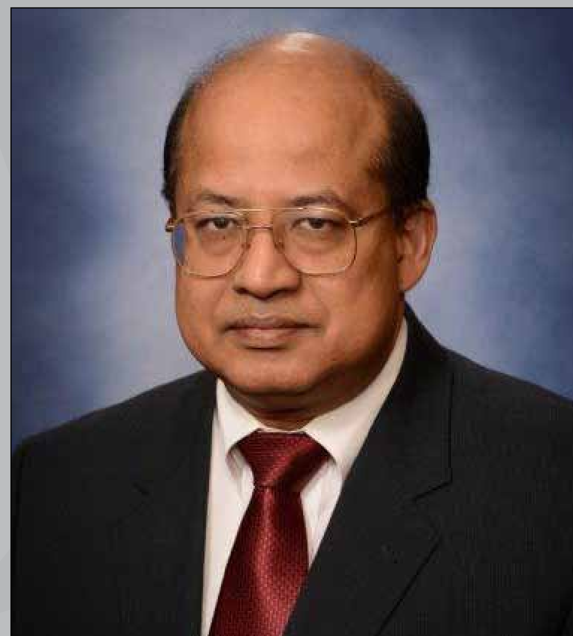
MARY KAY O'CONNOR PROCESS SAFETY CENTER

TEXAS A&M ENGINEERING EXPERIMENT STATION

2013-2014 RESEARCH HIGHLIGHTS

Note from the DIRECTOR



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

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.

"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.

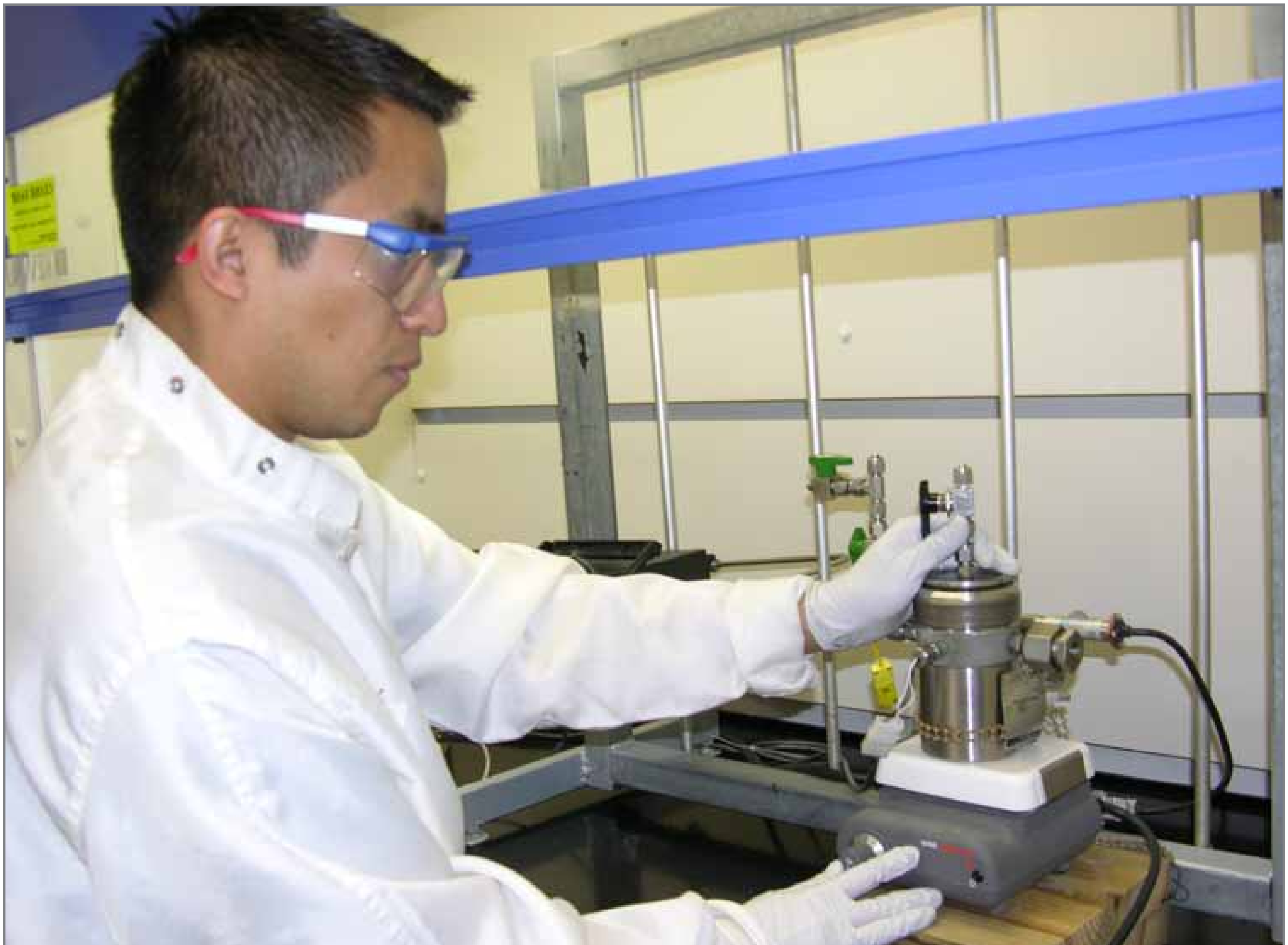
Industry Research Activities

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

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

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

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

"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.

"Relief Value Failure Sizing"

Adewale Awoniyi

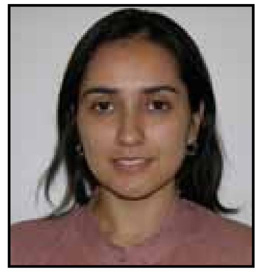
The relief valve is of great importance as it is often the last line of defense in many industrial process operations. Because of their common use in a lot of processes, relief valves are exposed to a large number of different operation conditions that could lead to their failure. For this reason, it is important that the selection and maintenance of relief valves be done very carefully. The most important criterion in the selection of a relief valve is sizing. For proper sizing, knowledge of the local codes requirements, the process conditions, and all other pressure-relieving aspects of the process are required. The purpose of this research is to better understand the factors that could lead to relief valve failures and how these failures can be minimized in order to maintain high levels of safety.

"The Development of the Material Sensor for Detecting Fire"

Julius Choi

The objective of this research is to develop the material sensor for smoldering/flaming fire detection. The tracer gas, which can be easily detected, will be stored in the tiny material sensor which can be embedded on the surface of paint. This material will be temperature sensitive, and the tracer gas will be released from this sensor at specific temperature where combustion or fire is supposed to occur. Then, released tracer gas will be noticed by a detector. This material sensor will be applied on surfaces prone to smoldering combustion such as wire insulation, cable trays, and electronic equipment

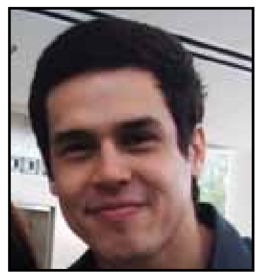
"Vapor Pressure Measurement of Formaldehyde Water Solution"



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.

"Optimal Placement of Gas Detectors in Process Facilities Considering Reliability and Voting"



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.

"Shock Interaction with Dust Layers"

Amira Chowdhury

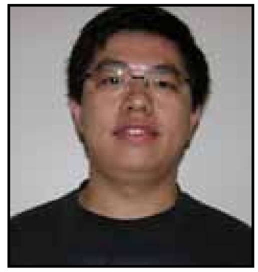
Secondary dust explosions can be far more destructive than a primary explosion due to the increased quantity and concentration of dispersed combustible dust, making this a very important issue in the industries. Secondary dust explosions occur when the shock of an initial explosion dislodges more accumulated 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 to Liquefied Natural Gas pool spreading on water: A study of key parameters"

Nirupama Gopalaswami

An accidental release of Liquefied Natural Gas can result in a formation of liquid pool and vapor cloud which can lead to hazards in the presence of ignition sources. Consequence analysis is used to evaluate the potential consequences arising from accidents and intentional acts. One of the initial steps in consequence analysis is source term modeling, which involves the determination of the amount of vapor generated from the spill along with its physical state. The source term modeling results are used as input to the dispersion model which describes how material is transported downwind at certain concentration levels. This has been studied extensively and it is now possible to determine the exclusion distance with a variety of modeling tools. The accuracy of exclusion distance determination depends largely on the source term assessment. For the past few years, a simplified source term for the release of LNG on water, which assumed a mean evaporation rate, was used for modeling, but the actual process involves a complex phenomenon which changes over time. The spreading of the LNG pool is influenced by various parameters, and the effect of parameters on the spreading LNG pool is studied and guidelines for proper source term modeling are developed.

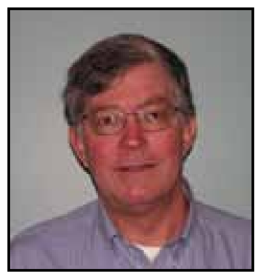
"The Temperature Effect on the Flammability of Hydrogen and Hydrocarbons Mixtures"



Ning Gan

The flammability 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 heat will be released in a short duration of time when combustible gas is ignited, and the extremely high temperature of the reaction will be a threat to the facility and people. Currently, Le Chatelier's Law is used to predict the flammability of gas mixtures in industry. The research objective is to study the flammability characteristics of combustible gases at different temperature ranges 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 satisfy all kind of reaction conditions.

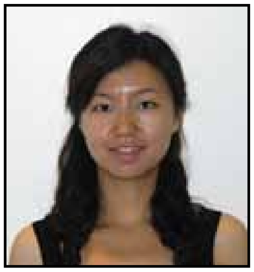
"Predictive Model for Stress-Corrosion Cracking"



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.

“NH4NO3 Reduction of Explosion Hazard while Maintaining Agricultural Benefit”



Zhe Han

Runaway reactions present a potentially serious threat to the chemical process industry. In general, this research topic will investigate the mechanisms that drive these reactions, develop predictive models, and create appropriate and effective mitigation strategies. Specifically, this project will look at reducing the explosion hazard associated with ammonium nitrate (AN) while maintaining its agricultural benefit. On one hand, the safety issues associated with the storage of AN will be considered. On the other hand, more efforts will be spent on developing the reactions stoichiometry, thermodynamic parameters, and kinetic parameters related to AN.

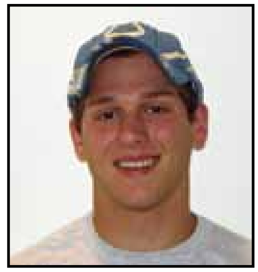
In this project, experimental analysis, theoretical methods, and a systematic approach for reactivity evaluation will be used to better study the mechanisms that result in explosion hazards. The first step is to study the decomposition of AN, using RSST, APTAC, and DSC/TGA. Some materials act as inert which results in the dilution of AN, and others tend to increase the chemical reaction zone to reduce the probability of explosion due to incorporation. Therefore, this study will look into the behavior of AN with additives. Except from that, weathering effect, humidity effect, and volume effect will be tested to find out how the storage condition will affect decomposition of AN. GC can be used to analyze the gas composition. Except for experimental work, modeling tools such as Gaussian and Material Studio will also be used to validate experimental data.

“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.

“Blast Decontamination Foam for Chemical Mitigation”



Brian Harding

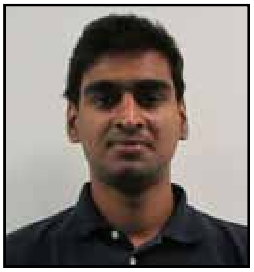
Decontamination foam is used to decontaminate surfaces, people, etc. from all types of contaminants. It is used because it has a fairly long residence time on surfaces, and is able to decontaminate them at a high level. On the surface, my research topic is concerned with the use of decon foam to stop 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.

“Cryogenic effect of LNG on Reinforced concrete”

Bilkis Islam

In recent years, the U.S. has experienced increasing demand of LNG which requires large quantities of LNG to be transported from one place to another. There are significant risks associated with the transportation of LNG. The massive size of LNG storage tanks and LNG tankers pose the potential for a very large incident in case of any containment releases in the facility or during transportation. Spillage of LNG can lead to pool fire, vapor cloud explosion, etc., and can lead to significantly damage of the roads or bridges. A spill of a significant amount of LNG can affect the durability of road materials such as reinforced cement concrete (RCC). This research will focus on the cryogenic effect of LNG on reinforced cement concrete in terms of change in thermal conductivity, ductility, and thermal stress. In general most key concrete properties such as compressive strength, tensile strength, modulus of elasticity, thermal conductivity, and permeability improve under cryogenic temperature if there is a single freezing cycle. A reduction of strength in concrete might happen due to a freeze thaw cycle. The research objectives will be a literature review on properties of concrete and steel that effects the thermal deterioration, development of a heat conduction problem using finite element methods to obtain thermal distribution data in a stressed concrete pavement slab, and development of methodology to find thermal stresses from the temperature distribution on the slab.

"In-situ Production of Hydrogen Peroxide for Oxidation Reactions"

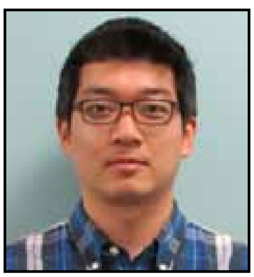


Sunder Janardanan

Hydrogen peroxide is vastly used as an industrial oxidant due to its high selectivity over oxygen. Also, it reduces the downstream separation problems as water is produced as the byproduct. However, hydrogen peroxide is highly unstable and decomposes to water and oxygen, releasing large amounts of heat. Hence, the storage of hydrogen peroxide poses high risk. The research aims at studying the production of hydrogen peroxide in-situ for oxidations reactions. A feasible synthesis technique for hydrogen peroxide will be integrated with the consequent oxidation reaction to design a one pot synthesis for the desired product.

The major manufacturing techniques of hydrogen peroxide are 1) Anthroquinone process, 2) electrolysis of water/ sulphuric acid/ sulphates, and3) Oxidation of secondary alcohols. Lab studies will be focused on finding the safest and economically viable option for the overall oxidation reaction.

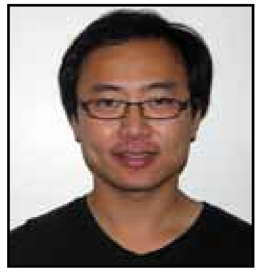
"Laboratory Design for Nanoparticles Hazards"



Jin Kim

Over recent decades, nanoparticles are increasingly produced as the result of the rapid development in nanotechnology to meet the needs of specific applications, most notably chemical industry, energy management and medical sciences. This results in an inevitable unintended exposure of humans to these nanoparticles. Following exposure, nanoparticles can access the body through the lungs, gastrointestinal tract, skin, injections and implantations. This exposure can cause serious diseases in the systemic organs. As the result, an increasing concern has been raised over the potential impacts of nanoparticles to human health. In light of this, research that will be discussed is: (1) understanding nanoparticles and their hazards to human health, (2) finding out current regulations and exposure limits for a variety of nanoparticles, (3) developing guideline for working safely with nanoparticles in laboratories, and (4) recommending safety considerations for MKOPSC Nanodust Explosion Laboratory.

"Measure Hybrid Mixtures Explosion Characteristics"



Jiaojun Jiang

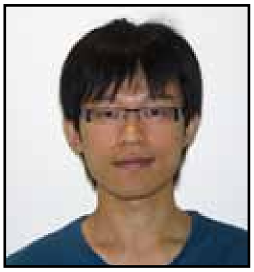
Hybrid mixtures consist of a flammable gas and a combustible dust which causes lots of accidents. They are encountered in various industries such as painting factories, mining, grain elevators or pharmaceutical. Each of them may be present in an amount less than its Lower Flammable Limit (LFL)/ Minimum 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, including Maximum Pressure (Pmax), Maximum Rate of Pressure Rise ([dP/dt]max), Limited Oxygen Concentration (LOC) and deflagration index (KSt). The goal is to provide important information for preventing hybrid mixtures explosion.

"Risk Analysis of Offshore Operations Focus on Response of Spill Accidents"

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.

"Aerosol Flammability Study"



Yan-Ru Lin

High flash point liquids (e.g., heat transfer fluids) are thought to be safe since they are relatively hard to be ignited. However, if they leak at a higher pressure and temperature from the pipeline (or other containers), then aerosols may be formed. The former researchers have shown that aerosols can develop into global flame under specific conditions. From the literature, flame speed of aerosols can be accelerated when aerosol size is at a specific transition range (5~30 μm). This transition range varies with different fluids. Therefore, the goal of this research is to upgrade the current electrospray device and study the phenomena by testing fluids with varied flash points and other properties. The study will also run modeling to verify the experimental results. Later, research on the lower flammable limit of aerosol will be conducted.

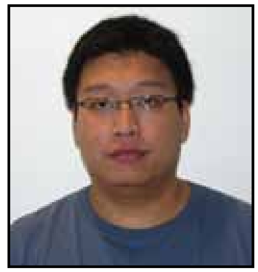
"Experimental and Theoretical Study of the Decomposition Reaction of tert-Butyl Peroxy-2-Ethylexhanoate (t-BPEH)"

Olga Reyes

T-BPEH is a peroxide widely use in the petrochemical industry as an initiator of the (co)polymerization of the most common types of monomers, i.e., ethylene, styrene and acrylates. The use of this peroxide poses an intrinsic risk due to the possibility of its highly exothermic self-decomposition and subsequent runaway reaction. During the runaway reaction, vapor and gases will be formed (creating a hybrid system), rising the pressure inside the reactor. However, depending on the boiling point of the solvent, the behavior of the system will differ during the runaway reaction. The fundamental understanding of the chemical reaction kinetics of this complex system is of paramount importance in the design of the full scale chemical reactor and its safeguards (venting and control systems).

The objective of this research is to combine the use of adiabatic and isothermal calorimetry experiments with computational chemistry in order to get a better understanding of the reaction path and kinetics of the decomposition of t-BPEH under runaway conditions, when diluted in two different solvents and with a difference in their boiling points of more than 100°C. This study is part of a work that aims to understand the dynamic, kinetic, thermodynamic, and fluid dynamic of a reactor carrying on the decomposition reaction of t-BPEH from the start of the reaction until the end of the venting step.

"Modeling of Uncontrolled Fluid Flow in Wellbore and its Prevention"



Ruochen Liu

Uncontrolled fluid flow in wellbore includes gas-kick, blowout, petroleum seep, and hydrate formation. Geological uncertainties, equipment failures, material fatigue, design deficiencies, or human errors might lead to those incidents. A blowout is always the most unwanted disaster for all the well operations, such as the Macondo incident. It might severely damage the environment, equipment, and materials; deplete the reservoir; cause fires and possibly explosions; injure or kill operators and personnel; lead to a large financial loss; and affect the companies' credibility.

"Offshore Facility Siting and Layout Optimization"

Josh Richardson

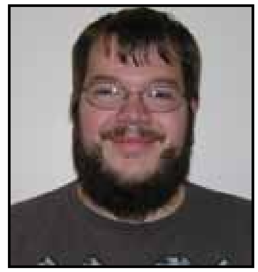
The use of mathematical modeling has recently been applied to onshore facilities to optimize the layout of process units and equipment in a plant setting. However, this approach has not been applied in an offshore context where there are several complicating factors and constraints to consider, such as lack of space, added confinement in the case of explosions, three-dimensional modeling and other related factors. The purpose of this research is to supplement and improve the current offshore design practice through the use of mathematical modeling and optimization techniques to minimize risk in the case of fire and explosion or other scenarios that may occur on a platform.

"Toward an Inherently Safer Process for Alkylpyridines N-Oxidation"

Alba Pineda

The N-oxidation of alkylpyridines is a reaction widely used in the pharmaceutical industry. Major hazards are associated with the undesired gas-generating decomposition of hydrogen peroxide, the oxidizing agent. The generation of oxygen from the decomposition reaction, combined with the flammability of the alkylpyridines, represents a serious hazard of fire and explosion for this process. Additional complications arise during the N-oxidation of higher order alkylpyridines, due to the separation of the organic and aqueous phases, which promotes the decomposition of hydrogen peroxide. The goal of this research is to develop an inherently safer and more efficient process for the N-oxidation of alkylpyridines. This will be achieved by integrating calorimetric and thermodynamic studies, inherent safety principles, and reaction engineering.

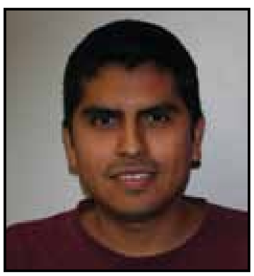
"Reactivity of Aromatic Nitro Compounds"



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 of industrial chemical processes. However, the process is highly exothermic and subject to runaway and the products, nitrocompounds, will undergo monomolecular decomposition at higher temperatures, releasing a massive amount of energy and often causing explosions. The process continues to produce industrial accidents. The process has been shown to exhibit complex phase behavior with between one and three simultaneous liquid phases. This makes understanding, modeling, and predicting the system behavior in a reactor even more difficult. It is therefore desired to better understand, model, and predict the phase behavior to improve reactor models and designs in order to improve the safety of the process.

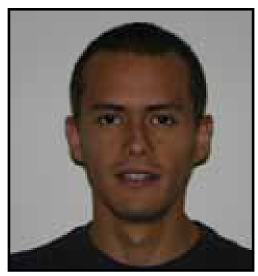
"Well Integrity Modeling and Risk Assessment in Sustained Casing Pressure Annuli"



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.

"Deflagration to Detonation Transition Studies"



Camilo Rosas

When referring to explosions, there are two different mechanisms. The first one is deflagration, which is a sub-sonic combustion wave with respect to the unburnt gas ahead of the flame. On a deflagration, it is possible to distinguish the flame front and the shock front from one another. The second mechanism is detonation, which is a supersonic combustion wave propagating at 1500-2000m/s in fuel-air and can produce overpressures up to around 2 MPa. On a detonation, the flame front and the shock front are coupled as one and it is very hard to distinguish one from another. Additionally, if the appropriate conditions are given, it is possible to have an abrupt transition from deflagration to detonation. This research project will focus 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.

"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.

"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˚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 LN2, 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.

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.

"Application of Risk Analysis Techniques in Industrial Situations"

Hanan Altabbakh

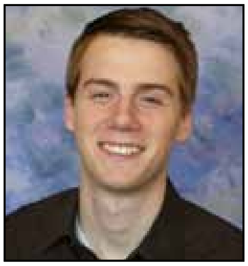
This study explores three different types of risk assessment techniques, namely Layer of Protection Analysis (LOPA), Risk in Early Design (RED), and Swiss Cheese Model (SCM) to evaluate risk and limitations of system safety programs in a variety of industrial situations. Industrial case studies are used to identifies strengths and weaknesses of each assessment technique and to assist engineers and managers in selecting the best risk assessment technique to mitigate risk and enhance safety for various situations.

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

Xiaohong Cui

Following Amundson and Bilous' landmark paper in 1955, which treated the stirred tank reactor as a dynamic system and used Lyapunov's method of linearization to give a pair of algebraic conditions for local stability and to depict the global picture on the phase plane, two streams henceforth have dominated most of the work of understanding stirred tank reactors behaviors. Based upon the methods of singularity 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. The dynamic branch emphasizes the question of stability of steady states and/or undamped oscillations and exhibits the dynamic behaviors via phase plots. The present work aims at identifying hazards of the reaction of N-oxidation of alkylpyridines by hydrogen peroxide in a CSTR from the perspective of the multiplicity of steady states and the dynamics of the reacting system, and proposing an inherently safer and more efficient reactor configuration of thermally coupling the exothermic reaction of the N-oxidation of alkylpyridines by hydrogen peroxide with a selected endothermic reaction in the same volume to achieve reactive cooling effect, i.e., the enthalpy released by the exothermic reaction is recovered in the chemical bonds of the endothermic reaction products.

"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.

"Mass Production of Solid State Systems for Harvesting Waste Heat from Process Industries"

Jinmoo Lee

Energy usage in the United States is predicted to increase exponentially over the foreseeable future, yet 56-57% of all energy produced is still rejected as waste heat. For example, a majority of the energy generated using petroleum ($\approx$ 92.8 %) is used by the transportation and industrial sectors. However, the petroleum industry by itself does not operate at top efficiencies, and it is estimated that refineries could cut their energy costs by 54% or $8.3 billion per year through the use of current state-of-the-art energy practices. Furthermore, a major portion of the energy generated by burning gasoline in automobiles is lost either in the engine coolant or through the exhaust. So, it is clear that a staggering amount of energy can be saved by recovering waste heat. Solid-state thermoelectric modules can be used for recovering this waste heat. These solid-state thermoelectrics modules have no moving parts, are portable and have very long operational lifetimes. Fabrication of these modules requires the mass production and large-scale assembly of nanomaterials that offer the potential of precisely controlling thermal and electrical transport through them. Synthesis of nanomaterial powders on an industrial scale, and their assembly into large thermoelectric modules, is essential for this purpose. The aim of this work is to accomplish the same, namely the development of a novel technology for the fabrication of large-scale thermoelectric modules based on inorganic compound semiconductor nanowires for scavenging waste heat.

"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.

"Pickering Emulsions and Foams for Process Safety"

Xuezhen 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).

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