

P2SAC FALL 2021 CONFERENCE

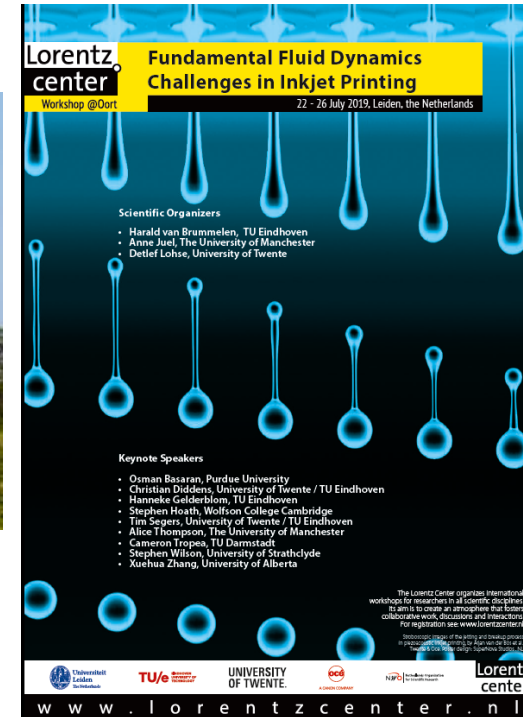
Welcome & Overview



Safety
(npr.org)



**Safety and
assurance**
(agdaily.com)



Flow assurance

Osman Basaran

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

Davidson School of Chemical Engineering/Purdue University

OUTLINE AND 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
- Primarily at the start of the second day, I will:
 - Provide an overview of P2SAC to *first-time attendees as well as long-standing industry members of the center* and *our students*
 - Highlight new PhD projects
- 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 once every 12 or 18 months)
 - **Flow assurance mini-conference** (to be held once every couple of years)
- A set of **tutorials** lasting half a day were then added to the program in Fall 2019 (to be held twice a year) and have now grown into a full-day program in Fall 2021

AGENDA FOR
FALL 2021 CONFERENCE
PURDUE PROCESS SAFETY AND
ASSURANCE CENTER (P2SAC)
December 6, 7 and 8

FALL 2021 CONFERENCE
PURDUE PROCESS SAFETY AND
ASSURANCE CENTER (P2SAC)

AGENDA AT A GLANCE

Monday-Wednesday, December 6-8, 2021

Monday, December 6, 2021: Tutorials

(8:00 am – 5:15 pm)

Tuesday, December 7, 2021: Safety conference

(8:00 am – 5:15 pm)

Wednesday, December 8, 2021: Discussions of
safety management systems

(9:00 am – 10:45 am)

FALL 2021 CONFERENCE
PURDUE PROCESS SAFETY AND ASSURANCE CENTER (P2SAC)

AGENDA FOR TUTORIALS

Monday, December 6, 2021

8:00 – 8:15	Osman Basaran (Professor of ChE and Academic Director of P2SAC): Welcome, overview and agenda
8:15 – 10:15	Jim McGlone and Edward Marszal (Kenexis): Fire and gas mapping for gas detector placement
10:15 – 10:30	Break
10:30 – 12:30	Elizabeth Raines (Fauske): Reactive vent sizing
12:30 – 1:15	Lunch

12:30 – 1:15	Lunch
1:15 – 2:15	Han Xia (Lilly): Explosive/self-reactive material classification/shipping around the world
2:15 – 3:15	George Harriott (Air Products): Pipeline dynamics (gas: leak location or liquid: leak detection)
3:15 – 3:30	Break
3:30 – 5:00	Min Sheng (Corteva): Practical use of ARC analysis for thermal stability
5:00 – 5:15	Ray Mentzer and Osman Basaran (Professors of ChE and Directors of P2SAC): Wrap up

FALL 2021 CONFERENCE
PURDUE PROCESS SAFETY AND ASSURANCE CENTER (P2SAC)

AGENDA FOR SAFETY CONFERENCE

Tuesday, December 7, 2021

- | | |
|---------------|--|
| 8:00 – 8:15 | Osman Basaran (Professor of ChE and Academic Director of P2SAC):
Welcome, overview and agenda |
| 8:15 – 8:45 | Ray Mentzer (Professor of ChE and Executive Director of P2SAC):
Welcome and overview of P2SAC research and teaching activities |
| 8:45 – 9:15 | Fareed Sayeed (Lilly): The use of quantum chemical calculations for
thermal hazard assessments |
| 9:15 – 9:45 | Connor Barrett and Jeff Sperry (Vertex): Bicyclo[1.1.1]pentanes – a rising
process safety challenge |
| 9:45 – 10:15 | Prasad Goteti (Honeywell): Connected process plants to improve safety
in the digital world |
| 10:15 – 10:30 | Break |

10:15 – 10:30	Break
10:30 – 11:00	Bryan Boudouris (Professor of ChE, Purdue): Low-power, low-cost gas sensors with high specificity for hydrogen gas
11:00 – 11:30	Erdem Arslan (Air Products): Reliability availability and maintainability (RAM) studies for industrial plants design and optimization
11:30 – 12:00	Abe Schuitman (Corteva): Sustainability metrics for small molecule development
12:00 – 12:30	Laurence Pearlman (Marsh) and Peter Rutigliano (Mercer Sirota): Using elements of safety culture as a predictor of process safety outcomes
12:30 – 1:15	Lunch

12:30 – 1:15	Lunch
1:15 – 1:45	Brett Savoie (Professor of ChE): Quantum chemical prediction of molecular thermodynamics to assess reaction safety and scale-up
1:45 – 2:15	Katherine Young (UG-Purdue) et al. (Purdue): Experimental versus predicted heats of reaction for some common reaction types in pharma industry
2:15 – 2:45	Vilas Pol (Professor of ChE): Battery safety
2:45 – 3:15	Daniel Valco (Corteva): Thermal instability and associated potential safety hazards of $[\text{Rh}(\text{ethylene})_2\text{Cl}]_2$ catalyst
3:15 – 3:30	Break

3:15 – 3:30	Break
3:30 – 4:00	Xuemin Chen (Dow): Industrial perspectives on highly energetic materials
4:00 – 4:30	Daniel Nguyen (ioKinetic): Leveraging the adiabatic calorimetry for optimal emergency relief sizing
4:30 – 5:00	Joe Jakubowicz (UG-Purdue) et al. (Purdue): Tool to calculate LFL and UFL of flammable mixtures with inerts
5:00 – 5:15	Ray Mentzer and Osman Basaran : Wrap up

FALL 2021 CONFERENCE
PURDUE PROCESS SAFETY AND ASSURANCE CENTER (P2SAC)

AGENDA FOR DISCUSSIONS OF SAFETY MANAGEMENT SYSTEMS

Wednesday, December 8, 2021

- | | |
|---------------|--|
| 9:00 – 9:15 | Ray Mentzer and Osman Basaran (Professors of ChE and Directors of P2SAC): preamble |
| 9:15 – 9:45 | Laura Turci, Ross Bass and Jonathan Slater (3M): 3M's EHS management systems – an element-based approach |
| 9:45 – 10:15 | Leslie Day and Thomas Noah (CountryMark): The application of management systems within CountryMark |
| 10:15 – 10:45 | Ray Mentzer and Osman Basaran (Professors of ChE and Directors of P2SAC): open discussion and conference conclusion |

P2SAC CONFERENCES: EVOLUTION AND OUTLOOK

- **Early years:** the first conference (Fall 2014) and about a half a dozen conferences after that consisted of very full, one-day meetings
- **Subsequent years:** multi-day mini-conferences consisting of
 - **General safety conference** (*twice a year*)
 - **Safety in the pharmaceutical industry conference** (*once a year*)
 - **Flow assurance conference** (*once every couple of years*)
 - **Tutorials** lasting one half to full day (*twice a year*)
- **First time this fall:** company-led session on discussion of **management systems**
- **We hope that the Spring 2022 Conference (05/22) will be in-person**

P2SAC SPRING 2022 CONFERENCE (TENTATIVE)

- Early to mid-May 2022
- **Program:** multi-day mini-conferences consisting of
 - **Tutorials** (*one half to full day*)
 - **General safety conference** (*full day*)
 - **Safety in the pharmaceutical industry** (*full day*)
 - **Flow assurance conference** (*full day, including several outside academic and industry speakers*)
 - **Company-led discussions on topic(s) of high-current interest** [*highly tentative*] (*a few hours and perhaps on the same day as tutorials or flow assurance*)
- We hope that the Spring 2022 Conference (05/22) will be FTF!

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



3M

Lilly

AMGEN

MARSH



سابك
sabic



CountryMark®

AcuTech
PROCESS RISK MANAGEMENT

KENEXIS

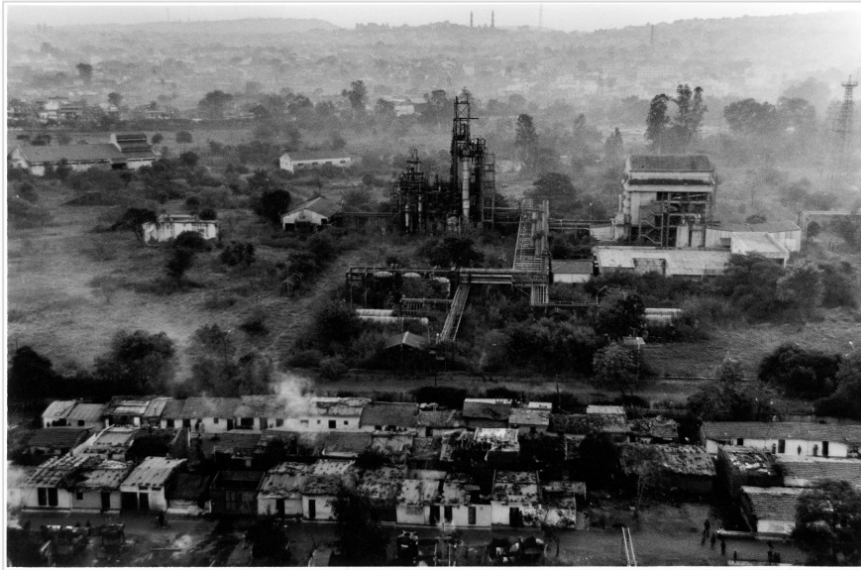
Endress+Hauser 
People for Process Automation




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

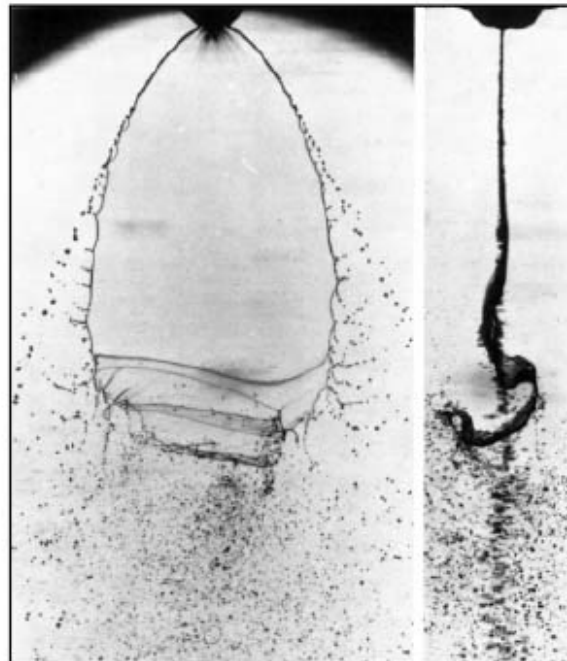


Imperial Sugar, Georgia (2008): 14 fatalities

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).
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)



12/6/2021

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: a listing of current projects will be provided
- 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

*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)

*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)

*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)

*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)

*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)

*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.