

# SPRING 2021 CONFERENCE

## PURDUE PROCESS SAFETY AND ASSURANCE CENTER (P2SAC)

### Welcome and Overview



***Osman Basaran***

Burton and Kathryn Gedge Professor and  
Academic and Founding Director of P2SAC

Davidson School of Chemical Engineering/Purdue University

<https://engineering.purdue.edu/P2SAC>

# ROADMAP/GOALS

- The common purpose of the presentations that I will give at the start of each day is first and foremost to go over the agendas/programs
- At the start of the second day, I will:
  - Provide an overview of P2SAC to *new and long-standing industry members of the center* and *students*
  - Go over the PhD projects selected for funding
- My presentation will be short on the first day and even shorter on the third day

# CENTER MANAGEMENT

- **Osman Basaran**, Burton and Kathryn Gedge  
Professor of Chemical Engineering:  
Academic and Founding Director (AD) of P2SAC  
[obasaran@purdue.edu]
- **Ray Mentzer**, Professor of Engineering Practice:  
Executive Director (ED) of P2SAC  
[rmentzer@purdue.edu]
- **Web site:** <https://engineering.purdue.edu/P2SAC>

# EVOLUTION OF TWICE-A-YEAR P2SAC CONFERENCES

- The first conference (Fall 2014) and more than half a dozen subsequent conferences consisted of very full, one-day meetings
- We then introduced multi-day mini-conferences consisting of:
  - Regular safety mini-conference (to be held twice a year)
  - Safety in the pharmaceutical industry mini-conference (to be held at least once a year)
  - Flow assurance mini-conference (to be held once every couple of years or at most once a year)
- A set of tutorials lasting half a day were then added to the program in Fall 2019 (to be held twice a year)

**AGENDA FOR SPRING 2021 CONFERENCE**  
**PURDUE PROCESS SAFETY AND**  
**ASSURANCE CENTER (P2SAC)**  
*May 13, 14, and 17*

## Day 1—Thursday, May 13, 1:00-5:30 pm: Tutorials

- |           |  |
|-----------|--|
| 1:00-1:15 | <b>Osman Basaran</b> , Academic Director P2SAC: Welcome, opening remarks, and overview of the programs for the Spring 2021 conference(s) |
| 1:15-3:15 | <b>Robert Bellair</b> , Flammability Leader, Dow:<br>Flammable ambiguity: challenges in flammability testing and application             |
| 3:15-3:30 | <b>Break</b>   |
| 3:30-5:30 | <b>Katie Mulligan</b> , Reactive Chemicals SME, Dow:<br>Practical applications, extensions and limits of reactive chemical testing tools |

**Day 2—Friday, May 14, 12:00-5:30 pm:**  
**General safety and assurance mini-conference**

12:00-12:15      **Osman Basaran**, Purdue: Opening remarks and welcome

12:15-12:45      **Ray Mentzer**, Purdue: Opening remarks and overview

- 12:45-1:15      **Kathy Shell**, aeSolutions and **Jaidev Amrite**,  
Sparkcognition: Put artificial intelligence and machine  
learning to use today to increase reliability and reduce  
incidents
- 1:15-1:45      **Vilas Pol**, Purdue: General talk on batteries and  
battery safety
- 1:45-2:15      **Elizabeth Rosene**, Purdue (UG): Organizational health-  
a new methodology and survey for measuring [project  
done in collaboration with ACC & Marsh]
- 2:15-2:45      **Sarah Eck**, Dekra: Truck unloading-human  
performance
- 2:45-3:00      Break



2:45-3:00	Break
3:00-3:30	<b>Tekin Kunt</b> , PSRG: Common cause failures – awareness and mitigation
3:30-4:00	<b>Abhijit Talpade</b> , Purdue (PhD candidate) and <b>David Moore</b> , AcuTech: Analysis of cybersecurity risks of proposed remote CISTAR facilities
4:00-4:30	<b>Wahid Wakil</b> , Smith & Burgess: Commonly missed overpressure scenarios in relief device sizing
4:30-5:00	<b>Jim Klein</b> , ABS Group: Sustaining effective process safety programs
5:00-5:30	<b>Xinyu Zhen</b> , Purdue (PMP graduate): Safety shower and eyewash systems - best practices

**Day 3—Monday, May 17, 12:00-5:15 pm:**  
**Mini-conference on safety and assurance in**  
**pharmaceutical and reaction engineering**

12:00-12:05      **Osman Basaran**, Purdue: (A very short) welcome

12:05-12:30      **Ray Mentzer**, Purdue: Introductory/opening talk

12:30-1:00	<b>Anthony Janes</b> , GSK: Predicting the fire and explosion properties of early phase active pharmaceutical ingredients
1:00-1:30	<b>Jeffrey Sperry</b> , Vertex: Assessing explosive properties of temozolomide (TMZ)
1:30-2:00	<b>Min Sheng</b> , Corteva: Heat loss in accelerating rate calorimetry (ARC) analysis and thermal lag for high self-heat rates
2:00-2:30	<b>Raj Gounder</b> , Purdue: General talk on catalysis and prevention through design (PTD)
2:30-2:45	Break

2:30-2:45

Break

2:45-3:15

**Brett Savoie**, Purdue: General talk on reactivity and property prediction using computational chemistry

3:15-3:45

**Caitlin Justice**, Purdue (UG): Comparison of computational models and experimental data for some reactions common to pharma industry (outcome of collaboration between six P2SAC cos and B. Savoie)

- 3:45-4:15      **Pushkar Ghanekar**, Purdue (PhD candidate):  
Promoting a safe laboratory environment using the reactive hazard evaluation and analysis compilation tool (RHEACT)
- 4:15-4:45      **Ayman Allian**, Lilly: How pharmaceutical companies are working together to make their facilities and the world safer
- 4:45-5:15      **Brittany Armstrong**, Merck: Process safety assessment of a diborane-generating reaction for pilot plant scaleup

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- **We hope that the Fall 2021 Conference (12/21) will be in-person!**

# WHAT IS P2SAC?

- P2SAC is an academic research center that is based in the Davidson School of Chemical Engineering at Purdue University.
- P2SAC was conceived in 2013 and launched in 2014 by Professor Osman Basaran who is the Academic and Founding Director of the center (henceforward the AD).
- Dr. Ray Mentzer joined the center as Executive Director (ED) in 2016.
- P2SAC is focused on problems that fall in the large subject of safety and process and/or product assurance (hence the name the *Purdue Process Safety and Assurance Center, P2SAC*).
- Approach adopted at P2SAC, while **driven by problems in industry**, is **research-based**. P2SAC is not involved in critically important but more applied safety issues, e.g. training of first responders.
- P2SAC is almost entirely funded by membership fees paid by its industrial member companies or sponsors.

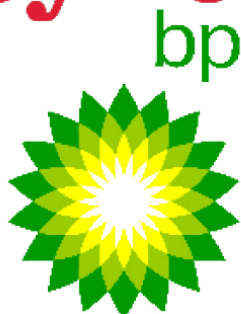
# CURRENT INDUSTRIAL MEMBERS/SPONSORS\*

**Honeywell**

**FAUSKE**  
& ASSOCIATES, LLC

**gsk**

**Pfizer**



**Chevron**

**3M**

**Lilly**

**AMGEN**

**MARSH**



**سابك**  
**sabik**

**DOW**



**CountryMark®**

**AcuTech**  
PROCESS RISK MANAGEMENT

**KENEXIS**

**Endress+Hauser**

People for Process Automation

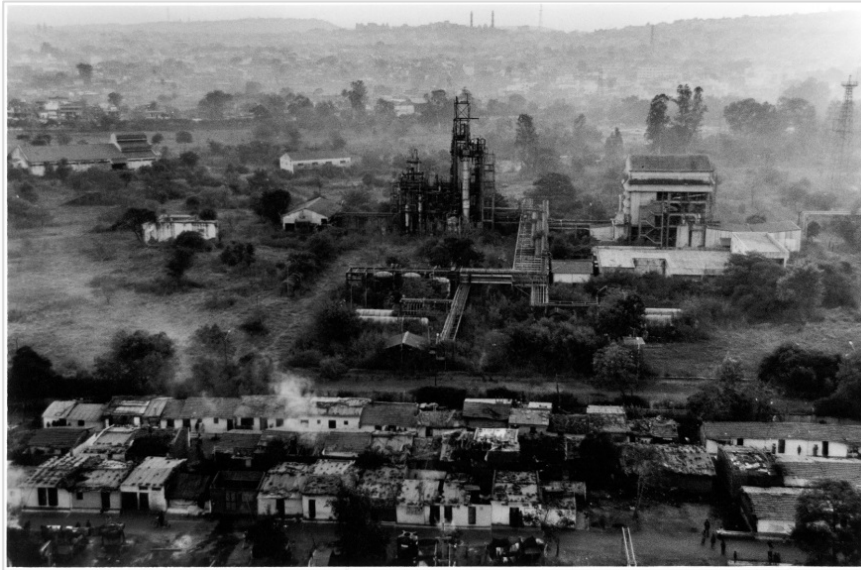


**CORTEVA**  
agriscience

\*The center's Advisory Board also includes **Air Products** and The National Institute for Occupational Safety & Health (**NIOSH**).



# PURDUE PROCESS **SAFETY** & ASSURANCE CENTER (P2SAC)



**Bhopal, India (1984):** At least 3,787 and over 16,000 claimed fatalities



**West Pharmaceuticals, NC (2003):** 6 fatalities



**BP Texas City (2005):** 15 fatalities

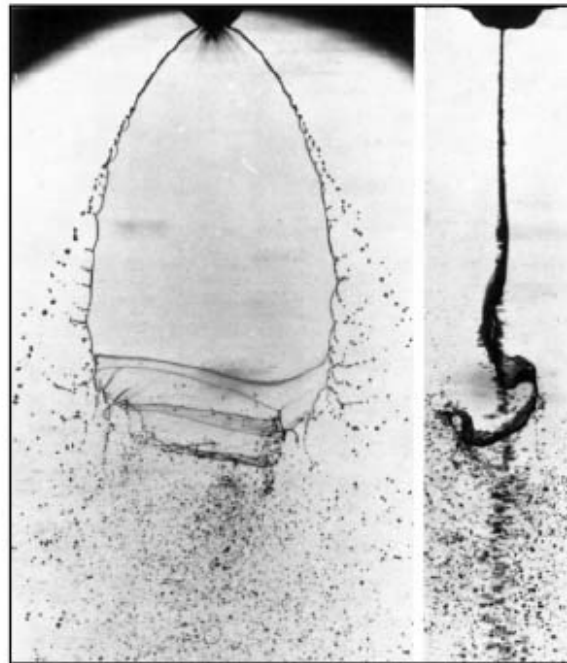


**Imperial Sugar, Georgia (2008):** 14 fatalities

# WHY **ASSURANCE**? SPRAY DRIFT EXAMPLE FROM CROP SPRAYING OR CROP PROTECTION



Liquid sheet from a fan spray nozzle  
(Crapper et al. JFM 1973; Villermaux  
ARFM 2007, Altieri and Cryer 2018)



**Small drops are undesirable because they lead to drift** (Basaran group research funded by Corteva).  
**Mystery: modern spray solutions do not disintegrate like pure fluids! Why?**



Spray drift is the most common cause of off-target movement of chemicals (e.g. pesticides) in crop spraying. It can injure or damage plants, animals, the environment or property, and even affect human health. “Drift” is the airborne movement of agricultural chemicals as droplets, particles or vapor.



# SAFETY

**Texas Fertilizer Plant Explosion (West, TX)**  
(April 23, 2013, Washington Post)



**Refinery explosion: How Philly dodged a catastrophe**  
(June 21, 2019, Philadelphia Inquirer)



5/14/2021

# ASSURANCE

## FLOW ASSURANCE:

- **Coalescers, dehydrators, desalters, and oil-water-gas separators (in O&G industry)**
- Hydrate formation in oil and gas pipelines
- **Spray drift in agriculture**
- **“Drop size-modulation” and “satellite droplet or misting prevention” in ink jet printing and additive manufacturing operations**
- **Bottle filling (detergent bottles or drug vials)**
- **Rupture/integrity of coated films on substrates and free thin films/sheets (important in atomization and polymer processing)**

## OTHER EXAMPLES:

- **Avoiding polymorphs in the pharma industry**
- **Personalized medicine: printing drugs on edible substrates**
- **Control of particle (or capsule) size as well as shape**
- **Safety, reliability, and durability of biomedical (e.g. implants) and surgical devices**

# CENTER ACTIVITIES AND UNIQUE FEATURES (I)

- Involve **multiple faculty** (rather than a single person), **PhD students** (2+ year projects), **PMP students** (intense summer projects mentored by member companies), and exceptional **undergraduates** in safety-related research.
- Additionally, P2SAC aims in the long term to become a leader in certain aspects of safety education through development and teaching of primarily undergraduate and graduate courses. *(According to informal polling of first year graduate students in our program, **Purdue ChE is one of a handful of departments nationally and internationally that requires all undergraduates to take a core course on safety in order to receive a BS degree**) (The course is also offered to graduate students, which is even more unusual.)*

# CENTER ACTIVITIES AND UNIQUE FEATURES (II)

- Our goal/mission is not to focus on a single or primarily one industry segment, e.g. we do not just want to have members that are oil and gas (O&G) producers
- Synergism: bring together people from different industries, e.g. pharma and O&G, who would normally not attend the same conferences and/or interact with one another on a regular basis

# **SUMMARY OF TYPES OF P2SAC RESEARCH PROJECTS**

- PhD research projects: to be covered here
- Professional Master's Program (PMP) capstone research projects: to be covered by Ray Mentzer
- Undergraduate (UG) research projects: also to be covered by Ray Mentzer

# PROCESS FOR DETERMINING AND FUNDING PhD PROJECTS

(Program managed by Osman Basaran, AD)

- There are two ways for coming up with new projects. Either
  - Faculty or groups of faculty (within and outside ChE) come up with project ideas on their own or
  - Industrial members work with faculty to develop new projects
- **Timing for formulating projects:** *summer and early fall*
- **Timing and mechanism(s) for proposing projects:** either by
  - Making an oral presentation/pitch during the fall conference or
  - Submitting a 1.5-page written project proposal to Osman Basaran (AD) in December
- **How are projects to be funded determined?** Member companies rank order the projects and send their rankings to the AD
- **Final determination on funding:** AD selects projects to be supported based on input received and availability of funds

# **NEW PhD PROJECTS APPROVED FOR FUNDING IN 2021-2022**

- Proposals for twelve (12) projects were submitted by the faculty
- Member companies were asked to rank-order the proposed projects
- Six (6) proposals were chosen to be funded
- An unexpected but desirable commonality among projects to be funded: all successful proposals involved participation and/or active involvement by one or more P2SAC member companies



# PhD PROJECTS APPROVED FOR FUNDING (2021-2022)

**Project title:** Quantum chemical prediction of molecular thermodynamics to assess reaction safety and scale-up\*

**PI:** Prof. Brett M. Savoie, Davidson School of Chemical Engineering, Purdue University

**Project suggested/proposed or championed by:** Brett M. Savoie (Purdue) and virtually all members of P2SAC from the pharmaceutical industry

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\*This is a recent and rapidly growing area of research in P2SAC, and its impact on safety-related work at member companies will become quite clear on Monday.

# PhD PROJECTS 2021-2022 CONT'D

**Project title:** Low-power, low-cost gas sensors with high specificity for hydrogen gas\*

**PI:** Bryan W. Boudouris, Davidson School of Chemical Engineering, Purdue University

**Project suggested/proposed or championed by:** Bryan W. Boudouris (Purdue) and Hariprasad Janakiram Subramani (Chevron)

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\*Research methodology can be applied to all sorts of sensors, i.e. hydrogen gas sensor is just one of many possibilities/targets.

# PhD PROJECTS 2021-2022 CONT'D

**Project title:** Prevention through catalyst design for applications in the petrochemical industry\*

**PI:** Prof. Rajamani Gounder, Davidson School of Chemical Engineering, Purdue University

**Project suggested/proposed or championed by:** Rajamani Gounder (Purdue)

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\*The idea for the center to do research at the intersection of catalysis and PTD (prevention through design) was born after a presentation by a member of the center's advisory board at a P2SAC conference.

# PhD PROJECTS 2021-2022 CONT'D

**Project title:** Predicting spray dynamics for flow assurance, minimization of fines, and prevention of drift\*

**PI:** Prof. Osman A. Basaran, Davidson School of Chemical Engineering, Purdue University

**Project suggested/proposed or championed by:** Pritish M. Kamat (Dow) and Osman A. Basaran (Purdue)

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\*Although the general area of sprays is an active research area in the Basaran group, the project was initially suggested by Dow.

# PhD PROJECTS 2021-2022 CONT'D

**Project title:** Real-time Li-ion battery monitoring using impedance spectroscopy and gas/pressure sensors for early thermal runaway detection\*

**PI:** Prof. Vilas Pol, Davidson School of Chemical Engineering, Purdue University

**Project suggested/proposed or championed by:** Vilas Pol (Purdue); Edward Marszal, James Mcglone (Kenexis) and Erich Binder (Worley)

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\*The proposal came together after weeks of back and forth between Prof. Pol and industry representatives.

# PhD PROJECTS 2021-2022 CONT'D

**Project title:** Understanding erosion at the microscopic scale\*

**PI:** Prof. Osman A. Basaran, Davidson School of Chemical Engineering, Purdue University

**Project suggested/proposed or championed by:**

Hariprasad J. Subramani (Chevron) and Osman A. Basaran (Purdue)

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\*Dr. Subramani and colleagues had been promoting the general area of erosion and this project in particular for a number of years until the idea finally gelled into a concrete proposal.