Purdue Process Safety & Assurance Center

- ***2015 – 2016 Accomplishments***
- ***2017 Research Program***
- ***Chemical Process Safety course; UG & Grad Students***

Ray Mentzer

May 3, 2017

P2SAC Accomplishments – ’15 -’16

- **Publication** “A MINLP Formulation and Solution Approach for Optimal Sensor Placement Under Non-uniform Sensor Failure”, Liu, J., and Laird, C.D., in progress, 2016
- **Presentation** “A Global Stochastic Programming Approach for the Optimal Placement of Gas Detectors with Non-uniform Unavailabilities”, Liu, J., and Laird, C.D., Mary Kay O’Connor Process Safety Symposium, 2016

- **Publication** ‘A systematic framework for process control design and risk analysis in continuous pharmaceutical solid-dosage manufacturing: a feeder-blender system’, Su Q, Moreno M, Giridhar A, Reklaitis GV, Nagy ZK, Journal of Pharmaceutical Innovation, 2016; submitted
- **Presentation** ‘Fault-tolerant control design and risk MAP based resiliency analysis of continuous solid dose manufacturing.’ Su Q, Moreno RM, Ganesh S, Giridhar A, Reklaitis GV, Nagy ZK, AIChE Annual Meeting. San Francisco, USA, 2016

- **Presentation** “Standing Wave Design of a Non-isocratic Three-Zone Simulated Moving Bed for Continuous Purification of Therapeutic Proteins,” Hoon Choi, David M. Harvey, Nicholas H. Soepriatna, George S. Weeden Jr., and Nien-Hwa Linda Wang, AIChE Meeting, San Francisco, Nov. 14 , 2016
- “Rare Metals and Elements from Coal Ash in the “Rare Metal Age,” Entrepreneur Leadership Academy, Purdue Foundry, April 11, 2017.
- **Provisional Patent Application**

P2SAC Accomplishments – cont'd

- **Publications:**
- "Active Site Dynamics and Microkinetic Modeling of Ethanol Dehydration on Sn-Beta Zeolites", [G]**Bukowski**, B., [G]**Bates**, J. S., **Gounder**, R., **Greeley**, J.*(**2017**) *to be submitted.*
- "Confining Environments Around Sn Atoms Isolated within Single-Site Zeolites Are Distinguishable Using DNP-NMR Spectroscopy", [G]**Harris**, J. W., Liao, W.-C., [G]**Di Iorio**, J. R., [UG]**Henry**, A. M., Ong, T. C., Comas-Vives, A., Copèret, C.*, **Gounder**, R.*, (**2017**) *under review*.
- "Controlled Insertion of Tin Atoms into Zeolite Framework Vacancies and Consequences for Glucose Isomerization Catalysis", [G]**Vega-Vila**, J. C., [G]**Harris**, J. W., **Gounder**, R.*, *Journal of Catalysis*, 344 (**2016**) 108-120.
- "A Transmission Infrared Cell Design for Temperature-Controlled Adsorption and Reactivity Studies on Heterogeneous Catalysts", [G]**Cybulskis**, V. J., [G]**Harris**, J. W., Zvinevich, Y., **Ribeiro**, F. H.*, **Gounder**, R.*, *Review of Scientific Instruments*, 87 (**2016**) 103101.
- "Identifying Sn Site Heterogeneities Prevalent Among Sn-Beta Zeolites", Wolf, P., Liao, W.-C., Ong, T. C., Valla, M., [G]**Harris**, J. W., **Gounder**, R., van der Graaff, W. N. P., Pidko, E. A., Hensen, E. J. M., Ferini, P., Dijkmans, J., Sels, B., Hermans, I., Copèret, C., *Helvetica Chimica Acta*, 99 (**2016**) 916-927.
- "Titration and Quantification of Open and Closed Lewis Acid Sites in Sn-Beta Zeolites that Catalyze Glucose Isomerization." [G]**Harris**, J. W., [G]**Cordon**, M. J., [G]**Di Iorio**, J. R., [G]**Vega-Vila**, J. C., **Ribeiro**, F. H., **Gounder**, R.*, *Journal of Catalysis*, 335 (**2016**) 141-154.
- **1 Provisional Patent Application**
- **25 Presentations / Posters at Technical Society Meetings**

- **UG Research with Prof Mentzer**
  - Combustible Dust Hazards in Chemical & Industrial Processes; AraOluwa Adaramola, F16
  - Process Safety in Agricultural and Pharmaceutical Industries; Divya Natarajan, F16
  - Reactive Chemical Hazards; Peter Hellwarth, F16
  - Nano Technology Safety; Nicole Szumigalski, F16
  - Comparison of Global Process Safety Regulations; Jennifer Besserman, S17

Potential P2SAC Research Projects – Industry Input, Nov '16

1) Reflecting on the current "Human Performance" discussion as it pertains to design criteria and operational use, how have past engineering design criteria accounted for normal human error mechanisms and "hardening" of a system to be tolerant to these known error types? (Phillips 66)
2) What does competence in the major hazards industry (O&G) in the form of critical decision making and task execution look like for senior managers, engineers, operators, etc? (Phillips 66)
3) Develop a small-scale predictive tool for the MIE of combustible dust based on the chemical structure. (Lilly; Fauske; SSPC)
4) Extend the batch-to-batch variation in modeling chemical processes to a 'Safety by Design' concept in order to incorporate lot-to-lot variability of reagents or solvents in safety analyses. (Lilly)
5) Conduct a process safety related benchmarking survey of the pharmaceutical and perhaps broader (O&G, petrochem, fine chemicals, Agriculture, etc) industries. (Lilly)
6) Compile safety data for the use of amid coupling reagents and a ranking of them/recommendation for their use based on thermal hazard data. Where data doesn't exist, conduct DSC and/or ARC experiments. (Lilly)

Research Projects – Industry Input – 2

7) Recognizing that high performance / safe operations require proper design, operations and maintenance, what steps are needed to improve the human interface through design features and ergonomics with particular attention to control room operators? (BP & ExxonMobil)

8) In today's work environment there is wide use of cell phones, FitBits, etc for personal use as well as tablets, etc for data capture, etc. What is known of the impact of such modern personal electronic devices as potential ignition sources in process areas? (ExxonMobil)

9) Extend Charpy impact curves for brittle fracture of pipelines to different metallurgies, most likely using a probabilistic approach. (ExxonMobil)

10) Address validation of the use of water sprays to mitigate overpressures. (ExxonMobil)

11) Conduct literature review of leak frequency and mechanisms for LNG metallurgy failures. (ExxonMobil)

Research Projects – Industry Input - 3

12) Risk and reliability of aged gas and product pipelines, in terms of incidents and causative factors. Quantify the residual risk of having certain types of pipeline failures under various inspection programs. (ExxonMobil, Prof Laird & RCP)

13) Review the current state and assumptions for common cause models and look for means to upgrade. To what degree are systemic failures addressed in risk analyses vs. random approach commonly deployed? (BP, Honeywell)

14) Validate large scale consequence modeling by reviewing studies that have been done comparing large scale field tests with Gaussian and CFD models. (BP & Kenexis)

15) What tools & models exist to detect subsea leaks in three phase produced fluids, particularly when the lines are sub-ambient? (BP)

16) What has the experience been with regard to corrosion under insulation, such as with wet insulation exposed to the environment? What methods are available to look for defects? (BP)

17) Re-examine current basis for gas & fire detector placement. (BP, Prof Laird)

Potential P2SAC Research Projects – Purdue Faculty Input

A) Strategically assess the cyber physical vulnerability of example chemical processes, make reasonable assumptions to generalize the results, and develop industry wide strategies to make chemical processes inherently more cyber physically secure. (Prof Joe Pekny & Eric Dietz, Director of the Purdue Homeland Security Institute)

B) Computational analysis of drop coalescence in emulsions to reduce retention times in oil-water separators. By means of simulations, clarify the effect of fluid viscosities, drop sizes, drop velocities, and surfactants on coalescence in oil-water separators and probe the effect of surfactants on breaking emulsions and influencing retention times in oil-water separators. (Prof Osman Basaran, School of Chemical Engineering)

C) Combine computational fluid dynamics and experiments to advance the understanding of erosion in pipelines. Particle-wall collisions will be studied using high-speed imaging by shooting particles at different angles of impact at solid walls and subsequently simulated using CFD. (Prof Osman Basaran, School of Chemical Engineering)

D) Robust model-based control for safe pharmaceutical manufacturing (Prof. Zoltan Nagy)

E) Prevention through catalyst design for applications in the petrochemical industry (Prof. Raj Gounder)

F) Advanced separation techniques for producing rare earth elements and other chemicals from coal fly ash (Prof. N.-H. Linda Wang)

P2SAC PROJECTS FOR 2017

Re-examine current basis for gas and fire detector placement (new project)

PI: Prof. Carl Laird Project suggested/proposed by BP

Type of project: PhD research

Optimal placement of gas detectors in process facilities: bringing optimization-based gas detector placement into practice (continuing project)

PI: Prof. Carl Laird Project suggested/proposed by Carl Laird

Type of project: PhD research

Validate large scale consequence modeling (new project)

Project suggested/proposed by BP

Type of project: MS research (with Kenexis as sponsor)

Prevention through catalyst design for applications in the petrochemical industry (new project)

PI: Prof. Raj Gounder Project suggested/proposed by Raj Gounder

Type of project: PhD research

Experience with LNG metallurgy failures (new project)

PI: Prof. Ray Mentzer Project suggested/proposed by: ExxonMobil

Type of project: UG research

P2SAC PROJECTS FOR 2017 – cont'd

Conduct a process safety related benchmarking survey of the pharmaceutical and perhaps broader industries (new project)

PI: Prof. Ray Mentzer Project suggested/proposed by Lilly

Type of project: UG research

Compilation of thermal hazard safety data for amide coupling reagents (new project)

Project suggested/proposed by Lilly

Type of project: MS (with Lilly as sponsor)

Robust model-based control for safe pharmaceutical manufacturing (new project)

PI: Prof. Zoltan Nagy Project suggested/proposed by Zoltan Nagy

Type of project: PhD research

Advanced separation techniques for producing rare earth elements and other chemicals from coal fly ash (new project)

PI: Prof. N.-H. Linda Wang Project suggested/proposed by N.-H. Linda Wang

Type of project: PhD research

Computational analysis of drop coalescence in emulsions to reduce retention times in oil-water separators (new project)

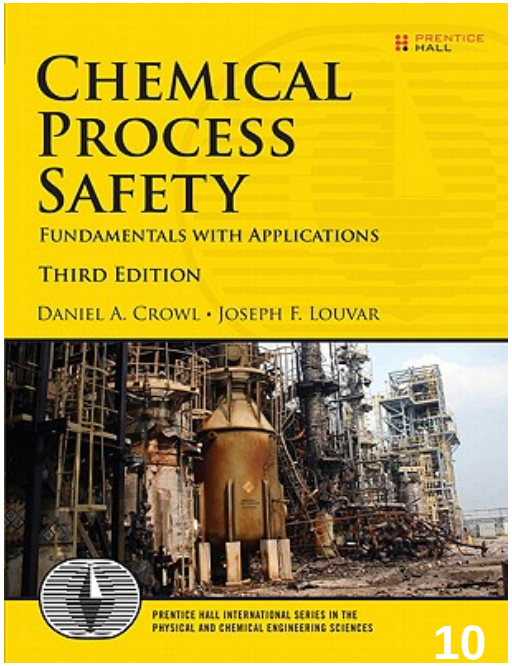
PI: Prof. Osman A. Basaran Project suggested/proposed by Osman A. Basaran & BP

Type of project: PhD research

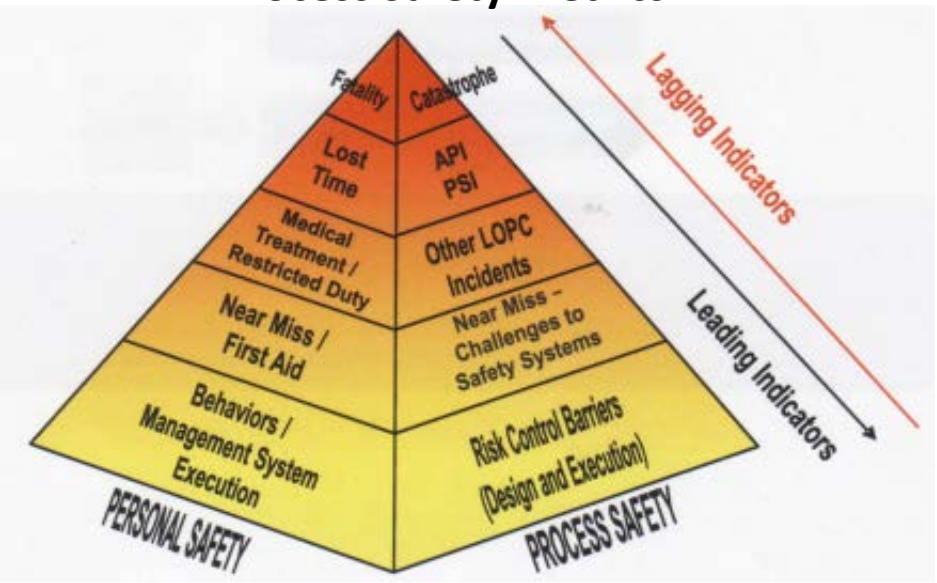
CHE 420 - Chemical Process Safety – core UG course

Safety Culture / Leadership
Personnel vs. Process Safety
& Metrics
Applicable regulations: OSHA
PSM, EPA RMP, etc
Source Term Modeling
Toxicants & Industrial Hygiene
Toxic/Flammable Gas Release
Dispersion Modeling
Fire & Explosion Protection
Chemical Reactivity
Relief System Design
Hazards Identification (HAZOP, ..)
Risk Assessment (Matrix, QRA, ..)
Accident Investigations

T-2 Laboratories, FL – ’09; 4 fatalities



Process Safety Metrics



Plume Model

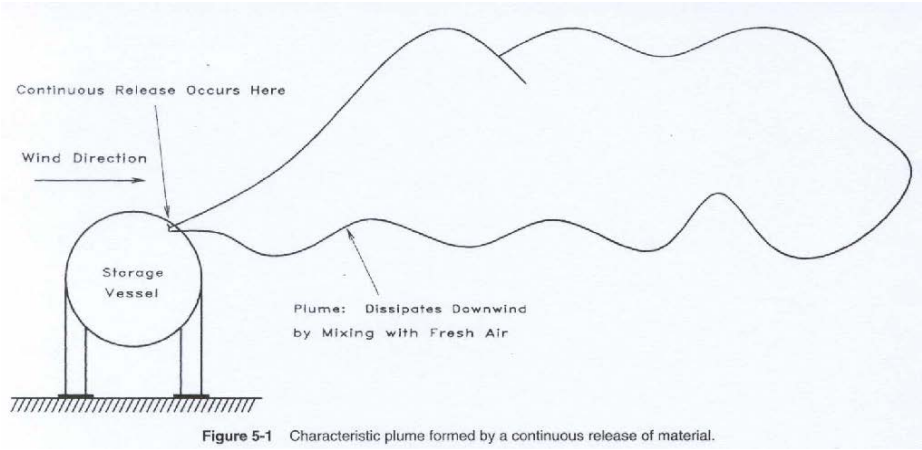
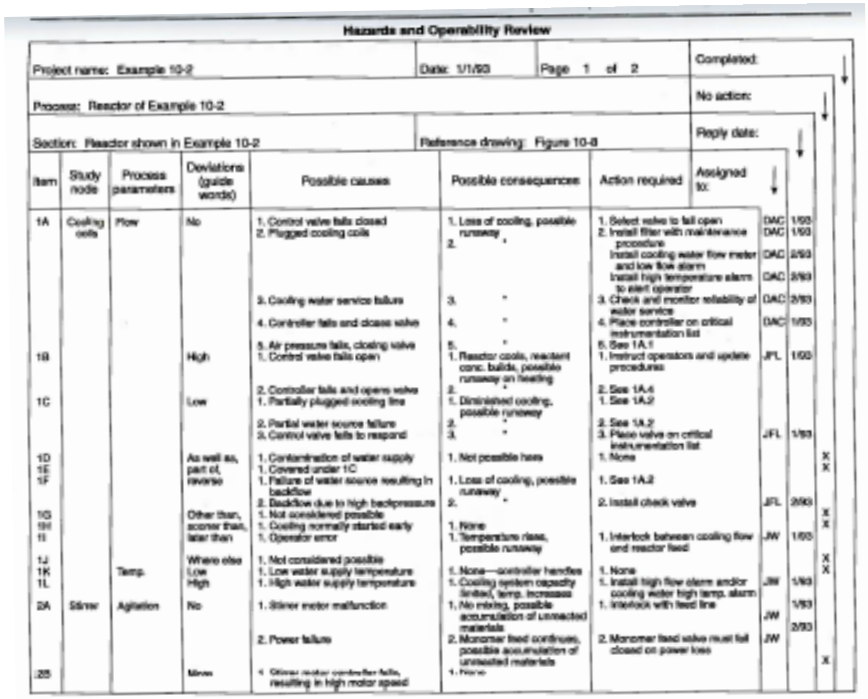


Figure 5-1 Characteristic plume formed by a continuous release of material.

HAZOP



Hazards and Operability Review

Project name: Example 10-2 | Date: 1/1/93 | Page 1 of 2 | Completed:

Process: Reactor of Example 10-2 | No action:

Section: Reactor shown in Example 10-2 | Reference drawing: Figure 10-8 | Reply date:

Item	Study node	Process parameters	Deviations (guide words)	Possible causes	Possible consequences	Action required	Assigned to:		
1A	Cooling coils	Flow	No	1. Control valve fails closed 2. Plugged cooling coils	1. Loss of cooling, possible runaway 2. "	1. Select valve to fail open 2. Install filter with maintenance procedure Install cooling water flow meter and low flow alarm Install high temperature alarm to alert operator	DAC DAC DAC DAC	1/93 1/93 2/93 2/93	
				3. Cooling water service failure	3. "	3. Check and monitor reliability of water service	DAC	2/93	
				4. Controller fails and closes valve	4. "	4. Place controller on critical instrumentation list	DAC	1/93	
				5. Air pressure fails, closing valve	5. "	5. See 1A.1			
1B			High	1. Control valve fails open	1. Reactor cools, reactant conc. builds, possible runaway on heating	1. Instruct operators and update procedures	JFL	1/93	
1C			Low	2. Controller fails and opens valve 1. Partially plugged cooling line	2. " 1. Diminished cooling, possible runaway	2. See 1A.4 1. See 1A.2			
				2. Partial water source failure 3. Control valve fails to respond	2. " 3. "	2. See 1A.2 3. Place valve on critical instrumentation list	JFL	1/93	
1D			As well as, part of, reverse	1. Contamination of water supply	1. Not possible here	1. None			X
1E				1. Covered under 1C					X
1F				1. Failure of water source resulting in backflow	1. Loss of cooling, possible runaway	1. See 1A.2			
1G			Other than, sooner than, later than	2. Backflow due to high backpressure 1. Not considered possible	2. " 1. None	2. Install check valve	JFL	2/93	X
1H				1. Cooling normally started early	1. Temperature rises, possible runaway	1. Interlock between cooling flow and reactor feed	JW	1/93	X
1I				1. Operator error					X
1J			Where else	1. Not considered possible	1. None	1. None			
1K		Temp.	Low	1. Low water supply temperature	1. Cooling system capacity limited, temp. increases	1. Install high flow alarm and/or cooling water high temp. alarm	JW	1/93	
1L			High	1. High water supply temperature	1. No mixing, possible accumulation of unreacted materials	1. Interlock with feed line	JW	1/93	
2A	Stirrer	Agitation	No	1. Stirrer motor malfunction	2. Monomer feed continues, possible accumulation of unreacted materials	2. Monomer feed valve must fail closed on power loss	JW	2/93	
				2. Power failure					
2B			More	1. Stirrer motor controller fails, resulting in high motor speed	1. None				X

Typical 4x4 Risk Matrix

Severity	Likelihood: Frequent	Possible	Rare	Remote
Major	Very High	Very High	High	Moderate
Serious	Very High	High	Moderate	Low
Minor	High	Moderate	Low	Low
Incidental	Moderate	Low	Low	Low

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