# Purdue Process Safety & Assurance Center (P2SAC)

# Overview


**Ray A. Mentzer**

**Professor of Engineering Practice**

**Associate Director, P2SAC**

Charles D. Davidson School of Chemical Engineering

Purdue University


*December 2, 2025*

# December 2025 Conference Registration

## **Sponsors**

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

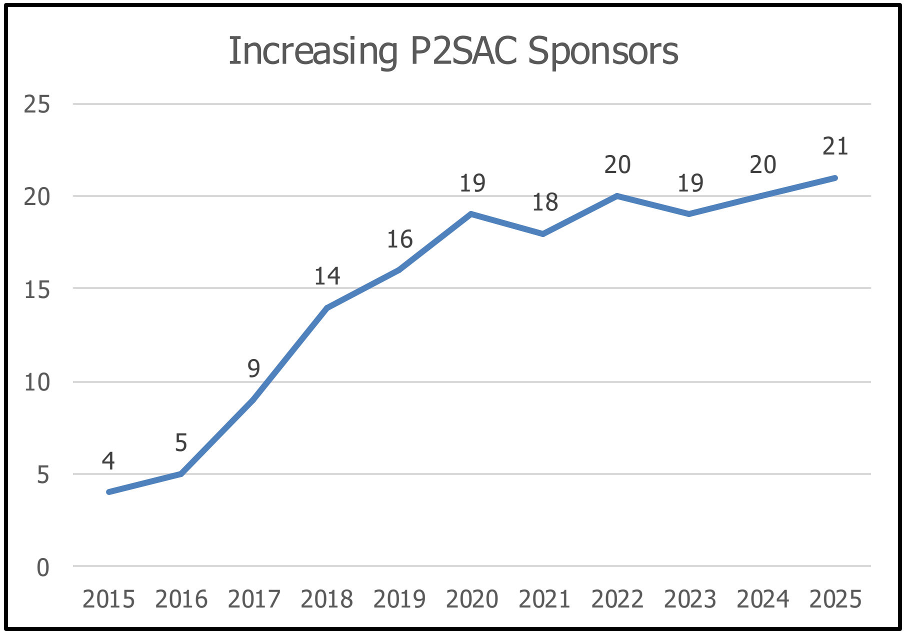
## **Guests**

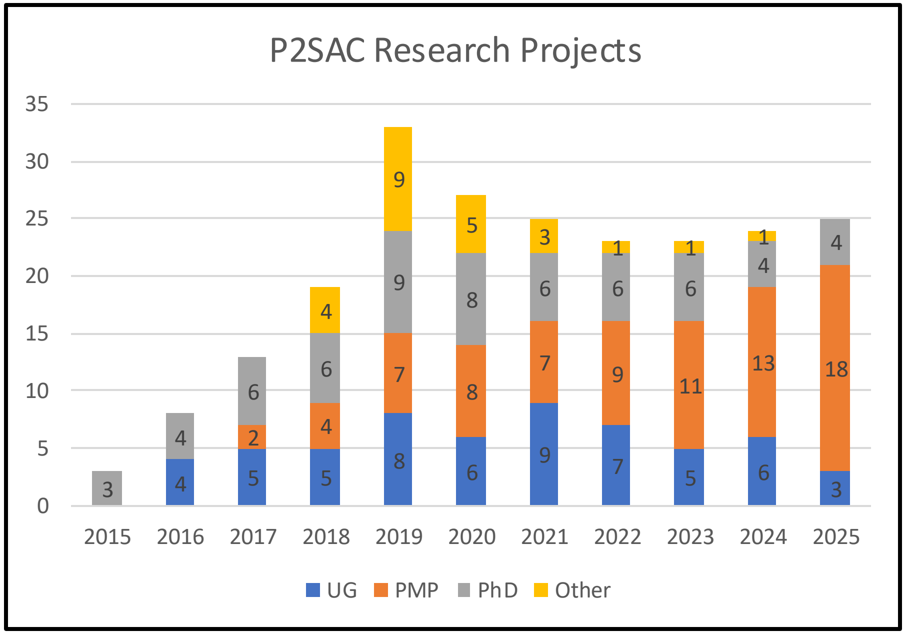
- AI-PSM*
- Baker Risk
- Cargill*
- Cummins
- Curia Global
- DEKRA
- Jensen Hughes
- Marathon Consulting
- Rolls Royce*
- Shell

**denotes 1st meeting*

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

# Growing Industry Participation & Projects in P2SAC



# Fall ‘25 Masters & UG Process Safety Research Projects

## Fall PMP Projects

Reactive Hazard Assessment Survey; Pharma, Chem & O&G - Lilly / Shell / Dow

Process Safety Assessments of Small to Medium Size Companies – PSRG

Pharma reactive chemistry modeling using CHETAH & TCIT; Part XIIII – Amgen, Vertex, Lilly, GSK, Pfizer, Merck …

Use of ChatGPT in a private cloud as a tool for inherent safety studies, HAZOPs, and other PHA methodologies; Part III – AcuTech

## UG Projects

Analysis of national oil companies by size & process safety performance, focusing on PEMEX incident history – (Prof Mentzer); fall

Continuation of prior projects to model heats of reaction of organometallics using TCIT software, Part VI - Johnson Matthey; fall

Use of Electrochemistry to Reduce Reactivity Hazards (Profs Tackett & Mentzer)

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# Summer & Spring ‘25 Masters Process Safety Research Projects

Spring PMP

- Heats of reaction for some common reaction types in pharma industry & comparison with CHETAH & TCIT predictions; Part XII; on-going ~5 years: w / 7 cos
- Estimation of minimum safe gas purge rates for open vents & flares – ExxonMobil
- Estimation of decomposition energies for organometallics & amine salt materials; Part IV – Johnson Matthey
- Management of Change – Safety & Consulting Associates
- Using Commercial AI tools to develop a HAZOP Augmentation & Automation chatbot – Kenexis & Dow
- Ammonia as a hydrogen carrier – PSRG
- Site specific decision trees for handling unstable materials, Part I - Evonik
- Improving the process of conducting inherent safety studies for safer technologies and alternatives analysis, Part I – AcuTech

Summer PMP projects

- Heats of rxn using CHETAH & TCIT; Part XIII – Amgen, Vertex, et al
- Organometallic combustion modeling using TCIT; Part V – Johnson Matthey
- Operator Competency – Safety & Consulting Associates
- Site-specific Decision Trees, Part II – Evonik
- Conducting inherently safer design studies, Part II - AcuTech

# Designing a Scalable Process Safety Performance Measurement System for Companies at Different Stages of Process Safety Maturity

**_Why_**

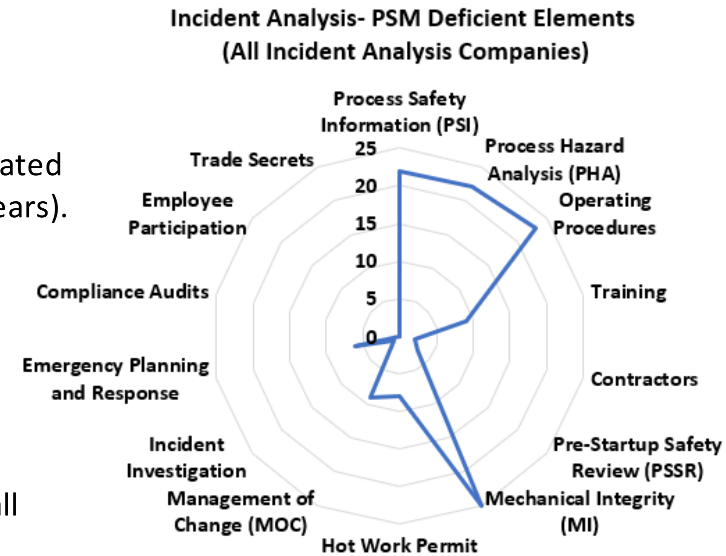
- ➢Reactive safety culture focused on compliance, not performance.
- ➢Fragmented data and inconsistent metrics across sites.
- ➢Repeat shortcomings in PSI, PHA, MI and OP.
- ➢The spider chart depicts the no. of companies that experienced incidents associated with failures in respective PSM element (Analyzed 30 CSB incidents from past 3 years).

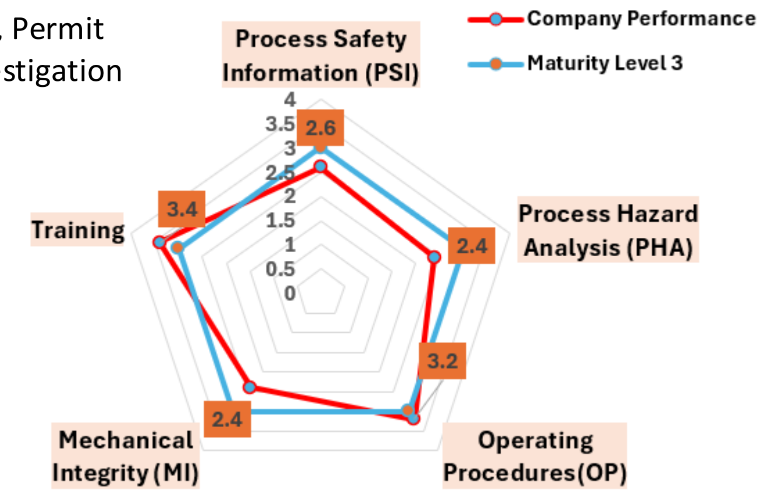
**_How_**

- ➢Our Solution: The Process Safety Performance Measurement System.
- ➢Integrates global best practices into a single measurable system.
- ➢Use leading + lagging indicators to quantify performance.
- ➢Build a single integrated framework across 10 key process safety elements.
    - ❑5 elements from OSHA 3908-03 2017 Process Safety Management for Small Businesses (PHA, PSI, Training, MI and Compliance Audits).
    - ❑5 elements from CSB incident investigations, RBPS and OSHA (MOC, OP, Permit System & Safe Work Practices, Contractor Management and Incident Investigation & Learning.
- ➢Convert raw data from a site into comparable maturity scores.

**_What_**

- ➢Identify weak elements (e.g., PSI 2.6, PHA 2.4, MI 2.4).
- ➢Strengthen strong areas (e.g., Training 3.4, OP 3.2).
- ➢Prioritize actions for all elements below Level 3.
- ➢Move plants from "reactive" to predictive performance.




Overall Maturity Level of the Pilot Case Study

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***Track what's strong. Fix what's weak.***
***Transform compliance into measurable performance.***

# Prediction of Heat of Reaction for Pharmaceutical Industry

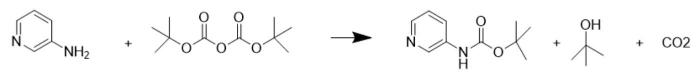
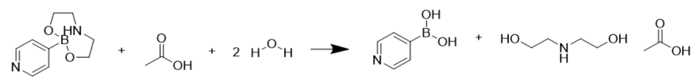
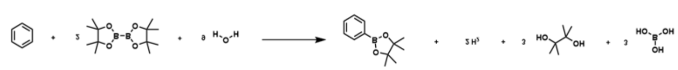
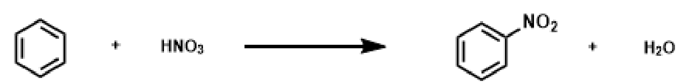
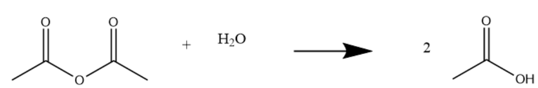
**Project Aim:**
Compare CHETAH and TCIT predicted ΔHrxn values with experimental data across diverse reaction types.

**Project Significance:**
1. Predict potential safety risk.
2. Improves accuracy of CHETAH and TCIT reaction predictions
3. Guides correct thermochemical methods for future modeling.

**Participating organizations:**
Amgen, GSK, Lilly, Merck, Pfizer & Vertex

**CHETAH:**
1. Group additivity method
2. Uses Benson Group principles
3. Limited for complex structures
4. SMILES input from ChemDraw

**TCIT:**
1. Quantum Chemistry Approach
2. G4 data integration
3. More comprehensive analysis
4. SMILES input from ChemDraw

| Reaction | Literature (kJ/mol) | CHETAH % Error | TCIT % Error |
|---|---|---|---|
|  | -17 | 63.64% | 325.76% |
|  | -12 | 789.89% | 15.41% |
|  | -112 | 206.16% | 0.58% |
|  | -263 | 43.2% | 347.14% |
|  | -56.6 | 1.9% | 1.68% |

**Key Findings:**
1. Gas-phase Benson groups (with correction) gave lower ΔHf error.
2. CHETAH and TCIT showed limitations with Boron and Nitro groups

**Strategic Trajectory:**
1. Expand comparison across more reaction classes to map limitations
2. Improve modelling for reactions involving charged species or missing Benson groups

# *Improving HAZOP Efficiency through AI Tool Integration*

## Participating Organization: AcuTech

**HAZOP Challenges**
Significant amount of manually entered information in traditional HAZOP studies, leading to time-intensive workflows and variable technical completeness.

**AI-Based Data Ingestion & Structuring**
Automated visual data extraction, data selection, and dataset creation using GPT-based tools to improve input quality and reduce manual effort.

**AI-Driven HAZOP Analysis**
Generation of preliminary deviations, hazards, and recommendations using AI models, enhancing the technical completeness of the study.

**Consequence & Scenario Development**
Building a dynamic consequence library, scenario-based outcomes, and analytics using historical and newly generated HAZOP datasets.

**HAZOP Review & Validation Session**
Conduct collaborative sessions with stakeholders to review AI-generated HAZOP data, validate extracted deviations and consequences, and refine outputs for practical use.

The Project aims to develop an AI-enabled tool to automate HAZOP data ingestion and selection, improving technical completeness and efficiency.

### Computational Approach

**AI-Enabled HAZOP Automation Tool:** Python-based backend using GPT models for visual data ingestion, and structured data generation to reduce manual effort

**Consequence & Scenario Engine**: Generates accurate, safety-aligned consequence outputs using rule-based logic applied to validated causes.

**Interactive Review Interface:** HTML-based user interface for uploading P&IDs, reviewing generated HAZOP outputs, and submitting corrected cause files for the second-stage consequence generation.

### Strategic Outcomes

**Improved Data Intelligence:** Expansion of data accuracy through the creation of a comprehensive consequence library, scenario-based consequence models, and structured analytics for historical HAZOPs.

**Advanced Hazard Insight & Knowledge Growth:** Long-term potential to identify recurring hazards, uncover missed deviations, and strengthen organizational understanding of emerging risk patterns.

### Current Status & Path Forward

- Core modules for equipment detection, cause generation, and consequence generation are completed and functioning reliably.
- Further improvements include refining the HAZOP output layout, expanding the consequence library, and enhancing speed and scalability for handling large batches of P&IDs.
- Generated HAZOP outputs are strong but still require safety-engineer review before use, so validation workflows and the User Interface will be further improved.
- These foundations position the tool for future capabilities such as advanced hazard insights and long-term learning from accumulated HAZOP data.

# Reactive Hazard Assessment

Mentors - Lilly, Dow, Shell

### *Objective:*

- To compare how Reactive Hazard Assessment (RHA) is conducted across academic, pharmaceutical, chemical, and petrochemical sectors - capturing definitions, tools, triggers, limitations, and documentation practices.

### *Approach to Achieving the Objective :*

- Conducted multi-phase stakeholder interviews across pharmaceutical, chemical, petrochemical, and academic research environments
- Mapped end-to-end reactive hazard assessment workflows - from prescreening→ scale-up → documentation
- Evaluated calorimetric testing platform including DSC, ARC, Phi-Tec systems, Easy Max, screening calorimeters, and sensitivity tests (impact, friction, ESD),
- Evaluated key references and resources such as Stossel, compatibility resources such as EPA, CRW, Bretherick's.
- Identified key drivers and constraints influencing RHA practices: personnel expertise, time availability, scale limitations, training depth, and data accessibility
- Identified information on prescreening and Advanced screening tools (DSC, ARC, etc.)

### *Next Steps:*

- Compare cross-industry risks - including dust explosibility, over-pressurization, chemical incompatibility, thermal - flammability behavior, and runaway reaction potential - to identify differences in hazard assessment practices

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## *Flow charts of RHA process for respective sectors*

**Lilly**

***Trigger Identified:*** Reactive functional groups / new chemistry / scale-up

↓

***Basic Screening:*** SDS → literature → internal guidelines → compatibility checks

↓

***Prescreening Tests :*** DSC → onset T → heat release → gas evolution

↓

***Advanced Quantitative Tools (If Flags) :*** ARC / RC-1 / TSU Evaluate kinetics, pressure rise, accumulation

↓

***Safety Controls & Scale-Up Decision:*** Cooling capacity / solvent selection / Addition rate control MOC

**Shell**

***Trigger Identified:*** Containment risk from large increases in pressure/temperature

↓

***Basic Screening:*** SDS → functional group check → Bretherick's → EPA/CRW tools (Literature as needed)

↓

***Prescreening Tests:*** Phi-Tec (pressure rise, heat release) Interpret yes/no for further study

↓

***Advanced Quantitative Tools (If Needed):*** ARC / VSP II with gas analysis Quantify exotherms & gas generation

↓

***Controls & Engineering Safeguards:*** Instrumentation (alarm and/or trip), designing relief systems

**Dow**

***Trigger Identified:*** New chemistry/ double/triple bonds / exothermic potential

↓

***Basic Screening:*** SDS → literature → internal literature (more trusted than SDS)

↓

***Thermal Screening:*** DSC → mixing calorimetry → TSU (pressure-enabled DSC) Check: onset T / rate / ΔH / gas evolution

↓

***Advanced Quantitative Tools:*** ARC / VSP II / Reaction Calorimetry Determine kinetics, runaway behavior, pressure limits

↓

***Controls & Engineering Safeguards:*** Define Controls & Safe Operating Window Cooling limits / accumulation analysis / solvent effects

**Purdue**

*based on interviews with Energetics Group

***Trigger Identified:*** new molecule, new formulation, energetic groups, unknown behavior

↓

***Basic Screening:***
- DSC (mandatory first test)
- Sensitivity tests: impact, friction, ESD

↓

***Secondary Assessment (If Needed):***
- DSC at different ramp rates (2–20°C/min)
- Compatibility tests (10°C & 120°C)
- Gas analysis only if expected

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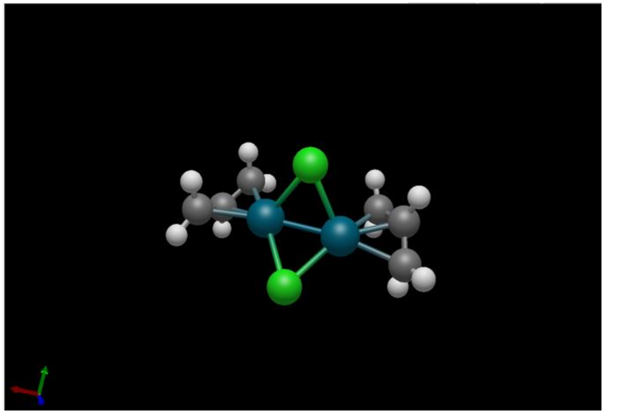
***Controls & Documentation:***
- Define limits (temperature, handling)
- Informal RHA Checklist template

# Estimation of Heat of Combustion of Organometallic Compounds

Mentor - Johnson Matthey



## Objective

Predict Heat of Combustion ($\Delta Hc$) for organometallic complexes using advanced computational tools and validate against experimental data.

## Experimental Data

-Experimental data was sourced from Johnson Matthey test results for Palladium, Ruthenium, and Iridium-based complexes.

-The NIST database has some experimental data for smaller metal oxides and chlorides, as well as a small amount of data for larger complexes.

## Computational Pathway:

-*Density Functional Theory (DFT),* used for geometry optimization and single-point energy calculations. Challenges with large ligands and unusual bonding geometries, but relatively inexpensive to run, yielding fast results.

-The Cambridge Structural Database (CSD) has experimentally-determined crystal structures for many organometallic complexes, and these were used as a starting point to skip the geometry optimization steps, when available.

-If unavailable, the molecules were drawn manually using Avogadro or Mercury and submitted for geometry optimization.

## Analysis

Modeled several Palladium, Ruthenium, and Iridium complexes, as well as metal chlorides and oxides (combustion products) to obtain heat of formation values.

Heat of Formation estimates were compared with those for predicted combustion products, allowing for direct estimation of $\Delta Hc$.

## Conclusions

-Iridium-containing compounds are particularly challenging and may require better baseline data before results are reliable.

-Palladium and Ruthenium-based compounds gave better results but differed from experimental values by up to 60%.

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# PEMEX Process Safety History

PEMEX

## Objective: Review of Process Safety Incident Rate Among Multi-National and Private Oil & Gas Companies

Scope:

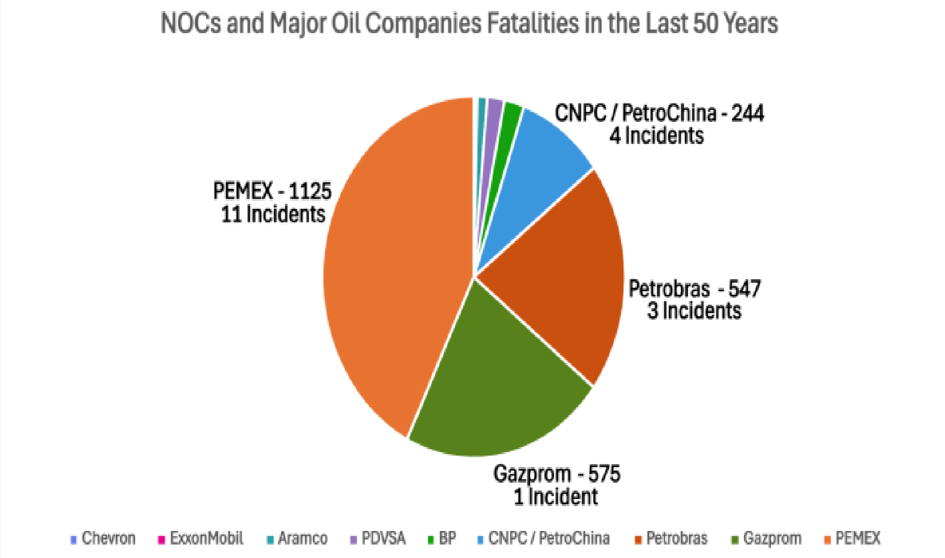
- National Oil Companies (NOCs): PEMEX, Aramco, CNPC, NIOC, Gazprom, PDVSA, Petrobras
- Major Oil Companies: Exxon, BP, Shell, Chevron

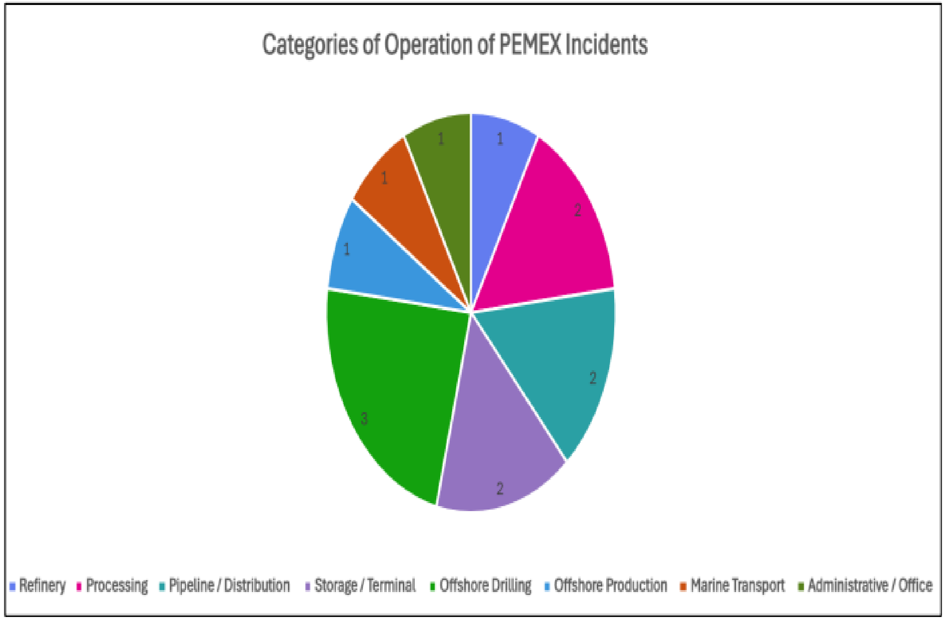
Process:

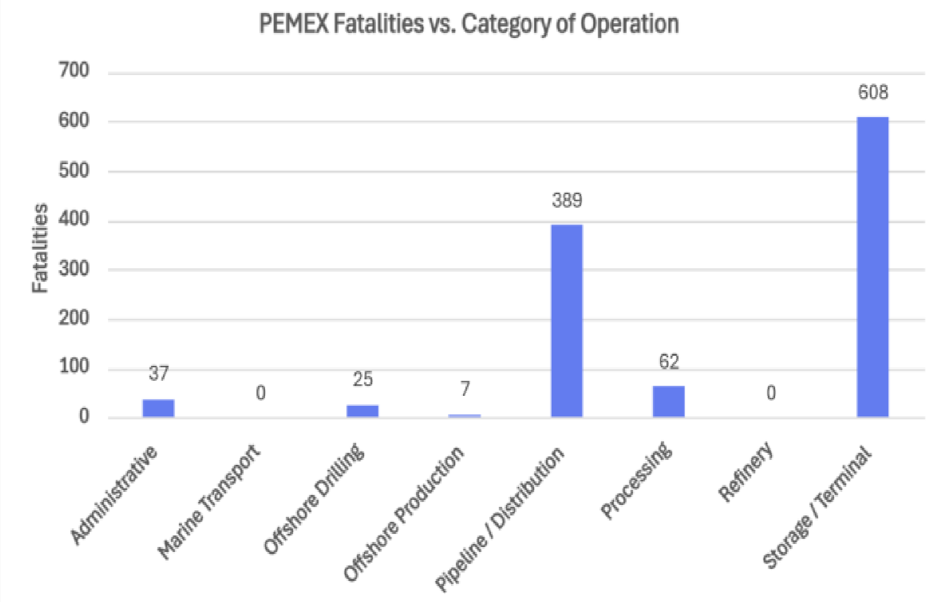
- Literature review for comparative analysis of companies
- Data collection and analysis of PEMEX incidents isolated and compared to other oil and gas companies
- Incidents defined using methodology incorporating fatalities, public/environmental impact, and operational/economic consequences

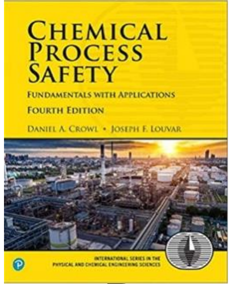
Conclusions:

- PEMEX has a history of repeated safety incidents
- Safety culture is lacking at PEMEX; not as high of a priority comparatively
- Repetition is due to poor administrative leadership
- Categories of operation that are more fatal include pipeline/distribution and storage/terminal
- Offshore drilling and pipeline/distribution have more frequent incidents



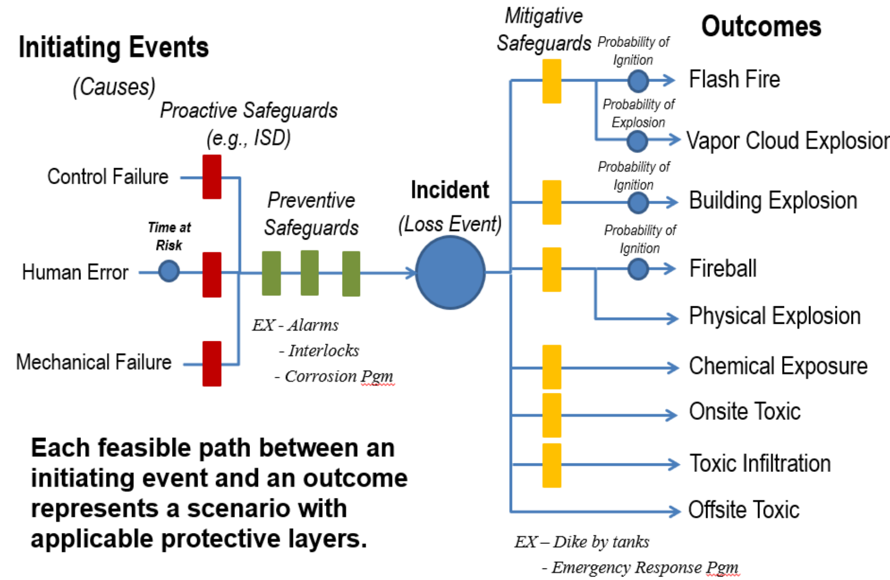






# Chemical Process Safety - Core Class

- 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.**

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


## 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 |

# P2SAC Corporate Sponsors

Lilly
AMGEN
Honeywell
DOW
VERTEX
KENEXIS
GSK
FAUSKE & ASSOCIATES, LLC
Pfizer
AcuTech PROCESS RISK MANAGEMENT
سابك sabic
CountryMark
CORTEVA agriscience
American Chemistry Council
ExxonMobil
JM Johnson Matthey
PSRG Process Safety and Reliability Group
EVONIK Leading Beyond Chemistry
Safety&
THT THERMAL HAZARD TECHNOLOGY
Takeda

# Process Safety Compliance Audits

Conduct Audit Every Three Years for OSHA PSM facilities; retain records of two most recent audits

Some companies have their own internal requirements beyond OSHA

Many considerations:

- internal or external auditors used
- how frequently; factors impacting (prior PSM score, hazards, size of operation, ...)
- composition and number on audit team, including duration (days, week, ...)
- what is audit based on ... Metric performance (Tier 1, ...), interviews, sampling of paperwork (e.g., work permits, MOC forms, ...)
- do you audit / assess each documented management system (14 OSHA elements, 20 CCPS, ...)
- how are scores calculated (e.g., 4 pt scale, with avg of 14 mgmt systems, ...)
- sharing and follow up on overall score (reviewed with VP, ... responsibility and timeline to close gaps)