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. Further, 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 serving all stakeholders, providing a common forum, and developing 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.
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 of 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
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.

**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.

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**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
Designing a Synergistic Flame Retardant System and Gaining Fundamental Understanding of the Synergistic Effect through Kinetic Modeling

Fire retardancy of plastics is becoming increasingly important due to its' widespread application in daily life and the subsequent fire hazard associated with it. Polymer nanocomposites have the potential to lead the way for better material performance with enhanced flame retardancy in the future. They offer an opportunity for exploring new behavior and functionality beyond what conventional materials have to offer. The main objective of the current work is to gain a 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

Boiling is one of the major areas of concern in source-term modeling. The 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. The 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.

Risk-based approach applied in Facility Siting and Layout

The main objective of this research is to incorporate the risk-based approach in the facility placement for a case study. Contrary to the worst case scenario approach, the risk-based analysis considers the range of all possible scenarios. It requires a good understanding of the frequency and the consequences associated with each potential scenario. The separation distance is obtained according to the risk acceptance criteria for the facility which can be related with individual or population risks. Besides the cost-benefit, it enhances more flexibility to the facility design by inserting the facility specifications with the use of probabilistic methods. Several studies associated with different methodologies for quantification of risk in the facility layout optimization have been reported; however, there are neither reported methodologies considering the entire range of all possible scenarios nor applications the risk acceptance criteria as a determining factor for the safe distances. In addition, the domino effect is considered for each scenario when applicable.

Human Factors in the Selection of New Technology for the Oil and Gas Industries

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 are not the best solution for the organization. When discussing Human Factors, an important issue is that there is no model or guide to explain which elements require more attention or where to invest more resources in order to select the best technology to reduce human error and improve the productivity. Moreover, it is difficult to identify, evaluate, and select new technology that can help people in organizations to facilitate the goals of reducing the likelihood of accidents. Therefore, the objective of this work is to develop a methodology for the identification, evaluation and selection of a new technology focused on Human Factors in order to achieve the next goals: present key elements about Human Factors related to the selection of new technology; impact Human Factors during the early process of selection of the new technology; and inform about the Human Factors and Ergonomics that can be considered in the selection of new technology.
With the potential of being net exporter from net importer of natural gas in the next 20 years as predicted by the Energy Outlook (2015), the USA will employ Liquefied Natural Gas (LNG) as a major mode of transport. This raises concerns about the safety of the LNG industry. This research will make an effort to establish a model to address the issue of feasibility to model LNG pool fires of larger diameters, incorporating the atmospheric effect to predict thermal radiation from the fire and predict the consequences using CFD tools. This analysis will be useful for deciding exclusion zones and emergency planning. The CFD model will be validated against available experimental data.

Dust explosions have been a persistent threat in the industry and have claimed lives and caused significant property damage. These explosions are characterized by their severity [Pmax, dP/dT, Kst] and ease of ignition [MIE, MEC, MIT]. Studies have found that these characteristics depend upon particle size, chemical composition and dispersity. However, the dependence of the explosion characteristics on shape and morphology has been neglected. Although, the variation of explosion characteristics with particle size is well understood for micro-dust those variations cannot be extrapolated to nano-size regime due to agglomeration and non-uniform dispersion of nano-dusts. The understanding of dispersion phenomena and its effect on agglomerate size and explosion characteristics of combustible nano-dusts is limited. The main objective of the current research is to address the influence of particle shape and morphology on the dust explosion characteristics such as Pmax, MIE, Kst. It also aims to study the effects of dispersion and the shear associated with it, on the nano-dust agglomerate size, particle size distribution and its explosion characteristics. This research will help to fill a gap in understanding dust explosion dependence on its particle properties and the dispersion effect on nanoparticle size and explosion characteristics.

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

Large amounts of substances are transported in pipelines worldwide. This activity represents a potential hazard that needs to be quantitatively assessed. The industry needs release models that are capable of accurately predicting the discharge rate from a pipeline. The near isentropic expansion following the rupture of a pipeline causes some liquids such as dense phase CO2 or LPG to produce a two-phase release. Current models cannot describe the behavior of a multiphase outflow following a pipeline puncture. Usually, when there is a puncture in a pipeline, the decompression rate is lower in comparison to a full bore rupture and the stratified regime predominates. Most of the models in the literature assume a homogeneous flow approach, which cannot describe this scenario accurately. This research focuses on proposing a model that includes the non-homogeneous assumption to estimate the inventory outflow during a pipeline puncture.

Tatiana Flechas

Flammability Characteristics of Light Hydrocarbons and their Mixtures at Elevated Conditions

Flammability limits of combustible gases like hydrogen, methane, and propane can be influenced by many factors such as temperature, pressure, and humidity. When combustible gas mixtures are ignited, large amounts of reaction energy are released in a short period of time, which can cause deflagration or even detonation. Moreover, the highly exothermic reaction poses threats to the facility and people. In this research, the objective is to study the flammability characteristics of combustible gases at elevated conditions (high temperature and high pressure) and propose corresponding methods to handling them safely. By using both experimental data and theoretical calculations, an improved Le Chatelier Law is postulated and tested to better predict the flammability limits of combustible mixtures.

Ning Gan

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

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 formation of a liquid pool and flammable vapor cloud, which can lead to major consequences in the presence of an 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, are the heat flux from water to the LNG pool and the turbulence in the cryogenic pool, are quantified using experiments. The results of the quantification of key parameters are implemented in the 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 this research can be used for emergency response planning for LNG facilities.

Nirupama Gopalaswami
Safety critical elements act as barriers to prevent major accident hazards. Several barriers may work conjointly to reduce risks to acceptable levels. However, it may not always be possible to immediately identify and repair or replace impaired barriers due to various reasons including supply and administrative delays and required equipment downtime. Evaluating multiple impairments and their associated cumulative risk remains a challenge given that information about these individual impairments need to be brought together and presented in a way that would enable realization of the overall picture of cumulative risk. The objective of this research is to determine the cumulative risk arising from impaired barriers such as safety critical elements under maintenance or changes in offshore resources. A cumulative risk assessment model is to be developed to provide an assessment of when an increased risk could occur that would help make decisions to reduce risks to ALARP.

Zohra Halim

Cumulative Risk Assessment Model to Analyze Increased Risk Due to Impaired Safety Critical Elements in Offshore Resources

Stress-corrosion cracking is a particularly insidious form of corrosion failure. It can occur with little to no warning and lead to the catastrophic failure of piping, structural materials and process equipment. Recently, DFT and Molecular Dynamics modeling has been used to predict the energy states along grain boundaries in BCC iron and 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 insight into the underlying mechanisms. Other researchers have recently published similar work using multi-scale modeling, extending 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.

Richard Gustafson

Predictive Model for Stress-Corrosion Cracking

Runaway reactions present a potentially serious threat to the chemical process industry. This project looks at reducing the explosion hazard associated with ammonium nitrate (AN) while maintaining its agricultural benefit. In general, this research investigates the mechanisms that drive these reactions, the development of predictive models, and the creation of appropriate and effective mitigation strategies. Experimental analysis, theoretical methods, and a systematic approach for reactivity evaluation have been used to better understand the mechanisms that result in AN explosion hazards. The decomposition of AN is studied using RSST and APTAC, including the effect of additives (inhibitors and promoters), weathering effect, humidity effect, and volume effect. The reactions’ stoichiometry, thermodynamic parameters, and kinetic parameters related to AN have been developed. In conclusion, the study will help identify the storage conditions that reduce AN hazards.

Zhe Han

NH4NO3 Reduction of Explosion Hazard while Maintaining Agricultural Benefit
**Decontamination Foam for Chemical Mitigation**

Decontamination foam is used to decontaminate surfaces or people from all types of contaminants. It is used because it has a fairly long residence time on surfaces, is able to decontaminate at a high level, and is non-toxic, non-corrosive, and environmentally safe. This research is concerned with the use of decontamination foam to prevent the spread of hazardous chemicals due to spills or other releases and remove the hazard by reacting with the chemical to form non-hazardous products. This research is aimed at effectively decontaminating chemicals that may be released in industrial incidents.

**Development of Nanocomposites Containing Zirconium Phosphate as Flame Retardant Materials**

The toxicity of widely used flame-retardant materials has sparked the development of many new kinds of materials. The polymeric nanocomposite is one such material which utilized nanoparticles embedded in a polymeric matrix. In an effort to better understand nanocomposites, the two main mechanisms for flame-retardancy are being studied separately and together for synergistic effects. The first of these effects is the catalytic charring effect, which forms a charred barrier between the flame and the burning polymer. Similarly, the physical barrier effect forms a protective barrier between the flame and polymer, but this is composed of agglomerated nanoparticles. These two effects give rise to a protective layer on the surface of the burning polymer, which acts as a shield for mass transfer and heat transfer. To analyze these two effects, current research includes heat transfer studies to better understand how heat flow within the polymeric material is affected by different mechanisms of flame-retardancy. To accomplish this, hybrid nanoparticles are engineered by attaching specific amounts of catalytic charring groups attached to physical barrier-forming nanoparticles, which are then embedded into polymer matrices. By varying the ratio of the catalytic charring groups attached to the physical barrier inducing nanoparticles, it should be possible to observe each mechanism separately, as well as synergistically.

**A Hybrid Fuzzy Logic and Probability Theory Method to Quantify the Uncertainty in Layer of Protection Analysis**

Layer of Protection Analysis (LOPA) is a semi-quantitative method to identify and analyze the significance of potential major incident scenarios 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 safeguard systems and with the assumption that the severity of consequences remains constant with the activity of independent protection layers (IPLs). These research gaps will be filled by a hybrid fuzzy logic and probability theory method. Fuzzy logic, a method to deal with uncertainty and imprecision, is an efficient tool to solve problems where no sharp boundaries are possible.
Resilience Engineering Framework Incorporating Prediction, Survival and Recovery Analysis

In the oil and gas industry, various risk assessment methods have been studied and developed to reduce undesirable events. However, incidents still happen so a better understanding of the risks and system safety aspects is necessary. A resilient facility would have the capacity to predict instabilities, 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 analysis framework including prediction, survival and recovery models. The framework developed would be applicable to both onshore and offshore installations primarily focusing on detection of unsafe zones, assessment of cumulative risks and prioritization of safety barriers during abnormal situations and reduction in response time resulting in mitigation of consequences. This approach is based on four basic abilities of a system to be resilient: anticipate unknown/uncertain 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.

Phase Equilibrium Studies on N-oxidation Systems to Identify Inherently Safer Operating Conditions

Alkylpyridine N-oxides are used in the pharmaceutical industries to synthesize analgesic and anti-inflammatory drugs. Currently, the N-oxides are produced in semi-batch reactors where alkylpyridines are oxidized with hydrogen peroxide (35% solution) and phosphotungstic acid catalyst. However, the N-oxidation is accompanied by the undesired, condition-dependent decomposition of hydrogen peroxide. A runaway of this reaction may result in a rapid generation of oxygen and temperature rise in the alkylpyridine flammable environment, with the additional potential to over pressurize the reaction vessel and/or trigger secondary decompositions of the product. The decomposition of hydrogen peroxide is exacerbated during the N-oxidation of higher order alkylpyridines due to the mass transfer resistance caused by the formation of an organic phase and an aqueous phase. The water-soluble catalyst causes severe decomposition of the peroxide, jeopardizing the safety of the process, and reducing its efficiency.

This research is focused on predicting the phase equilibrium for an alkylpyridine-Noxide-water-catalyst system. According to previously published literature, the N-oxide increases the solubility of alkylpyridines in water phase. The equilibrium studies would identify the component compositions for which a homogeneous system prevails. The improvement in the selectivity and yield of the N-oxide synthesis reaction, when conducted homogeneously, will also be studied.

Development of a Smart Sensor for the Detection and Mitigation of Microbiologically Influenced Corrosion (MIC)

Microbiologically Influenced Corrosion (MIC) is a form of corrosion that is either caused or accelerated by the presence of microbiota on the surface of metals and other materials of construction. It is a widespread problem in multiple industries, such as oil and gas, chemical, nuclear, power, water networks and utilities. 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/pseudo real-time would be a great tool to help combat MIC at an early stage before it becomes widespread through bio-film formation. The objective of my research is to develop a sensor-based on a nano-wire matrix which is functionalized with bio-molecules which can detect these microorganisms on a real time basis. These sensors are aimed towards high precision and specificity owing to their large surface areas functionalized with bio-molecules. The sensors may be mounted on pigs (devices used in maintenance of pipelines) or at locations where MIC is suspected and the local concentration of biota could be monitored.
Comparative Risk Analysis between LNG Import and Export Terminals

The increasing global demand for natural gas entails a rising need for safer practices in production and transportation of this energy resource. The most recent U.S. economic perspectives have influenced the environment for changes in natural gas trading, particularly in the development of LNG export terminals. Existing import terminals and projected export terminals contain different processes. These differences represent a new set of risks and hazards that must be evaluated before new or modified facilities are put into operation. For the case where an existing import plant is intended to become an export terminal, it is necessary to perform a thorough hazards assessment that will indicate the new area of impact in the case of an incident. This project intends to identify the different risks derived from the particular processes (basically regasification and liquefaction) performed at each type of terminal in order to identify which are the potential critical issues in the development of these new facilities.

Integration of Electron Impedance Spectroscopy and Microfluidics for Investigating Microbially Influenced Corrosion Using Co-culture Biofilms

Susmitha Purnima Kotu

Guido Lamus

Microbially influenced corrosion (MIC) is a major problem in various sectors including chemical process plants, on-shore and off-shore oil and gas, pipelines, marine and aviation industries. Annual losses associated with MIC in the United States are estimated to be $50 billion. MIC often develops as a result of biofilm formation by multiple microbial species that form well-defined and organized structures. Development of effective mitigation strategies for MIC requires a fundamental understanding of how biofilms are formed. The aim of this study is to investigate the factors underlying formation and development of dual-culture biofilms. Using Shewanella oneidensis as the model aerobic biofilm forming species and Desulfovibrio vulgaris as the model anaerobe and sulfate reducing bacterium, we investigated the dynamics of biofilm formation using a microfluidic flow cell. The experimental system consists of a flow channel in a microfluidic device made of polydimethylsiloxane that is bonded to a glass slide with coated metal electrodes. Co-culture biofilms of S. oneidensis and D. vulgaris developed in this system are used to develop a correlation between the thickness of biofilm as measured by confocal laser scanning microscope (CLSM) and impedance measurement from electron impedance spectroscopy (EIS). The effect of hydrodynamic factors like flow rate, shear stress on biofilm dynamics would be investigated. In addition, the effect of various typical biocides on these co-culture biofilms would be studied with respect to biocide penetration, efficacy of the kill and biofilm regrowth.

Flame Propagation Speed of Aerosols Generated by Electrospray

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

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. This is always the most unwanted disaster for all the well operations, an example being the Macondo incident. Consequences of a blowout include damage to the environment, equipment, and materials; personnel injuries and fatalities; loss of production; and damage to the companies’ credibility.

At present, there are research 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 in the environment. Therefore, the purpose of the research is to establish an 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 a model studies the onshore and offshore oil, gas, and oil/gas well blowout behaviors. Considering the uncertainties of geological parameters, such as permeability, porosity, and reservoir pressure, a site specific blowout risk picture is depicted by using the blowout model and the distribution of geo-uncertainties. In addition, after fully understanding the mechanism of blowout behaviors, suggestions will be made concerning the monitor and control of blown-out wells.

Analysis of the Thermal Decomposition of Untempered Peroxide Systems

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.

Deflagration to Detonation Transition Studies

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 present, 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. 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.
A life cycle of a product starts from the extraction of raw materials from nature and ends with the disposal of the product and waste after consumption. Every part of the life cycle has interaction with humans and environment. Hence, every part has concerns for safety of 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 this project. Safety in each part of the supply chain is often inter-related. Finding a good quantification of safety for the supply chain, as an overall objective, 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 especially for the gas processing industry.

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

Nitin Roy

Safety Climate Assessment for Chemical Process Industries

Since disasters such as The Chernobyl Nuclear incident occurred, safety culture has gained more and more attention for managing safety within an organization. Many researchers and organizations have found that safety culture strongly influences people’s perception of risk and behavior in the workplace. Safety culture can be regarded as underlying forces that drive the organization while safety climate is a snapshot of the safety culture at a certain moment, which changes over times. In this respect, much effort was made to develop the effective and accurate ways of measuring safety climate of an organization. Although many safety climate assessment tools have been developed for various purposes, there are few that cover the characteristics of chemical process industries. Therefore, studying the existing methods and developing safety climate inspection methods for chemical process industries will give benefits to those seeking to measure and improve their safety culture.

Changwon Son

Leading Indicators Analysis for Offshore Operations with Emphasis on Drilling

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 operations emphasizing on drilling. Blowouts and gas kick incidents have been analyzed to identify key causal factors divided into four categories – technical, operational, human and organizational factors (HOF) and system of organizations. Primary focus is made on validating technical and operational aspects of leading risk indicators with available drilling safety and reliability data. With the proposed set of leading indicators and physical observables, interactive algorithms will be constructed relating the indicators with causal factors and other process elements. Finally, leading indicators based risk modeling approach will be developed to identify critical events with relevant barriers and actions to prevent offshore incidents.

Nafiz Tamim
**Integration of Human Factors in Offshore Risk Assessment**

Human failures often contribute to major offshore incidents, but are usually not considered in traditional offshore risk assessment. Several human reliability analysis methods have been developed for the aviation and nuclear industry. Some methods have been applied in offshore, but the efficiency of these approaches in offshore drilling is still questionable. Also, there is no uniform category to classify human factors in the 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 objectives of this research are: 1) Identify human factors in offshore drilling; 2) Develop models incorporating human factors in offshore drilling risk assessment quantitatively; 3) Perform a sensitivity analysis to identify the most influencing factors; 4) Provide guidance to effectively improve human performance. The human factors that will be considered in modes are categorized as individual factors, group factors and organization factors. Models based on Hybrid Causal Logic (HCL) framework have been developed to integrate human factors in offshore drilling by event tree, fault tree and Bayesian network.

**LNG Vapor and Fire Hazards Mitigation Using High Expansion Foam**

The mitigation effects of high expansion foam on LNG vapor and fire hazards were studied experimentally. An LNG spill on land will be followed by vigorous vaporization. Due to the dense gas behavior, the LNG vapor cloud travels to a long distance at the ground level if it is not mitigated, which is the vapor hazard. Once the vapor cloud is ignited, the fire flashes back to the pool and causes a pool fire hazard. For LNG vapor hazard mitigation, the blanketing effect could reduce 70% of the heat from convection and radiation for LNG vaporization. The warming effect, an effect to increase LNG vapor buoyancy by warming the vapor, was studied in the lab with a self-built foam generator and a foam test apparatus. For the LNG pool fire mitigation, a large scale field test was conducted using an industrial foam generator. The mitigation effect was studied in terms of mass burning rate, thermal radiation, flame temperature, flame size and other parameters.
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. Some specific characteristics (i.e., type, chemical and surface composition, size), 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 experimental results have proved it. This research aims at identifying fire hazard and explosibility (deflagration index Kst and minimum explosive concentration) of some nanoparticles and finding out properties affecting nanoparticles’ combustion and explosion behavior to improve the current understanding of nanoparticles’ fire and explosion hazard.

Jiaqi Zhang

Heavy Gas Dispersion Model for Hydrogen Sulfide

A potential release source containing hydrogen sulfide concentration greater than or equal to 100 parts per million (ppm) could present a hazard to humans as well as the environment. The main purpose of this research is to better understand the behavior of hydrogen sulfide gas dispersion and how different components of the gas mixture behave inside the sour gas cloud once it leaves the leak source. Currently, the available models treat gas mixtures as one component, while real life incidents indicate that different components behave differently. Understanding this information will have significant implication on process safety of oil production facilities and the way we assess hazardous zones around toxic handling facilities.

Jiayong Zhu

Nitro Aromatic Compounds are important intermediates in the chemical industry. Mononitrotoluene (MNT) and Dinitrotoluene (DNT) are two typical nitro aromatic compounds used in the production of dyes, rubber chemicals, flexible foams and agricultural chemicals. However, incident history demonstrates inadequate recognition and evaluation of reactive hazards of nitro aromatic compounds. Tests prove that nitro aromatic compounds if held at elevated temperatures for an extended time are susceptible to thermal decomposition and may react at temperatures lower than the predicted ‘onset temperature.’ Moreover, contaminants such as nitric acid, sulfuric acid, and traces of salts may lower the thermal stability of nitro aromatic compounds. Therefore, MNT or DNT if held at elevated conditions may result in temperature and pressure runaway. Accordingly, a comprehensive risk assessment for the nitro aromatic compounds in the presence of other chemicals is essential to prevent incident occurrence.

Wen Zhu
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**

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 the systematic determination of the maximum number of steady-state solutions of a CSTR where several chemical reactions occur simultaneously and prediction of all possible types of diagrams describing the dependence of a state variable of the reactor on a design or operating variable. 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. 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. Furthermore, the benefits of the design would be verified and compared by proper risk and economic assessment methods.

**Burning Velocity of Suspended Dust Mixtures**

Finding fundamental properties, such as flammability limits and burning velocity, of flammable gas and combustible dust are vital to understand and prevent incidents 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 experiments. 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**

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).