically in the condensed phase by forming a surface layer which limits the supply of the polymer (fuel) to the fire and oxygen to the burning polymer. The combustion behavior of polymer nanocomposites is due to a twofold mechanism brought about by nanofillers: a physical barrier effect and a chemical charring catalytic action occurring in the condensed phase. The main objective of the current work is to gain fundamental understanding of the flame retardancy of polymers through the synergistic interaction among the nanofillers, ones that cause a physical barrier effect and the others that cause catalytic charring effect in the condensed phase, by studying the kinetics and the mass and heat transfer processes during pyrolysis.

## “LNG Source Term Modeling - Cryogenic Boiling”



Monir Ahammad

Boiling is one of the major areas of concern in source term modeling. Realistic estimation of cryogenic hazards (e.g., LNG and LN2) primarily depends on the accurate determination of its boil-off rate due to the heat transfer from the substrate. Computational estimation of the boil-off rate after a release is not trivial because of the complicated physics of boiling regimes, the time dependent nature

of pool spreading, the nature of the substrate, etc. The aim of this study is to simulate pool boiling of cryogenic mixtures for more accurate estimations of LNG source term modeling. To accomplish this, user defined physics functions of boiling and CFD will be used.

## “Vapor Pressure Measurement of Formaldehyde Water Solution”



Bibian Amaya

Formaldehyde is an important chemical with many uses in the chemical industry. Formaldehyde is highly reactive and therefore commonly handled in aqueous and / or methanolic solutions. The water formaldehyde system has been studied intensively. However, the problem of characterizing its vapor-liquid equilibrium is to date open as far as experimental measurements

are concerned and the definition of a satisfactory theoretical model capable of predicting vapor-liquid equilibrium for wide ranges of temperature and composition. The objective of this research is experimentally to figure out the vapor pressure of formaldehyde water solution at different concentrations and temperatures, in order to provide accurate evaporation rate as one of essential data in source term model for its release.

## “PEMEX Process Safety Procurement International”



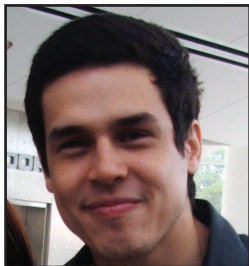
Jehova Arenas

Technology, human behavior and processes evolve every day in order to provide safer and more efficient operations, but in many cases the equipment or technology arrive late, are incorrectly incorporated, or aren't the last generation technology because the people or the departments in charge of these procedures do not have the knowledge, preparation, or experience to select the type of

solution that the company requires.

Therefore, my thesis will be focused in the necessity of develop a new division or strengthen the procurement international department in PEMEX, with the creation of an area dedicated to develop and incorporate safety, health, and environmental solutions. This division will be in charge of evaluate the actual necessities of the process, drilling, and transportation, in order provide the equipment or technology that the company needs to eliminate or administrate risks. Likewise, I want to raise awareness about the necessity of establish agreements with the best universities in the world and other oil companies to develop the solutions that PEMEX needs because we understand that maybe we cannot find all that we need in the market.

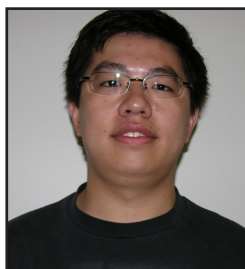
### "Mathematical Programming Formulations for the Placement of Imperfect Detectors in Mitigation Systems with Applications to Flammable Gas"



Alberto Benavides

Current strategies to place gas detectors in industrial settings are based upon heuristics or semi-quantitative approaches. Optimal sensor placement is difficult due to the large number of unknown variables that influence the risks associated with gas leaks. Heuristic and semi-quantitative approaches can give results that are far from optimal in terms of cost and risk reduction; a structured quantitative approach is necessary. Actual research is focused on the adaptation of a previously developed stochastic Mixed Integer Linear Programming (MILP) detector placement formulation. This adaptation accounts for two essential features in detection systems: voting and reliability. In order to avoid false positives, release events are not considered detected until multiple detectors acknowledge the release (voting architecture). Additionally, to consider the possibility of false negatives, the detectors' probability of failure on demand was incorporated into the formulation. Current results greatly outperform traditional placement schemes, demonstrating the capabilities of optimal sensor placement using stochastic programming in order to improve safety systems.

### "Flammability characteristics of hydrocarbons and its mixtures at elevated conditions"



Ning Gan

The flammability characteristics of combustible gases like hydrogen, methane, and propane is related to the temperature and pressure of the gas and air mixture when it is ignited. Large amounts of reaction energy will be released in a short duration of time which can cause deflagration or even detonation, also the extremely high temperature of the reaction will become a threat to the facility and people. The research objective is to study the flammability characteristics of combustible gases at elevated conditions (high temperature and high pressure) and propose the corresponding methods to handling them safely. By using both experimental data and theoretical calculations, an improved Le Chatelier' Law will be raised and tested to better predict the flammability limits of combustible mixtures.

### "Shock Interaction with Dust Layers"



Amira Chowdhury

Secondary dust explosions can be far more destructive than a primary explosion due to the increased quantity and concentration of dispersed combustible dust, making this a very important issue in the industries. Secondary dust explosions occur when the shock of an initial explosion dislodges more accumulated dust resulting in additional dust dispersed into the air. Therefore the problems of lifting and dispersing of a dust layer behind the propagating shock wave must be understood. This research aims to study shock interaction with dust layers. This research focuses on building experimental equipment with optical access to provide high speed flow visualization including measurement of dust dispersion, particle drag and shock attenuation.

### "Application of Computational Fluid Dynamics (CFD) to Liquefied Natural Gas (LNG) Pool Spreading and Vaporization on Water"



Nirupama Gopalaswami

A ship-ship/ship-shore collision of an LNG marine tanker or a rupture of the LNG loading and offloading lines can result in accidental spillage of LNG on water. This can result in a formation of liquid pool and flammable vapor cloud which can lead to hazards in the presence of ignition source. Safety analyses for the protection of the public and property involve the determination of consequences of such accidental releases. The evaluation of consequences resulting from an accidental spill of LNG on water involves the determination of the rate (source term) at which flammable hydrocarbon vapor is produced and the dynamics of the spreading pool. Two key parameters which affect pool spreading and vaporization phenomenon namely, the heat flux from water to the LNG pool and the turbulence in the cryogenic pool are quantified using experiments. The results of quantification of key parameters are implemented in CFD model to study the pool spreading and vaporization behavior. The CFD model is validated with LNG design spill experiments. The proposed study employs both experimental and modeling work to improve the consequence analysis techniques for LNG marine operations. The results of the research are used for emergency response planning for LNG facilities.



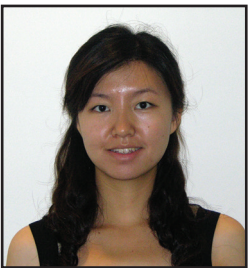
### “Predictive Model for Stress-Corrosion Cracking”



Richard Gustafson

Stress-corrosion cracking is a particularly insidious form of corrosion failure. It can occur with little to no advanced warning and lead to the catastrophic failure of piping, structural materials, and process equipment. Recently, DFT and Molecular Dynamics modeling was used to predict the energy states along grain boundaries in BCC iron, FCC nickel as atoms were inserted into lattice vacancies. This work resulted in a fundamental model that qualitatively correlates with experiential results of stress corrosion cracking in iron and nickel alloys and offers potential further insight into the underlying mechanisms. Other researchers have recently published similar work using multi-scale modeling to extend from the atomic to the continuum level for specific systems. The extension of this preliminary work and development of a general predictive model for stress-corrosion cracking based on a fundamental understanding of the stress-corrosion cracking mechanism could be used to reduce and avoid stress-corrosion cracking. The purpose of this research is to develop and validate such a model.

### “NH<sub>4</sub>NO<sub>3</sub> Reduction of Explosion Hazard while Maintaining Agricultural Benefit”



Zhe Han

Runaway reactions present a potentially serious threat to the chemical process industry. This research topic will look at reducing the explosion hazard associated with ammonium nitrate (AN) while maintaining its agricultural benefit, including investigating the mechanisms that drive the reactions, developing predictive models, and creating effective mitigation strategies. The reaction stoichiometry, thermodynamic parameters, and kinetic parameters related to AN explosion will be developed. Both experimental analysis and theoretical approach will be used to study AN hazards. The first step is to study the decomposition of AN, using RSST, APTAC, and DSC/TGA, under various conditions such as being in the existence of additives, in a confined space, under humid environment, weathering effect, and gas atmosphere. Recommendations on how to properly store AN will be provided. GC can be used to analysis the gas composition. Except for experimental work, modeling tools such as Gaussian and Material Studio will also be used to validate experimental data.

### “Blast Decontamination Foam for Chemical Mitigation”



Brian Harding

Decontamination foam is used to decontaminate surfaces, people, etc. from all types of contaminants. It is used because it has a fairly long residence time on surfaces, and is able to decontaminate them at a high level. On the surface, my research topic is concerned with the use of decon foam to stop the spread of chemical hazards due to spills or other releases of large quantities of potentially hazardous chemicals. This research is aimed at determining effective decontamination of biological and chemical agents from terrorist attacks.

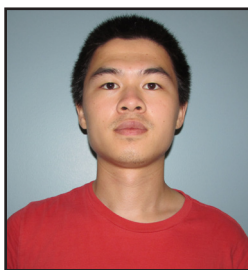
### “Development of Nanocomposites Containing Zirconium Phosphate as Flame Retardant Materials”



Logan Hatanaka

Cheap flame retardant materials with low toxicities are highly sought after for industrial and commercial purposes. Previous research has shown that inorganic-organic nanocomposite systems can yield cheap, low toxicity, and effective flame retardant materials. At elevated temperatures, these materials have reduced heat fluxes, a reduced mass loss rate, and improved viscosity properties. With this in mind, current research focuses on the flame retardant properties of zirconium phosphate as a nanofiller dispersed in various polymer matrices. The properties of zirconium phosphate make it a promising choice for utilization in these nanocomposite systems.

### “Fuzzy logic in Layer of Protection Analysis (fLOPA)”



Yizhi Hong

Layer of Protection Analysis (LOPA) is a method to identify and analyze the significance of potential major accident scenario associated with the processing or handling of highly hazardous chemicals. As a risk assessment method, LOPA has some disadvantages, mostly connected with limited availability and uncertainty of the failure rate of all safeguards systems and with the assumption that severity of consequences remains constant with the activity of independent protection layers (IPLs). These problems will be considered in fuzzy Layer of Protection Analysis. Fuzzy logic, a method to deal with uncertainty and imprecision, is an efficient tool to solve problems where no sharp boundaries are possible. Moreover, fLOPA will be compared with other methods, such as Bayesian Network, to give an evaluation of different risk assessment methods.

### “Risk management strategy for LNG transportation”



Bilkis Islam

Liquefied Natural Gas is playing an important role in the energy market recently. It is transported through different modes of transportation- waterways, roadways and pipelines. A part of LNG has been transported in truck tankers through roadways. Also in the near future use of LNG as road transportation will be increased due some significant advantages. Since LNG has some safety hazard,

risk management process is essential to ensure minimum risk during transportation of LNG. In this project, a database has been created with all LNG road transportation accidents to identify risks and hazards associated with it. A HAZID has been done for the identification of risks and hazards associated with LNG truck tankers and heavy duty vehicles using LNG fueling. To perform a risk analysis risk matrix is being formed for the hazards identified by HAZID. In the future, risk ranking of hazards will be evaluated and based on the ranking and current guidelines, recommendation for improving risk management will be discussed based on location category, protection goal and expected impact of hazard.

### “Phase equilibrium studies on N-oxidation systems to determine homogeneous mixture conditions”



Sunder Janardanan

The N-oxidation of alkyl pyridines is used extensively in pharmaceutical industries to produce N-oxides. The process is carried out in a semi-batch mode where aqueous hydrogen peroxide (30%) solution is added gradually to a mixture of alkyl pyridine and water-soluble phosphotungstic acid catalyst. N-oxide is formed as a major product, which is used in the preparation of

analgesics and anti-inflammatory drugs.

The decomposition of hydrogen peroxide and the liquid-liquid phase separation are the two challenges encountered during the reaction. The decomposition process is exothermic and can lead to over-pressurization of the system due to the release of oxygen gas. The presence of two phases during the reaction can affect the selectivity of the process drastically due mass transfer limitations. Moreover, the presence of the catalyst in the aqueous phase can promote the decomposition of hydrogen peroxide. Hence, it is extremely essential to determine the compositions and the operating conditions at which homogeneity exists.

According to previous research, it was observed that the presence of N-oxide tends to homogenize the system. Phase observation tests will be conducted on alkyl-pyridines, N-oxide and water system to understand the phase behavior at various temperatures and compositions. An attempt would be made to determine the conditions beyond which single-phase system exists.

### “Resilience Engineering in Offshore Safety”

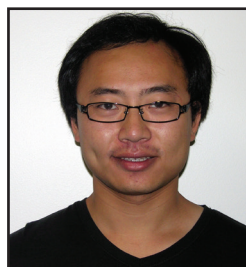


Prerna Jain

In the oil and gas industry, various risk assessment and management methods have been studied and developed to reduce undesirable events. However, offshore incidents still happen so a better understanding of the risks and system safety aspects is necessary. A resilient facility would have the capacity to overcome disruptions and continually transform itself to

meet the challenging needs and changing expectations over time. The main focus of this research would be to propose a resilience framework for process safety assessment in offshore process facilities. The resilience framework and model developed in this research would be applicable to offshore process installations primarily platform and drilling operations. This approach is based on basic four abilities of a system to be resilient: anticipate unknown and uncertain initiating events, monitor routine operations, learn from past events, and respond to events for quick recovery. It is important to understand the complexities involved and develop methods to make the system survive, adapt, and organize into new configurations as per demand.

### “Measure hybrid mixtures explosion characteristics with 36L vessel”



Jiaojun Jiang

Hybrid mixtures consist of a flammable gas and a combustible dust which cause lots of accidents. They are encountered in various industries such as painting factories, mining, grain elevators or pharmaceutical. Each of them may be present in an amount less than its Lower Flammable Limit (LFL)/ Minimum Explosible Concentration (MEC), and still give rise to an

explosible mixture. However, data concerning hybrid mixtures remain scarce. In this research, experiments with a 36L explosion sphere will be used to determine the influence of dusts and vapors concentration on the severity of explosions, include Maximum Pressure ( $P_{max}$ ), Maximum Rate of Pressure Rise ( $[dP/dt]_{max}$ ), and deflagration index (KSt). On the likelihood side, LFL of hybrid mixtures will be tested. The goal of studying the hazard of hybrid mixtures is to provide important information for preventing hybrid mixtures explosion.

## “Development of a smart sensor for the detection and mitigation of Microbiologically Induced Corrosion (MIC)”

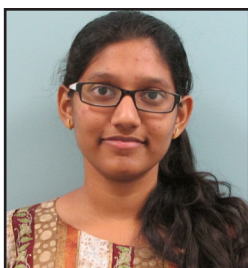


Pranav Kannan

Microbiologically Influenced Corrosion (MIC) is a form of corrosion, which is either caused or accelerated by the presence of micro-biota on the surface of metals and other materials of construction. It is a widespread problem in multiple industries including Oil & Gas, Chemical, Nuclear, and Power etc. This problem is only exacerbated by the recent surge in Fracking operations that also

use large quantities of water, and makes it imperative to detect and mitigate MIC. MIC control is achieved primarily through the use of biocides, which come with associated economic and environmental costs. Hence, an early-detection system, which is real-time, or pseudo real-time would be a great tool to combat MIC at an early stage before it becomes widespread through bio-film formation. This early detection is even more important for systems in harsh environment, such as sub-sea pipelines. The Objective of my research is to develop a sensor based on nanowire matrix – Functionalized with Bio-molecules, which can detect these microorganisms in a real time basis. These sensors are expected to be sensitive due to their large surface areas (Nanomaterial-matrix) and specific due to the biomolecules functionalization. The sensors could be mounted on pigs (Devices used in maintenance of pipelines) or at multiple locations where MIC is suspected and the local concentration of biota could be monitored which would be a great tool for devising mitigation strategies.

## “Aerosol Flammability Study”



Susmitha Kotu

Microbial Corrosion or Microbially Induced Corrosion (MIC) is an electrochemical process where metabolic activity of micro-organisms initiates, accelerates or facilitates corrosion reaction. MIC and bio-fouling cost 3.1% of US GDP. About 75-90% of internal pipeline leaks are due to localized corrosion, of which MIC is the most predominant form. In harsh environments like in the case of

MIC, micro-organisms form biofilms, a self-producing matrix of extracellular polymeric substance with complex consortia of multiple species. A fundamental understanding of MIC requires an understanding of how biofilms are formed and the major determinants of biofilm formation. Lab experiments would be done to find the dominant factor and the relative magnitude of other major factors among hydrodynamic factors, biochemical factors and internal gene expression. This would allow us to fine-tune these factors to control biofilm formation. The experimental plan includes developing a model consortium of biofilm of selected species in microfluidic devices and incorporating Electron Impedance Spectroscopy (EIS) into these devices to allow continuous and non-destructive monitoring of biofilm formation through both microscopy and EIS.

## “Comparative Risk Analysis between LNG Import and Export Terminals”

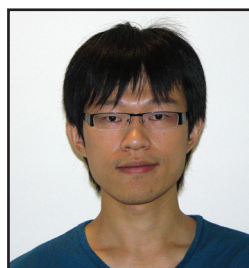


Guido Lamus

The increasing demand for natural gas entails a rising need for safer practices in production and transportation of this energy resource. Several studies oriented to forecast the LNG behavior during accidents have been done for onshore operations. However, there are particular factors involved in the offshore activities (currents, waves, and winds) that generate a wider

range of exigencies that are required to be incorporated in the fluid dynamic models. The quantitative results obtained from the fluid dynamic analysis will be incorporated to GIS (Geographic Information System) in order to provide a pragmatic approach on the possible scenarios that can be held during an event under these particular environmental conditions. The main goal of this research is to contribute with robust information about the nature of LNG spill accidents in order to support the most accurate mitigation plans.

## “Flame Propagation Speed of Aerosols Generated by Electro spray”



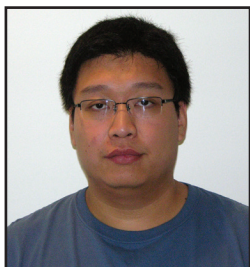
Yan-Ru Lin

Flash point is widely used as the parameter to categorize liquid flammability in various standards. However, this categorization methodology does not consider liquid behavior under extreme conditions, e.g., high pressure and high temperature. When a liquid is released from containment under such conditions, aerosol or mist will form, and the flammability of aerosol

is still not clearly defined, even though it has been studied for decades. Since the potential hazards of aerosol are not recognized and addressed properly, the consequences of aerosol hazards may be more severe than flammable vapor hazards. Moreover, the flame speed of aerosol may be higher than that of vapor under certain conditions. Therefore, several hydrocarbons were tested and the trend of their flame propagation speeds is also discussed to resolve the contradiction between different theories.



## “Modeling of Uncontrolled Fluid Flow in Wellbore and its Prevention”

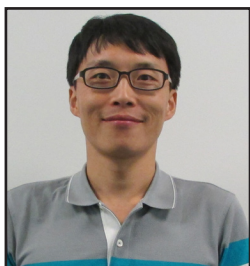


Ruochen Liu

Uncontrolled fluid flow in wellbore includes gas-kick, blowout, and hydrate formation. Without proper control strategies, a kick might turn into a blowout event quickly. It is always the most unwanted disaster for all the well operations, such as the Macondo incident. Consequences of the blowout include the damage to the environment, equipment, and materials; personnel injuries and fatalities; lost of production; and

hurting the companies' credibility. At present, there are some papers that investigate the risk and consequence analysis of a blowout, but only few of them address the mechanism of a blowout with respect to the flow rate of a blowout and the total amount of hydrocarbons discharged to the environment. Therefore, the purpose of the research is to establish a analytical or semi-analytical mathematical model of uncontrolled fluid flow based on the basic physical phenomenon, including heat transfer and fluid dynamics, to estimate the blowout rate and total production loss. Such model studies the onshore and offshore oil, gas, and oil/gas well blowout behaviors. Depending on the conditions of reservoir and well configurations, sonic velocity might be achievable for some of the blowout events. In addition, after fully understanding the mechanism of blowout behaviors, some suggestions are given to monitor and control the blown-outtwells.

## “Process Safety Study for Organizational Change”



Younggil Park

Many companies have been tried to change their organization in order to improve their business profits and meet environmental changes. Also oil & gas and chemical industries take this for granted. General types of organizational changes from downsizing, mergers and acquisitions are organizational structure changes, organizational policy changes and personnel and their roles changes. But the problem

is that organizational change is less apparent than physical change of facility. Even subtle changes of organization could affect serious impact to process safety part. The lack of an organizational change management has been found to be root causes and contributing factors in many incidents. In order to prevent loss of corporate knowledge, safety and reduce the impact of process safety management programs and its performance, sufficient planning and analysis of the organizational change management should be necessary. In order to achieve successful organizational change management, the key of the system is how effectively to assess the risk of this change. In this study, the following key questions could be discussed: (1) What are the organizational changes that affect risk, (2) How do these changes influence risk, and (3) How much do they influence risk.

## “Reactivity of Aromatic Nitro Compounds”



William Pittman

Aromatic Nitration is an important industrial process necessary for the production of a wide variety of products. Nitration by mixed acid is among the oldest industrial chemical processes. However, the process is highly exothermic and subject to thermal runaway. The products of the reaction, the aromatic nitrocompounds, will undergo monomolecular decomposition at

higher temperatures, releasing a massive amount of energy, often leading to explosions. The process continues to produce catastrophic industrial accidents. More recently the process has been shown to exhibit complex thermodynamic and multi-phase behavior which allows between one and three liquid phases to coexist. This is thought to be the result of a microemulsion forming within the system. This makes understanding, modeling, and predicting the behavior of the system behavior in the reactor and in the rest of the process potentially even more difficult. The research currently undertaken therefor aims to better understand the thermodynamic behavior of the system to determine what, if any, improvements need to be made to current modeling and process simulation efforts for this system.

## “Analysis of the Thermal Decomposition of Untempered Peroxide Systems”



Olga Reyes

Emergency relief systems are one of the most commonly selected measures to protect reactors from thermal explosions. In this research Dicumyl Peroxide (DCP) and Cumene Hydroperoxide (CHP) were chosen to be studied, because from a pressure relief point of view they have been classified as gassy (mainly gases are formed during the runaway) and hybrid (vapor and gases are formed

during the runaway) systems, respectively. These two kinds of systems typically show an untempered behavior: the temperature increases even after the relief operation. Existing vent sizing methods focus their attention mainly on vapor systems and may lead to oversizing when dealing with untempered hybrid and gassy systems.

The objective of this research is to combine the use of adiabatic and pseudo adiabatic calorimetry experiments with computational chemistry in order to: (1) understand the behavior of the thermal decomposition of DCP and CHP under runaway conditions, (2) identify the influence of experimental conditions, and the accuracy of the correction methods to scale up the parameters obtained at lab scale, and (3) use computational chemistry and molecular simulations in order to get a better understanding of the thermal decomposition mechanisms of CHP and DCP.

## “Facility Layout Optimization for Offshore Operations”



Josh Richardson

The initial and ongoing layout of any facility is a key component of safe operations. Offshore operations present unique challenges due to tight spacing and remoteness of the platform, leading to the chance that any process safety event could turn catastrophic. In order to minimize this probability and the consequence should an event arise, an MINLP formulation

has been created to optimize the layout of equipment with respect to fire, explosion, and toxic dispersion hazards on an offshore platform. This formulation allows for equipment of user-defined footprint areas and operating conditions to be placed in a multi-floor environment, minimizing a risk-based objective where both probability of an event and consequence of the event are considered. Further, the model optimizes muster points and escape routes to avoid particularly hazardous areas. The model can be used for initial layout, placing new equipment, and sensitivity analysis when considering changes in parameters such as building larger platforms, platforms with more or less floors, and changing footprint areas of equipment. Mitigation systems and extended applications of the model are being implemented as part of future work.

## “Deflagration to Detonation Transition Studies”

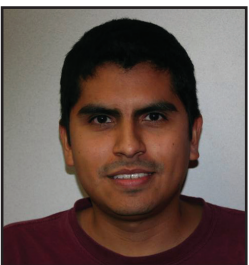


Camilo Rosas

When referring to explosions, there are two different mechanisms, deflagration and detonation. If the appropriate conditions are given, it is possible to have an abrupt transition from deflagration to detonation. This research project focuses on the transition from deflagration to detonation and combines theoretical, experimental, and modeling approaches in order

to achieve a better understanding of this phenomenon. Currently, there is no Computational Fluid Dynamics (CFD) model capable to predict the abrupt rise in pressure when DDT occurs. However, there is a model that predicts the likelihood to obtain DDT in a particular scenario. Currently, such tool is being validated with available literature data. Additionally, using this CFD model, it has been observed that the non-uniformity of obstacles' shapes and blockage ratios can decrease the run-up distance to obtain DDT. However, experiments have to be performed in order to prove whether or not this is correct. Therefore, experiments are focused on evaluating the effect on the run-up distance to obtain DDT due to the non-uniformity distribution of obstacles with different shapes and different blockage ratios along the detonation tube.

## “Well Integrity Modeling and Risk Assessment in Sustained Casing Pressure Annuli”

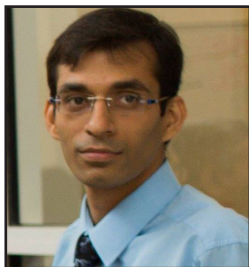


Tony Rocha-Valadez

Compromised well integrity can have catastrophic consequences on both environmental and safety aspects. The consequences of not detecting and managing well integrity issues can go from the activation of rupture discs to a release of oil/gas, fire and/or explosion during a blowout. Sustained Casing Pressure (SCP) is any pressure that builds up after having bleed-off any gas in the

casing. Most diagnostic testing of SCP and other casing pressure problems require long testing periods, arbitrary criteria from qualitative assumptions and, in some cases, specialized equipment. The goal of this research is to develop analytical models that can mimic the behavior of the gas migrating through the casing and generating SCP, as well as other phenomena that lead to increase casing pressure that may compromise the integrity of the well. With this type of model, early time diagnostics can be provided and the estimation of important non-measurable parameters, such as cement effective permeability and flow rate, is possible without the need of specialized equipment. An earlier diagnostic and parameter estimation that reflects the integrity of the well barriers, can serve as tools for risk based decision making by identifying the severity of a leak and evaluating the risk for a release and its safety and environmental impact.

## “Developing Integrated Process Safety Metrics for an Industrial Supply Chain considering the Life-Cycle Analysis (LCA) of the Product”



Nitin Roy

A life cycle of a product starts from the extraction of raw materials from nature and ends on the disposal of the product after consumption. Every part of the life cycle has interaction with humans and environment. Hence, every part has concerns for safety of the people and the environment. Quantifying the safety level in each facility in the life cycle i.e. the supply chain

is the major objective of the project. Safety in each part of the supply chain is often inter-related and hence to find a good quantification of safety for the supply chain as an overall has never been done before. The final objective of the project is to apply this developed overall metric in the general supply chain optimization problem in the industry especially the gas processing industry. The project is in its first phase and the literature survey of the existing metrics has been completed and a general review paper is expected to be done by summer.



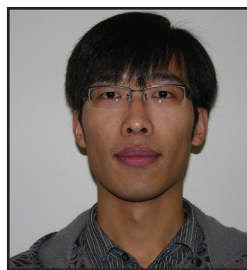
## “Leading Indicator Analysis for Offshore Operations with Emphasis on Drilling”



Nafiz Tamim

Offshore oil and gas operations have always been very challenging due to technological and operational complexity in combination with harsh environmental conditions. Geological uncertainties, high pressure flammable fluids in presence of ignition source, complicated structural layout, limited response time allowance, difficulty of control and communication are some of the critical factors that possess clear threats towards safe operations and may result in high consequence events. Developing well specified risk indicators for robust safe work guidelines is quite a difficult job to achieve due to such highly correlated factors and multifaceted operations. This research work primarily undertakes the task of defining and analyzing leading risk indicators specific to offshore energy industries. Blowouts and drilling incidents will be analyzed in terms of addressing the technical aspects of leading risk indicators and a database containing information on root causes with observed parameters prior to failure will be constructed. Additionally, successful technologies and approaches adopted by industries will also be studied for understanding effective barrier performances. With analyzed incident and operational control data, advanced algorithms of incident path from initiating events will be developed with optimize use of preventive barriers. Finally, methodologies for identifying and killing of gas kick, which is considered to be a major leading indicator for blowout, will be proposed with analysis of some potential response scenarios.

## “LNG Vapor Hazard Mitigation Using High Expansion Foam”



Bin Zhang

The use of liquefied natural gas (LNG) for ease of transportation and storage raises safety concerns with facilities, the community, and the environment. The spilled LNG will vaporize violently with a boiling temperature of  $-162^{\circ}\text{C}$ . The vaporized liquid will expand 600 times, and migrate downwind to generate a huge vapor cloud at the ground level with heavier-than-air behavior at the boiling temperature. The LNG vapor cloud is hazardous since it is flammable with a concentration between 5-15 (v/v) percent in the air. The huge vapor cloud increases the possibility of ignition to escalate the incident. The vapor hazard can be mitigated by reducing the vaporization rate to generate less vapor and warming the vapor to raise the vapor buoyancy. High expansion foam has been recommended by NFPA 11 and NFPA 471 as a measure for LNG hazard mitigation. The foam blanket provides the ability of blocking the convective and radiant heat to suppress LNG vaporization and warming the vapor to enhance the dispersion. The mitigation effects of high expansion foam will be studied through small-scale experiments using LN<sub>2</sub>, and a theoretical study will be conducted to develop models based on the experimental results for the consequence estimation of an LNG spill with high expansion foam application.

## “Integration of Human Factors in Offshore Risk Assessment”



Ming Zeng

Human failures often contribute to major offshore incidents, but they are usually not considered in traditional offshore risk assessment. Several human reliability analysis methods have been developed so far in aviation and nuclear industry and some of them have been applied in offshore, but the efficiency of these approaches is still questionable. Also, there is no uniform category to classify human factors in offshore industry. If the important factors are not identified, it could overestimate the risk. Therefore, the appropriate human factors need to be included in the risk assessment. The objective of this research are to : 1) Category of human factors in offshore industry. 2) Develop models to incorporating human factors in offshore risk assessment quantitatively. 3) Perform a sensitivity analysis to identify the most influencing factors 4) Provide guidance to effectively improve human performance.

## “Nanoparticles Flammability and Explosion”



Jiaqi Zhang

In recent years, very little attention has been given to the fire and explosion hazards associated with engineered nano-materials, while the need for these materials has increased significantly. The specific characteristics (type, chemical and surface composition, size, etc.), effect of agglomeration and mixing and turbulence, might cause a significant gap between the flammability and explosion of nanoparticles and that of micro-size particles. Some experiment results have proved it. By using a 36 L explosion sphere, this research plans to figure out the effect of characteristics mentioned above on the flammability and the sensitivity and severity of explosion. The goal of this research is to find out the mechanism and build a model for nanoparticles combustion and explosion, and then provide information for prevention and mitigation of nanoparticles combustion and explosion.



## “Comprehensive Risk assessment of Hydrogen Peroxide Catalyzed by Tungstic Acid”



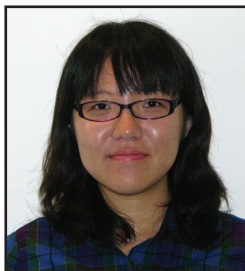
Wen Zhu

Hydrogen peroxide catalyzed by tungstic acid is a popular reagent for the oxidation of olefins, alcohols, and sulfides and many other chemicals. Since the oxidation reaction by hydrogen oxide is economical and environmental friendly, there is a trend to use  $H_2O_2$  as an oxidant for large scale processes in industry such as caprolactam synthesis and propylene oxidation. However, tungsten species could catalyze the decomposition of hydrogen peroxide at low onset temperature. Moreover, concentrated hydrogen peroxide may decompose violently in contact with iron, copper, chromium, and other metals, so the construction materials of processing equipment should also be carefully assessed. Therefore, the tungsten-catalyzed hydrogen peroxide oxidation accompanied by metals may result temperature and pressure runaway due to the acceleration of decomposition. Accordingly, a comprehensive risk assessment for the hydrogen peroxide oxidation process with the tungstic acid is essential to prevent incident occurrence.

## Faculty Fellows Program

In order to serve all of its stakeholders, the Mary Kay O'Connor Process Safety Center has developed a group of faculty with expertise in various fields of research. This group includes Texas A&M University faculty members from Industrial Psychology, Chemistry, Chemical Engineering and Mechanical Engineering. In addition, the center brings in visiting scholars from throughout the world to work with its students and research staff. Students in the Faculty Fellows Program are involved in important safety-related research efforts supported by the center.

## “Steady-state and Dynamic Analysis of N-oxidation of Alkylpyridines by Hydrogen Peroxide in a CSTR”



Xiaohong Cui

Two streams have dominated most of the work of understanding stirred tank reactors behaviors. Based upon bifurcation theory, the static current focuses on systematic determination of the maximum number of steady-state solutions of a CSTR and prediction of all possible types of bifurcation diagrams describing the dependence of a state variable of the reactor on a design or operation parameter. The dynamic branch emphasizes the question of stability of steady states and/or undamped oscillations in the form of limit cycles and exhibits the dynamic behaviors via phase plots. Pyridine and its derivatives are widely used as starting materials for pharmaceuticals and agrochemicals syntheses. This work aims to seek safer and more efficient reactor design and operation for N-oxidation of alkylpyridines via reactor modeling and system analysis. Specifically, a CSTR setup is adopted and the reactor design and operation plane is demarcated based upon system steady-state and dynamic characteristics predicted by bifurcation theory and displayed on different types of bifurcation diagrams and phase plots. Conditions that are promising for operation at safe stable steady states without sacrificing production capacity are identified.

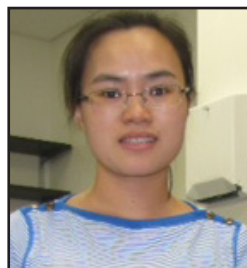
### “An Empirical Test of the Incremental Validity of Industry-Specific Safety Climate”



Nate Keiser

Safety climate is broadly defined as shared employee perceptions of safety policies, procedures, and practices (Zohar, 2003). Safety climate exists at all levels within an organization, and encompasses the formal written policies and procedures as well as the unwritten practices that actually take place (Jex, Swanson, & Grubb, 2013). As a psychological construct, safety climate is defined independent of the various industries and organizations in which it exists. However, Zohar (2003) also advocated for the inclusion of industry-specific safety climate items. The value of industry-specific compared to general safety climate items has not been tested empirically. Consequently, I seek to test if industry-specific items provide incremental validity in the prediction of safety behavior and incidents and result in higher levels of agreement about climate among workgroup members.

### “Pickering Emulsions and Foams for Process Safety”



Xuezheng Wang

Surface modified single ZrP (Zirconium Phosphate) nanosheets can be used to stabilize either emulsions or foams, which are called Pickering emulsions or Pickering foams, respectively. Pickering emulsions and foams have found various applications in areas as diverse as the food industry, oil industry, polymer and ceramic fields, paint products, fire distinguishing materials, and pharmacy areas. They are becoming the most popular type of soft matter, attracting world-wide attention. Here, we are trying to extend the use of ZrP nanosheet-based foams to the area of expansion foams as a mitigation measure for LNG spills and fire, and use the ZrP nanosheet-based emulsions for oil spill treatments. The optimum conditions for the application of the Pickering foam or emulsion are studied based on the particle size, the surface modification, and the choice of gas (for foam) or oil (for emulsion).

### “Burning Velocity of Suspended Dust Mixtures”



Travis Sikes

Finding fundamental properties, such as flammability limits and burning velocity, of flammable gas and combustible dust are vital to understand and prevent accidents involving aerosols that can occur in manufacturing. In traditional aerosol experiments, there is an unknown amount of turbulence and uniformity which results in facility dependent data that is less reliable when building models and predicting dust explosions. To improve on this, a schlieren system is being used in conjunction with the spherically expanding flame method to photograph the propagation of the flame front during the experiment. This allows the flame speed to be determined from both pressure and optical data. Having such a large optical access allows verification that the experiment is laminar and opens up the possibility of using new methods to check for repeatability and uniformity. These improvements will lead to a more quantitative experiment and better measurements to prevent future catastrophes.



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