

# Purdue Process Safety & Assurance Center (P2SAC)

## Overview

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# P2SAC

## Celebrates 10th Anniversary

Established 2014, **Purdue's Process Safety & Assurance Center** (P2SAC) began with a handful of company representatives and members of the Davidson School of Chemical Engineering's (ChE) Industrial Advisory Council. A decade later, P2SAC now hosts biannual conferences on Purdue's campus, with over a hundred registrants, 23 sponsor companies and a growing number of interested companies in attendance.

P2SAC serves as a nexus for advancing chemical process safety education and research. The focus is on specific industry safety sectors such as oil and gas, chemical, pharmaceutical and technological industries. P2SAC collaborates with industry partners via research, specialized courses and consultation to help contribute to improving safety standards worldwide.



# May 2024 Conference Registration

## Sponsors

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

## Guests

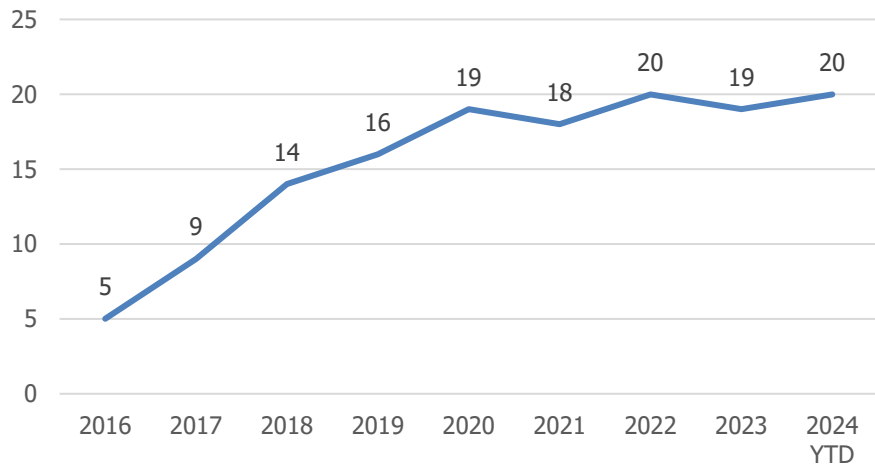
- Bristol Myers Squibb
- CCPS
- Gilead
- Grace
- Marathon Consulting\*
- Merck
- Operational Sustainability\*
- PHMS\*
- Scitegrity\*
- Spark Cognition\*
- Thermal Hazard\*
- Toellner Consulting\*

*\*denotes 1<sup>st</sup> meeting*

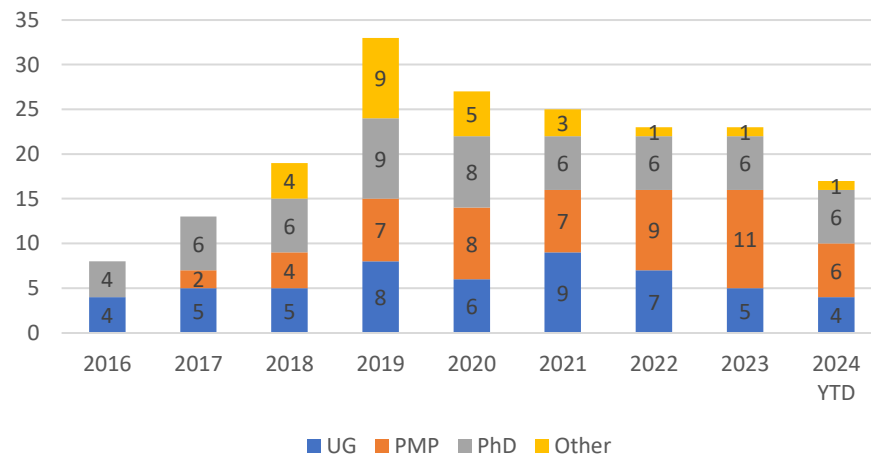
On-going dialog with other Depts:  
ABE, CHEM, IE, IPPH & ME

# Growing Industry Participation & Projects in P2SAC

## Increasing P2SAC Sponsors



## P2SAC Research Projects



# ChE Professional Masters Program

Program Growth: 9 students in '15 / '16 academic year to 51 in Fall 2023 (33% female; 90% int'l)

Placement: \$82-86k avg starting salary 2023, 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

Companies participating: Abbvie, AcuTech, Allergan, AMGEN, Biotech, BP, Bristol-Myers Squibb, Chevron, Cook, Corteva, Dow, Evonik, ExxonMobil, Fauske, Fresenius Kabi, GSK, Kenexis, Lilly, Marsh, Merck, Pfizer, Phillips 66, 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.

# 2023 / 2024 AY Professional MS Research

- Correlating Flammability Limits to Laminar Burning Velocity – **ExxonMobil**
- Is it time to introduce Virtual Logic Solvers in the Process Industry – **Honeywell**
- Estimation of Decomposition Energies for Organometallic Materials – **Johnson Matthey**
- Design of a detonation trap in liquid handling service of a Reactive Nitro-Organic; Toluene Ambient Air Analyzers – **SABIC**
- Using Commercial AI Tools to Develop a HAZOP Augmentation and Automation Chatbot - **Kenexis**

# 2023 / 2024 AY Undergraduate Research

Heats of reaction for some common reaction types in pharma industry & comparison with TCIT & CHETAH predictions; on-going ~3 years - **8 cos**

Prediction of Gas Evolution in Common Reaction Solvents with ASPEN; continuation of PMP - **GSK, Amgen & Lilly**

Hazards & risks associated with proposed H<sub>2</sub>, NH<sub>3</sub>, ... CO<sub>2</sub> pipelines – **ExxonMobil & BP**

Use of AI for process safety studies – **PSRG** and Profs Li & Bernal

Summarize AI process safety related techniques and develop training materials for industry – **ACC** and Profs Li & Bernal

Assessment of ChatGPT's use in process safety - **ACC & PSRG** and Prof Li

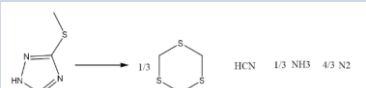
Investigate whether a correlation exists between the laminar burning velocity and LFL under known conditions - **ExxonMobil**

Estimation of Decomposition Energies for Quaternary Amines Using TCIT – **Johnson Matthey**

# Predicting Heats of Reactions Common In Pharma Industry – UG / PMP

- Project uses experimental reaction data from pharmaceutical companies, including Amgen, Corteva, GSK, JM, Lilly, Merck, Pfizer, and Vertex to compare with predictions of:
  - CHETAH – widely used, licensed by ASTM since 1974, based on Benson groups
  - TCIT – novel Purdue methodology, combines quantum chemistry & G4 data
  - YARP – new Purdue methodology, generates potential decomposition products without any user provided reaction data
- Programs calculate the heat of rxn when given the molecular structures in SMILES string format, generated through ChemDraw
- Study included: decomposition reactions for various tetrazole based compounds in TCIT and CHETAH, 1H-tetrazole and methyl tetrazole decompositions in YARP
  - CHETAH cannot handle SMILES string for any tetrazole compound, tetrazoles modeled manually using Benson groups
  - 8 different tetrazoles studied
- Sample reactions shown below
- CONCLUSIONS:** TCIT calculations have an average 20 % error; Overall TCIT results were better than CHETAH heat of reaction results; neither method can currently handle ionic and free-radical groups. YARP successfully predicted expected products for 1H tetrazole and methyl tetrazole
- NEXT STEPS:** continue with TCIT & CHETAH comparison for different reactions, use of YARP to predict decomposition products

Reaction	Measured $\Delta H_{rxn}$ (kJ/mol)	CHETAH $\Delta H_{rxn}$ (kJ/mol)	TCIT $\Delta H_{rxn}$ (kJ/mol)	% DIFF CHETAH	% DIFF TCIT
1H-tetrazole $\rightarrow$ HCN + 1/3 NH <sub>3</sub> + 4/3 N <sub>2</sub>	-160.5	-232.98	-208.91	45.16	30.16
Methyl Tetrazole $\rightarrow$ CH <sub>3</sub> CN + 1/3 NH <sub>3</sub> + 4/3 N <sub>2</sub>	-242.07	-228.59	-201.24	5.56	16.87
5- (methylthio)-1H tetrazole	-156.33	-217.35	-187.9	39.03	20.19

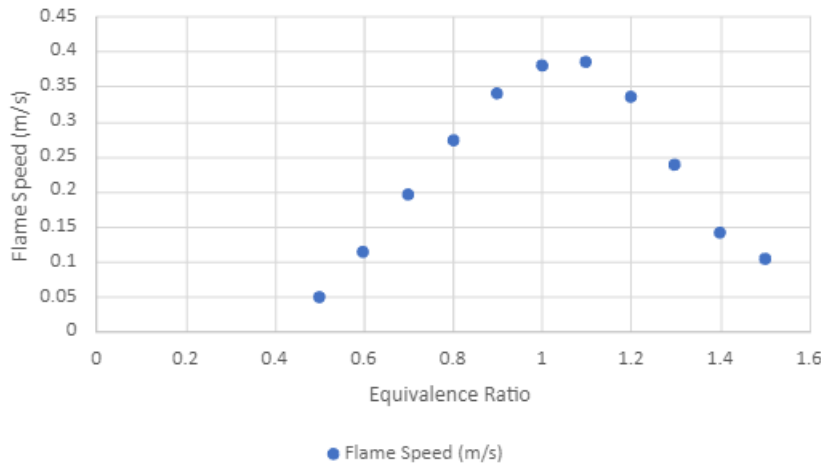




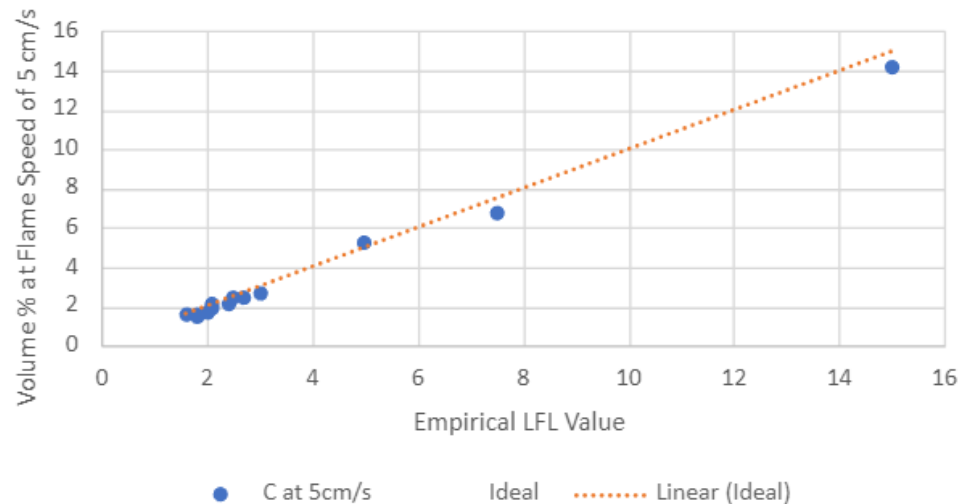
# Correlating Flammability Limits to Laminar Burning Velocity – UG (w / ExxonMobil)

- Python combustion program developed by ExxonMobil allows for determination of laminar flame speed for given temperature, pressure, and composition of fuel
- Compositions were found for flame speed choices (2,4,5 cm/s) and were compared to the LFLs for 13 species at ambient conditions. The flame speed that predicted LFLs most correctly was chosen as ideal flame speed (5 cm/s). At this choice, compositions only deviated by roughly 8.5% per species from their LFL.
- Similar process was conducted at elevated pressure (up to 10 bar) with 3 species due to more limited empirical data

Flammability Graph for Methane-Air Fuel at Ambient Conditions



Flame Speed of 5 cm/s at Ambient Conditions



US LFL (Methane)	Volume % at 0 cm/s (model LFL)	Vol % at 2 cm/s	Vol % at 4 cm/s	Vol % at 5 cm/s
5	4.223	4.517	5.063	5.267

# AI in Mechanical Integrity

Mentors – ACC, PSRG, Kenexis

Systems studied: ChatGPT + GPT-builder, Gemini

## Study included

- Literature review of current AI applications in mechanical integrity
- Building a GPT model to answer mechanical integrity related questions (e.g. failure modes, preventive maintenance tasks)
- Training it with sample plants to extract process safety advice

## Conclusions

- Can perform well for materials of construction
- Adequate for failure modes, root cause analysis and preventive maintenance tasks

## Next steps

- Modify ChatGPT API (coding experience required)
- Explore quantitative AI models
- Generate synthetic data to train the model

Ten publicly available CSB Reports relating to mechanical integrity were fed to train ChatGPT. **Dialog:**

*There were a series of explosions at a refinery. What are the possible root causes of this incident?*

ChatGPT ...

*What type of mechanical integrity failure could have occurred?*

ChatGPT

‘Mechanical integrity failures in a refinery setting can occur due to a variety of reasons, often related to the physical condition and operational capabilities of equipment and structures. Here are some common types of mechanical integrity failures that could lead to serious incidents, including explosions: **Corrosion; Erosion; Fatigue; Creep; Stress Corrosion Cracking (SCC); Hydrogen Induced Cracking (HIC); Brittle Fracture; Improper Material Selection or Installation; Weld and Joint Failures; Overloading and Overpressurization:**

Preventing these types of mechanical integrity failures requires a robust maintenance and inspection program, proper material selection, design according to industry standards, and adherence to operational limits. Regular inspections, testing, and monitoring are essential to identify and mitigate the risks associated with mechanical integrity issues.’

*Could you be even more specific?*

ChatGPT ...

# Chemical Process Safety - Core Class

## 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

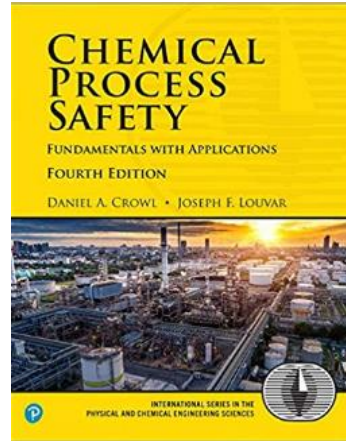
Chemical Reactivity

Relief System Design

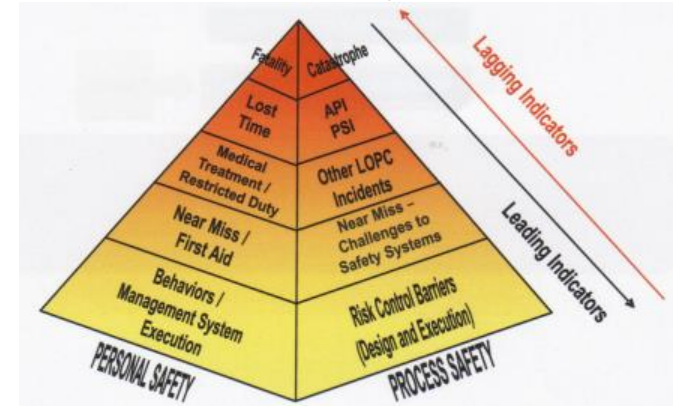
Hazards Identification (HAZOP, ..)

Risk Assessment (Matrix, QRA, ..)

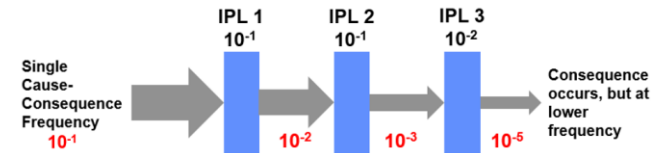
Accident Investigations



## Process Safety Metrics



## LOPA Frequencies



## Typical 4x4 Risk Matrix

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

## HAZOP

Node # \_:

Design Intent:

Parameter	Guide Word	Deviation	Causes	Consequences	Recommendations

# 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.



# P2SAC Sponsors



*Lilly*

**AMGEN**

**Honeywell**



**KENEXIS**



**FAUSKE**  
ASSOCIATES, LLC



**curia**

**AcuTech**  
PROCESS RISK MANAGEMENT

سابك  
*sebic*



**CountryMark.**

**Endress+Hauser**  
People for Process Automation



**American  
Chemistry  
Council**

**ExxonMobil**

**JM Johnson Matthey**  
Inspiring science, enhancing life

**PSCG**  
Process Safety and Reliability Group