Process Intensification: Concepts and Applications

Phillip R. Westmoreland

Department of Chemical and Biomolecular Engineering
North Carolina State University
Process Intensification

Process Science and Technology

How is Process Intensification defined?


• Or isn’t that just sound process development?
  – Would include all of catalysis.
  – Improved separations, heat transfer, mass transfer, mixing.
  – Process control.
  – Process optimization.

• Points toward “Process Science and Technology” as a more general goal for advances.
  – New and improved process technologies and the science that underpins them.
(a) Increased productivity = intensification.
The same trend is worldwide (2000 data).

Thanks to Jim Wei, emeritus Dean of Engin'g, Princeton.
(b) It is Process Technology that puts ChEs into the “Manufacturing Enterprise.”

- In the U.S. government, manufacturing is a top topic, partly because of jobs.
  - To the public, Manufacturing = Using machines / machining /assembly lines to make durable goods.
  - They easily accept that processes making fuels or polymers or pharmaceuticals or potato chips is manufacturing, too.

- New generations of manufacturing focus on process- and property-driven manufacturing.
(c) Opportunity: Today’s academic ChE research in the US emphasizes products, not processes.

- John Chen surveyed 40 ChE department heads about research interests of their 620 tenure-track faculty members plus emeritus faculty.
- Reported as fractional interests in six areas;
- Three process-dominated areas:
  - “UO” (process sciences like thermo, transport, separations)
  - Reaction engineering (kinetics, catalysis, reactors)
  - Analysis / Modeling (simulation, process dynamics and control)
- Three product-dominated areas:
  - Materials (material science, surface science, polymers)
  - Bio (biotechnology, medical science, life science)
  - Nano (nanoscience and nanotechnology)
The results showed this dominance of “product”.

- Compare findings for the categories:
  - Bio 28%
  - Materials 20% 55%
  - Nano 7%
  - UO 16%
  - Rxn Engineering 14% 45%
  - Analysis/Modeling 15%

- UO and Bio illustrate the shift over time (Opportunity!):
Try again: How is Process Intensification different?

- **European view**: Create new processes through…
  - **Reduced size**
    - Beat economy of scale, directly or through other attributes.
    - Cost = Capital + Operating (feed, utilities, people) but also Distribution + Hazard/risk + Demand amount
  - **Use of “extreme forces” or unusual contacting phases**
    - Electrical, g-forces, high shear, microwaves, sonochemistry, oscillation; supercritical fluids, ionic liquids, azeotropic distillation
  - **Process combinations and reconfigurations** (reactor-separator, reactive distillation, divided-wall distillation).
- Still a subset of good Process Science and Technology, but it provides some bases for distinction.
My focus is on reaction kinetics: Bio-oil production, fuel and process chemistry, data science.
PI relevance of five areas from our group.

- **Thermal & catalytic kinetics for chemicals from biomass.**
  - Federally sponsored, partly in collaboration with industry.

- **High-intensity liquid-liquid reactions.**
  - DoD-sponsored, collaboration with Purdue Aero Engineering.

- **Coking-free cracking of hydrocarbons.**
  - DoD-sponsored.

- **Mechanisms of gas-phase homogeneous catalysis.**
  - Industry collaboration.

- **Developing an international data cyberinfrastructure.**
  - Multiple Federal agencies, Combustion Institute, collaboration with Michael Frenklach at UC Berkeley.
Thermal & catalytic kinetics: Chemicals from biomass.

- Interest in bio-oils seems to be moving from fuel toward chemical feedstocks.
  - Distributed, fairly small-scale units are necessary:
  - Collection/transportation of wet, bulky lignocellulosic biomass.
- Experimentally, we pyrolyze 5-15 mg solid in a Pyroprobe or a TGA/DSC, analyzing with GCxGC-TOFMS.
Thermal & catalytic kinetics: Chemicals from biomass.

- Also: Pyrolyze or burn vaporizable intermediates and model compounds in flow reactors, CSTRs, and packed-bed reactors with exhaust analysis by molecular-beam mass spectrometry (MBMS).
Tubular reactor design

Swagelok Cap with Machined Orifice
ID: 0.254mm

Flow at Mach=1 through orifice
Thermal & catalytic kinetics: Chemicals from biomass.

- Model with elementary-reaction kinetics.
  - Transition-state theory using quantum chemistry TSs.
  - Thermally/chemically activated reaction theories.
- Detailed cellulose pyrolysis kinetics from glucose: e.g., break the chain to make cello-n-san + cellulose oligomer:
Thermal & catalytic kinetics: Chemicals from biomass.

- Empirical and predicted selectivity and rates form a solid foundation for reactor engineering in intensified processes.
- Catalysis is a classic way of intensifying processes and making reactions more selective.
- Accurate models of performance, even if only of trends, will aid catalyst creation/selection and combined use of catalysis reactors and separations.
PI relevance of five areas from our group.

• Thermal & catalytic kinetics for chemicals from biomass.
  – Federally sponsored, partly in collaboration with industry.
• High-intensity liquid-liquid reactions.
  – DoD-sponsored, collaboration with Purdue Aero Engineering.
• Coking-free cracking of hydrocarbons.
  – DoD-sponsored.
• Mechanisms of gas-phase homogeneous catalysis.
  – Industry collaboration.
• Developing an international data cyberinfrastructure.
  – Multiple Federal agencies, Combustion Institute, collaboration with Michael Frenklach at UC Berkeley.
SMART MANUFACTURING (SM)
Building Infrastructure | Powering Smart Decisions

Affordable, Accessible, Innovative & Secure
Intelligent, Seamless & Collaborative
Networked-Based SM Platform

Business Systems, ERP

Supply Chain

Smart Grid

Smart Factory

Distribution Center

Customer
Concluding remarks.

• PI research on distributed energy sources.
  – Compact, high-efficiency, intensified generation of electrical power, including microcombustors and fuel-cell units.
    • Application to homes, single buildings, vehicles, and even electronic devices.
  – Coupled, small-scale energy or chemicals production, distributed around areas of waste biomass generation.
    • Natural partnering with R&D for integrating distributed renewable-energy sources into the electric-power grid.

• Smart Manufacturing is a way to leverage PI process development and impact.
  – Using PI to develop new processes and products would fit naturally into the Smart Manufacturing paradigm.

• Renew focus on Process Science and Technology.
Acknowledgments

• Ph.D. students Vikram Seshadri, Pat Fahey, Craig Needham, Sara Jo Taylor, Scott Crymble.
• Army Research Office (Gelled hypergols MURI).
• Air Force Office of Scientific Research (Endothermic Fuels for Hypersonic Flight).
• DOE / NREL / RTI International (Biomass Pyrolysis).
• DOE BES (Flame MBMS).
• Eastman Chemical.
• Multi-Agency Coordinating Committee for Combustion Research and NSF (Data cyberinfrastructure).

• Photo credit (Monument Valley): http://desktopwallpaperonline.info/Wallpapers--3983/roads%20and%20paths/On%20the%20Road%20Again,%20Monument%20Valley,%20Arizona.jpg