Purdue Process Safety & Assurance Center (P2SAC)

Overview

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Charles D. Davidson School of Chemical Engineering
Purdue University

December 4, 2024

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December 2024 Conference Registration

Sponsors

ACC – Am Chem Council
AcuTech
AMGEN
Corteva
CountryMark
Curia Global
Dow
Endress+Hauser
Evonik
ExxonMobil
Fauske & Associates
GSK
Honeywell
Johnson Matthey
Kenexis
Lilly
Pfizer
PSRG
SABIC
Safety&
Thermal Hazard Tech
Vertex

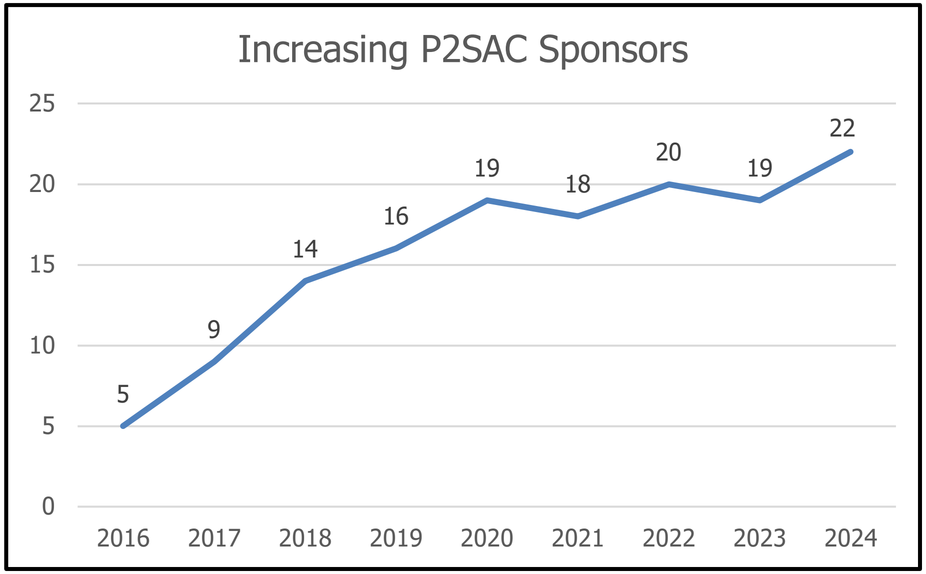
Guests

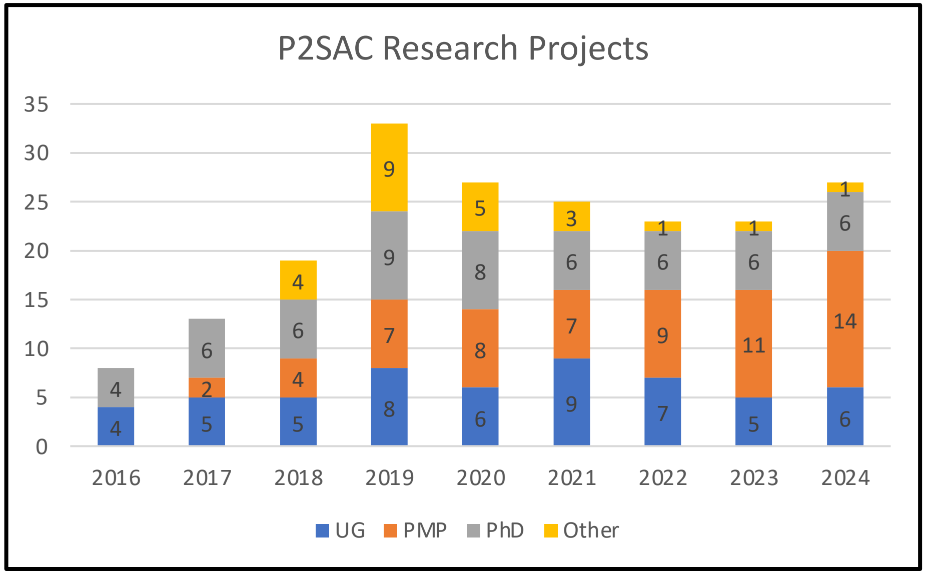
- CCPS
- Kiewit*
- Marathon Consulting
- Operational Sustainability*
- Safety Mgmt Group*
- Sandia Nat'l Labs
- Takeda*
- Univ of Illinois (UIUC)*

**denotes 1st meeting*

On-going dialog with other Depts:
ABE, CHEM, IE, IPPH & ME

Growing Industry Participation & Projects in P2SAC





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ChE Professional Masters Program

Program Growth: 9 students in ‘15 / ‘16 academic year to 62 in Fall 2024 (34% female; 81% int’l)

Placement: $86 - 90.5 k avg starting salary 2024, 94% placement within 6 mos

Seven areas **of** concentration: Energy Systems Fundamentals & Processes; Kinetics, Catalysis, and Reaction Engineering; Biochemical Engineering; Polymer Science and Engineering; Pharmaceutical Engineering; Gas and Petroleum Engineering; Data Science

Program completion in one year:

Students take 2 core courses; 3 electives in area of concentration; 3 in Management;

6 Credit hour Capstone project

Additional semester required for those without BS in chemical engineering

Capstone projects are typically suggested and led / mentored by industry

Students remain on campus with ~30-minute weekly call with industry mentor

+400 hrs of ‘free’ research

Typically, 1/3 –1 /2 of summer projects process safety related; 14 students and 11 projects this fall

Companies participating: Abbvie, AcuTech, Allergan, Amgen, Biotech, BP, Bristol-Myers Squibb, Chevron, Cook, Corteva, Dow, Evonik, ExxonMobil, Fauske, GSK, Johnson Matthey, Kenexis, Lilly, Marsh, Merck, Pfizer, Phillips 66, PSRG, Safety & Consulting, Shell, Siemens, Vertex, Whirlpool, 3M

~ 6 students in off-campus paid internships each semester

Intern companies include: Tesla, Bayer, Catalent, GSK, RiKarton Inc., Electric Hydrogen Co, Eurofins, Regeneron Pharm.

Spring & Summer ‘24 UG & Masters Process Safety Research Projects

Undergraduates

- Estimation of Decomposition Energies for Organometallic Materials Using TCIT – Johnson Matthey
- Continuation of molecular energetics modeling of molecules of interest to pharma industry including tetrazoles using CHETAH, TCIT & YARP - GSK, Vertex, ~6 pharmas
- Assessment of ChatGPT’s use in process safety - American Chemistry Council & PSRG
- Investigate whether a correlation exists between the laminar burning velocity and the LFL under known conditions - ExxonMobil

Professional MS

- Using Commercial AI Tools to Develop a HAZOP Augmentation and Automation Chatbot - Kenexis & Dow
- TCIT & YARP reaction modeling - GSK, Vertex, et al
- Kinetic modeling autocatalytic decomposition reactions – Amgen
- Dynamically Modeling High Pressure Releases for Complex Fire Suppression Systems - Fauske
- Determination of Common Root Causes of +300 Global Process Safety Incidents - Mentzer

Fall ‘24 UG & Masters Process Safety Research Projects

Professional MS Projects:

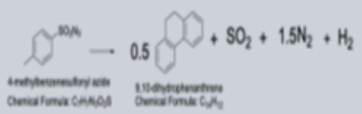
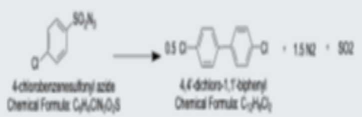
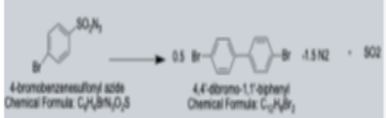
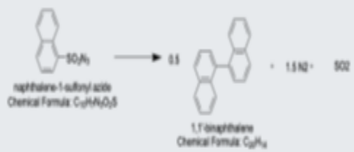
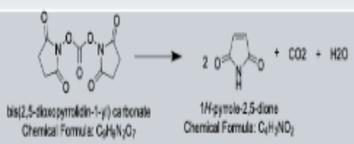
- Conducting Inherent Safety Design Studies Through AI-tool Integration - AcuTech
- Estimation of minimum safe gas purge rates for open vents and flares - ExxonMobil
- Comparison of predicted & experimental heats of decomposition for various reactions of interest to the pharmaceutical industry – GSK, Vertex, Amgen +3
- Estimation of Decomposition Energies for Organometallics – Johnson Matthey
- Advances in Management of Change in Hazardous Industries - Safety&
- Using Commercial AI Tools to Develop a HAZOP Augmentation and Automation Chatbot – Kenexis / Dow
- Ammonia as a Hydrogen Carrier - PSRG
- Site-specific decision trees for handling unstable materials – Evonik

- Two part-time PhDs & contract CS MS candidate engaged in NSF laboratory safety project since 2018

UG Projects:

- Use of Electrochemistry to Reduce Reactivity Hazards - Mentzer & Tackett
- Investigating Hazards Related to Carbon Sequestration and Storage - PSRG

Prediction of Heat of Reaction for Pharmaceutical Industry

REACTION	(% DIFF From Literature) CHETAH	(% DIFF From Literature) TCIT
	-36%	10%
	2%	9%
	8%	4%
	-15%	9%
	-15%	+15%

Project Aim

1. Accurately predict heat of reactions.
2. Develop robust computational methods.

Significance

1. Predict potential safety risks.
2. Predict reaction mechanisms and possible products.
3. Minimize experimental costs.

Participating organizations

Amgen, Corteva, GSK, JM, Lilly, Merck, Pfizer, Vertex

Computational Approaches

CHETAH

- Group additivity method
- Uses Benson group additivity principles
- Limited for complex structures
- SMILES input from ChemDraw

TCIT

- Quantum chemistry approach
- G4 data integration
- More comprehensive analysis
- Handles complex molecules
- SMILES input from ChemDraw

Compounds Tested:

•Sulphonyl Azide, NDSC

Key Findings:

•TCIT showed < ± 20% average error for DI-azo reactions.

Limitations:

•Neither TCIT nor CHETAH supports ionic or free-radical group analysis

Strategic Trajectory

- Expand methodology comparisons across diverse reaction types.
- Continue to enhance TCIT decomposition prediction capabilities.

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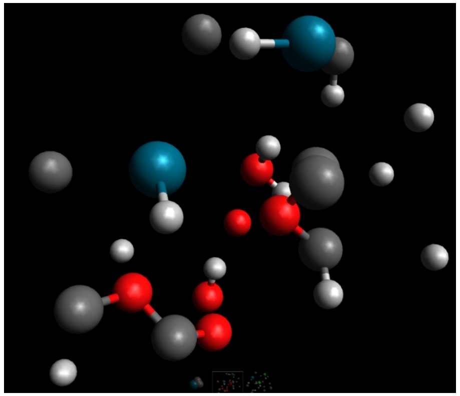
Estimation of Decomposition Energies of Organometallic Compounds

(w/Johnson Matthey)



Objective

Predict decomposition energies for organometallic complexes using advanced computational tools, validated against experimental data.

Experimental Data

Experimental data was sourced from industry-standard DEKRA reports, providing data for palladium complexes and phosphine ligands.

Computational Tools

Thermochemical Intensity Theory (TCIT), quantum chemical inputs (e.g., G4 data) with thermochemical datasets. Applied to calculate gas-phase heats of formation and sublimation enthalpies.

*CHETAH (ASTM Licensed), e*stimates thermodynamic properties based on Benson groups.

*Density Functional Theory (DFT), u*sed for geometry optimization and single-point energy calculations. Challenges with large ligands like palladium-phosphine complexes.

Modeled compounds primarily with ChemDraw, but used Avagadro for more complex structures

Analysis

Modeled: phosphine ligands (e.g., PPh3, PCy3, AmPhos, and JohnPhos) and their corresponding palladium complexes.

Sublimation enthalpies were integrated into gas-phase predictions to refine energy estimations.

Conclusions

TCIT predictions aligned closely with experimental data for most compounds, particularly PPh_3 & Pd complexes (<5%). High error (~56%) for PCy_3 attributed to deviations in sublimation enthalpies.

CHETAH exhibited significant underestimation for complex structures like AmPhos & JohnPhos.

Conducting Inherent Safety Design Studies through AI-Tool Integration

ISD Strategies

Implement strategies like Minimize, Substitute, Moderate, and Simplify to proactively reduce hazards at the design stage, ensuring safer and more sustainable processes.

Process Data and Regulatory

Regulatory guidelines and process safety datasets are used to align the ISD implementation with industry standards and compliance requirements.

ISD implementation with AI-Tool

Integrate AI tools to automate hazard analysis and provide actionable ISD recommendations, enhancing the efficiency and accuracy of safety evaluations.

Result Data Refining

Refine raw data from AI outputs to extract meaningful insights, ensuring clarity and applicability in decision-making processes.

Process and Hazard Wise Segregation

Categorize hazards and processes to prioritize ISD strategies effectively, focusing on critical areas with the highest risk potential.

ISD Brainstorming Session

Conduct collaborative sessions with stakeholders to evaluate AI-generated ISD recommendations and adapt them for practical implementation.

Participating Organization: Acutech

- The Project aims to develop an AI-based tool to integrate Inherently Safer Design (ISD) principles for process safety management, automating hazard identification, risk evaluation, and decision-making.
- **Computational Approach**
  - AI-Driven Tool: Python backend with Flex API OpenAI GPT-4o for ISD-related process dataset analysis.
  - Interactive Interface: HTML-based UI for output and users to interact and review ISD strategy.
- **Strategic Outcomes**
  - Restricting Approach to ISD recommendations within the periphery of the Project and data.
  - Reduced Time and Increased Efficacy in Data Analysis.
  - A streamlined, redundancy-free approach to hazard recommendations ensures efficiency and impact.
- Quality and detail datasets significantly enhance the efficiency and accuracy of AI-driven ISD recommendations, enabling more robust, actionable, and context-specific safety strategies.
- **Next Steps:** The analysis and integration of diverse real-time datasets to enable continuous refinement and optimization of safety strategies, enhancing the precision and adaptability of AI-driven ISD recommendations to address evolving risks effectively.

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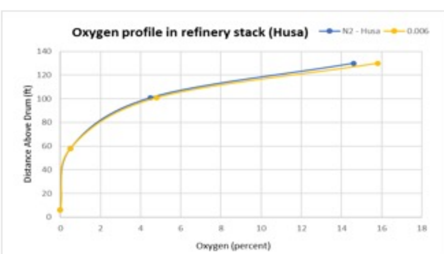
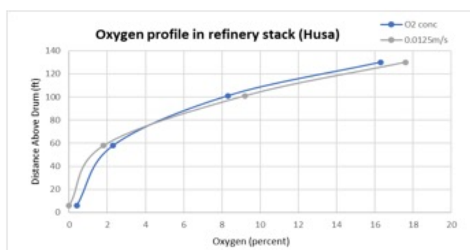
Simulating Oxygen Displacement in Flare Stacks Using CFD – (w / ExxonMobil)

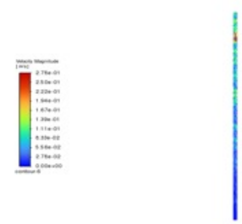
- CFD simulations were conducted using ANSYS Fluent to analyze oxygen displacement in flare stacks under varying conditions of purge gas compositions and velocities, originally studied by Husa (1964).
- The simulations revealed discrepancies in Husa's predicted purge gas velocities. For some gases, the predicted velocities were overestimated, while for others, they were underestimated. Conclusions were drawn by selecting velocities that matched the observed profiles from Husa's experiments for specific gases.
- When comparing the selected velocities to those predicted by the API RP 537 correlation, it was found that the chosen velocities closely aligned with the API standard's predictions. This suggests that the API correlation provides a more balanced estimation of purge velocities across different gases.
- To confirm the accuracy of the API standard across a broader range of conditions, further simulations are being conducted using additional gases, including hydrogen.



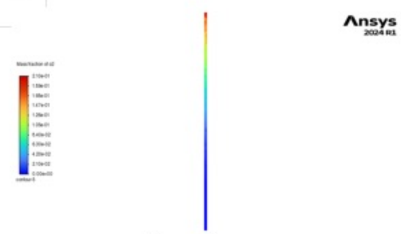
O_2 profile for N_2 as Purge gas



O_2 profile for Methane as Purge gas


Velocity contour

N_2 contour



O_2 contour

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Investigating Hazards Related to Carbon Sequestration and Storage (w / PSRG)

Objective: This project aims to identify and evaluate the risks and potential hazards associated with CCS technologies, as well as the safety protocols and technology used to mitigate risk.

CCS sites studied:

Project	Operator	Location	CO2 Source	Size Mt/yr	CO2 Sink	Status	Year(s)
Quest	Shell	Alberta	Steam-Methane	1.2	Saline	Operational	2015
Ketzin	GFZ	Germany	H2 Production	(Total 0.067)	Saline	Completed	2008-2013
Gorgon	Chevron	Australia	Natural Gas	3.4	Saline	Operational	2016
Decatur	MGSC	Illinois	Ethanol Production	(Total 1)	Saline	Completed	2011-2014
Citronelle	SECARB	Alabama	Carbon Capture	(Total .115)	Saline	Completed	2011-2014

Outlook: 43 sites are currently in operation, 33 under construction and 488 in various stages of development, corresponding to 50, 35 and 336 MTPA (million tons per annum) of CO2.

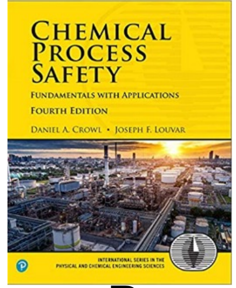
The risks associated with CCS involve loss of containment of CO2 once underground; during injection or post-injection. Potential areas of impact are the soil, underground drinking water, atmosphere & wildlife.

The factors that impact the safety of a site include: the cap rock, depth, porosity, permeability, proximity to faults and underground drinking water, and injection pressure.

Monitoring, Measurement, and Verification (MMV) technologies have been developed to improve safety of CCS sites, including pre-injection tests (e.g., seismic surveys, well bore logging) and measurements made during injection (e.g., downhole P & T gauges).

The main areas of concern or leakage pathways are: (1) man-made well seals (2) natural reservoir cap rocks (3) undiscovered faults and (4) small local permeability heterogeneities.

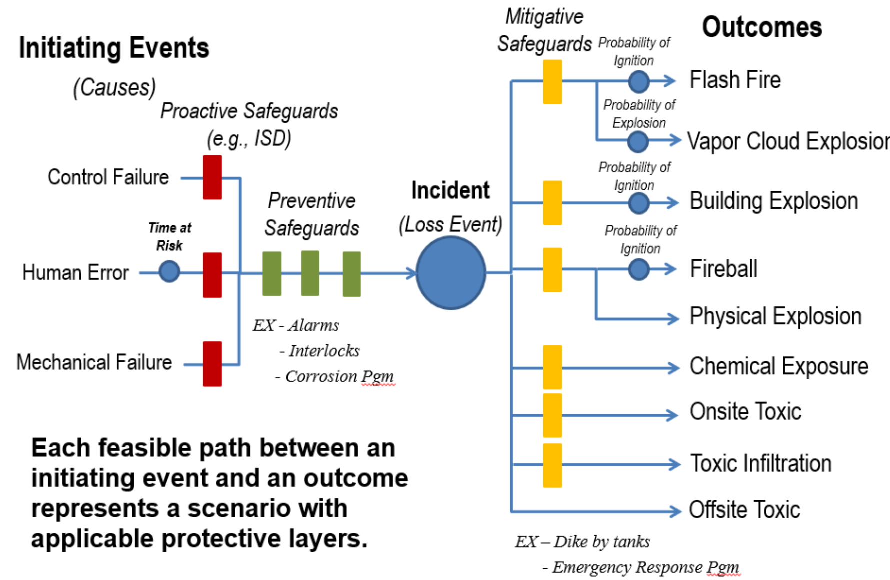
Conclusions: *The long-term stability and integrity risks of CCS are not fully understood. However, the overall safety of CCS relies largely on developing the correct site selection criteria, implementing appropriate MMV techniques, and the appropriate injection of CO2.*



Chemical Process Safety - Core Class

- Personnel vs. Process Safety
- 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
- Emergency Response

Bow-tie Diagram



Each feasible path between an initiating event and an outcome represents a scenario with applicable protective layers.

HAZOPs & Cyber Security

Threat	General Threat History	Specific threat history	Capability	Motivation/ Intent	Potential Actions	Overall Assessment	Threat Ranking
Cyber Attack	Previous cyberattacks like Triton, Maroochy water services breach, etc. have focused on targeting ICS components to cause significant physical and economic damages to the organization.	No history at this facility	Severe physical damage can be inflicted by cyber-attacks on the pressure controller (across TD-R), temperature controller (across TD-R and OLI-reactors) and the flow controller (TANK-1)).	Sophistication of cyber criminals is out stripping the ability to effectively counter the attacks, resulting in increased malicious events, loss of data and physical damage.	Malicious intent, personal enrichment, political or religious motivation.	The exposure to these proposed small remotely operated gas processing plants assets by cyberattack was evaluated by the team and determined within the next 10 years that the cyber-attack potential on these facilities will make this a 'Medium' threat.	Medium

Chemical Facility Anti-Terrorism Standards (CFATS) … and **Chemical Security …**

Threat Spectrum

Global Chemical and Biological Security

Benefits from Being P2SAC Sponsor

- Direct engagement in suggesting & selecting process safety research projects at all levels – PhD, PMP and UG.
- Priority in serving as mentor for process safety related Professional Masters Project of your choice.
- Attendance at biannual meetings to review research progress and learn from outside expert presentations.
- Sharing among companies of process safety learnings and challenges.
- Contact with students as they develop process safety expertise and enhance the science.

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JM Johnson Matthey Inspiring science, enhancing life
PSRG Process Safety and Reliability Group
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