# Process Intensification: Concepts and Applications

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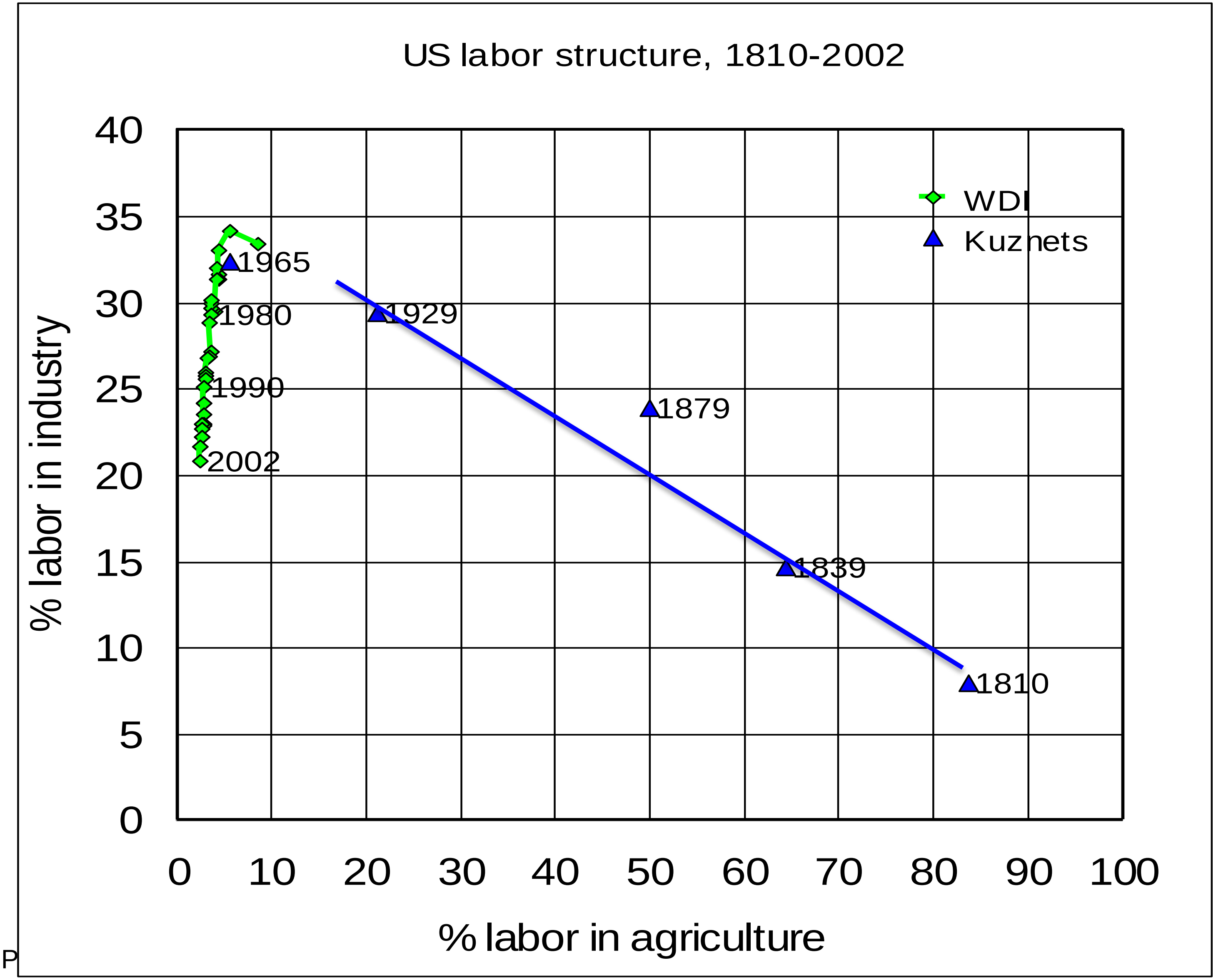
Proc Synthesis, Proc Systems Engineering, Proc Optim, Proc Control

# How is Process Intensification defined?

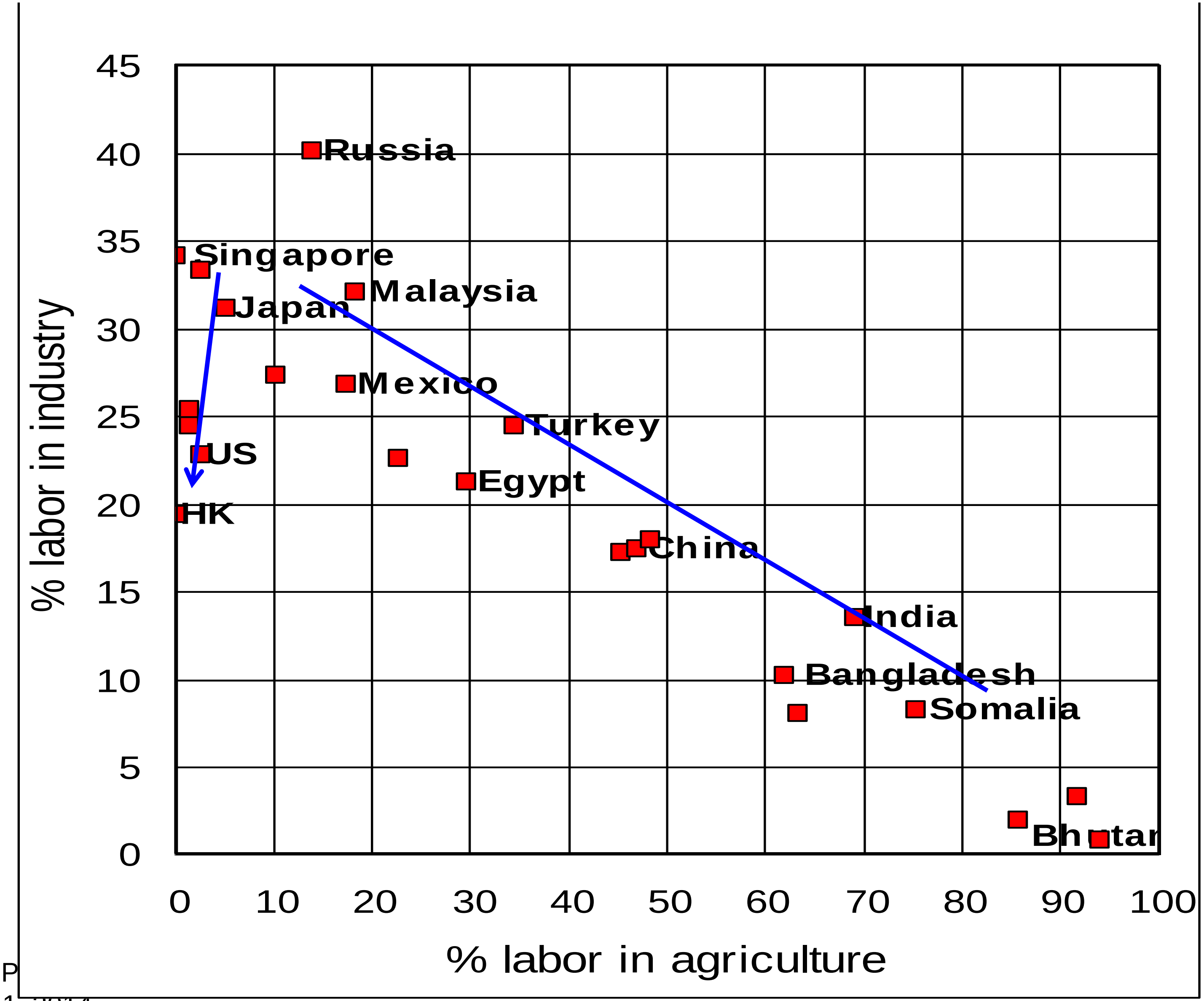
- "Any chemical engineering development that leads to a substantially smaller, cleaner, safer, and more energy-efficient technology is process intensification." -- Reay, Ramshaw, Harvey, *Process Intensification*, Oxford: Butterworth-Heinemann, 2008, p 21.
- Or isn't that just sound process development?
  - 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.




*Thanks to Jim Wei, emeritus Dean of Engin'g, Princeton.*

# The same trend is worldwide (2000 data).

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# (b) It is Process Technology that puts ChEs into the "Manufacturing Enterprise."

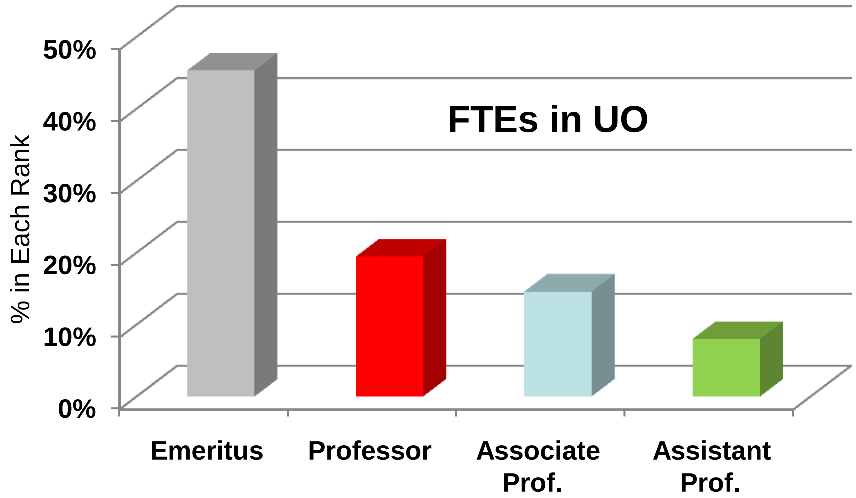
- In the U.S. government, manufacturing is a top topic, partly because of jobs.
  - To the public, Manufacturing = Using machines / machining /assembly lines to make durable goods.
  - They easily accept that processes making fuels or polymers or pharmaceuticals or potato chips is manufacturing, too.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

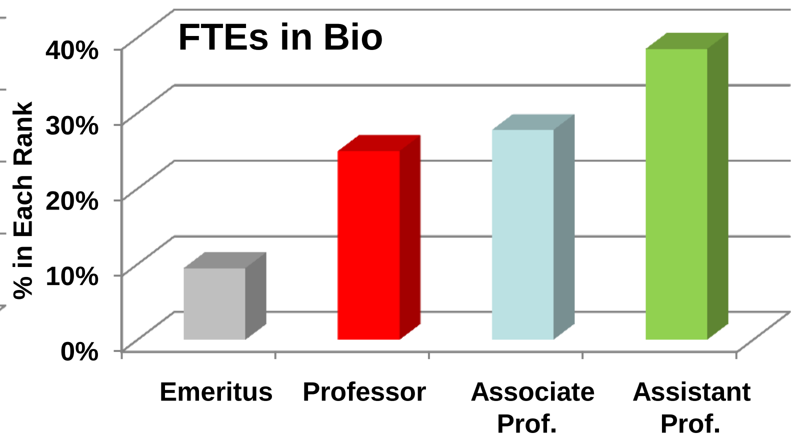
# (c) Opportunity: Today's academic ChE research in the US emphasizes products, not processes.

- 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%
  - Nano 7%
  - } 55%
  - UO 16%
  - Rxn Engineering 14%
  - Analysis/Modeling 15%
  - } 45%
- UO and Bio illustrate the shift over time (Opportunity!):

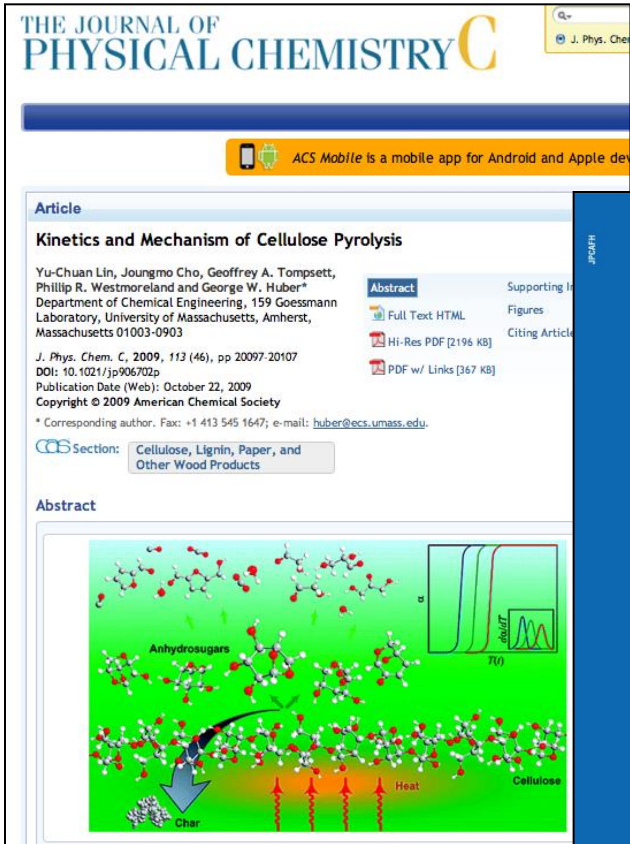


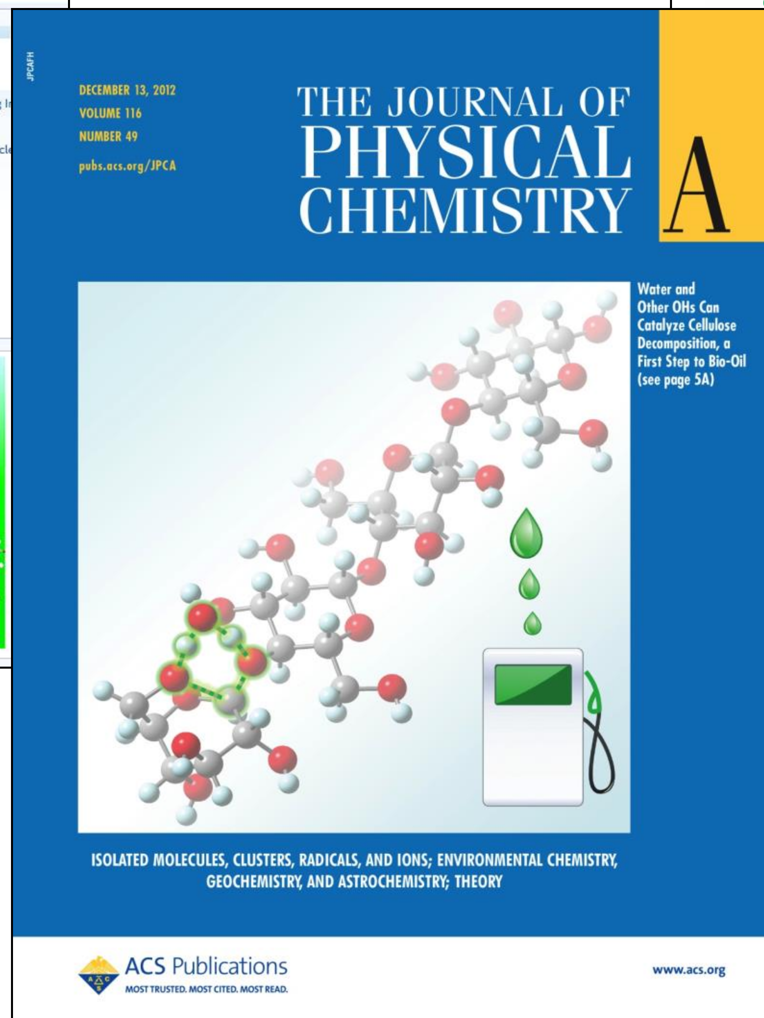



# Try again: How is Process Intensification different?

- **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
    - $$d\underline{G} = -\underline{S}dT + \underline{V}dP + \sigma\, d\underline{A} + \sum_j \left( \mu_j + m_j \phi + \frac{m_j u^2}{2} \right) dN_j + \underline{V}_s \mathcal{E}\, d\underline{D} + \underline{V}_s \mu_0 H dM$$
  - **Process combinations and reconfigurations** (reactor-separator, reactive distillation, divided-wall distillation).
- Still a <u>subset</u> 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.



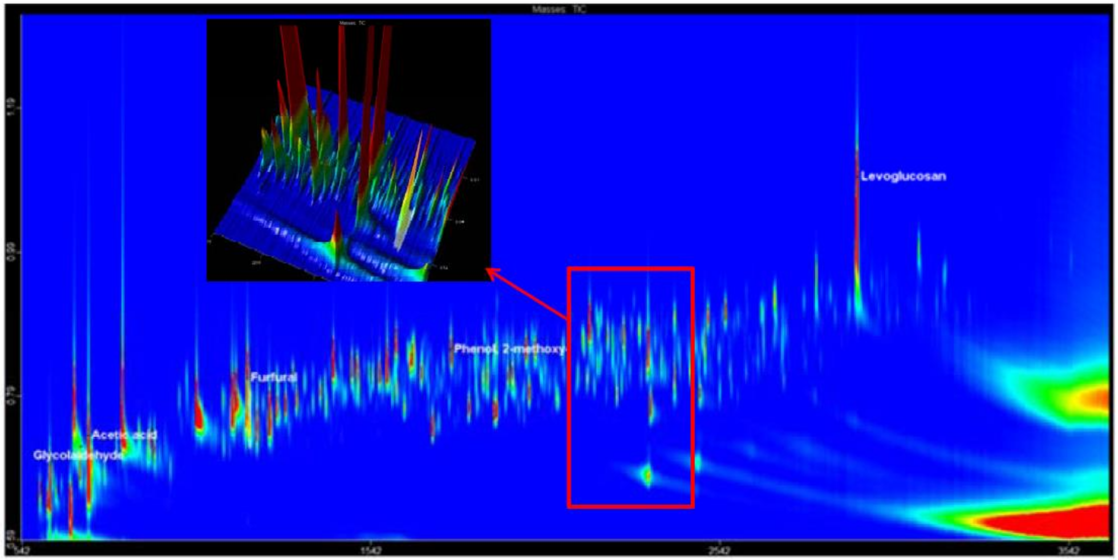




# PI relevance of five areas from our group.

- 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.

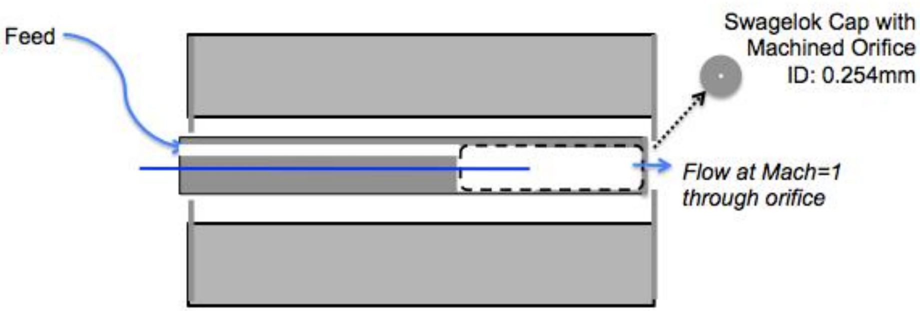
# Thermal & catalytic kinetics: Chemicals from biomass.

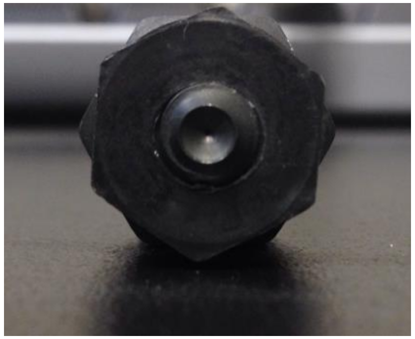
- Interest in bio-oils seems to be moving from fuel toward chemical feedstocks.
  - Distributed, fairly small-scale units are necessary:
  - Collection/transportation of wet, bulky lignocellulosic biomass.
- Experimentally, we pyrolyze 5-15 mg solid in a Pyroprobe or a TGA/DSC, analyzing with GCxGC-TOFMS.

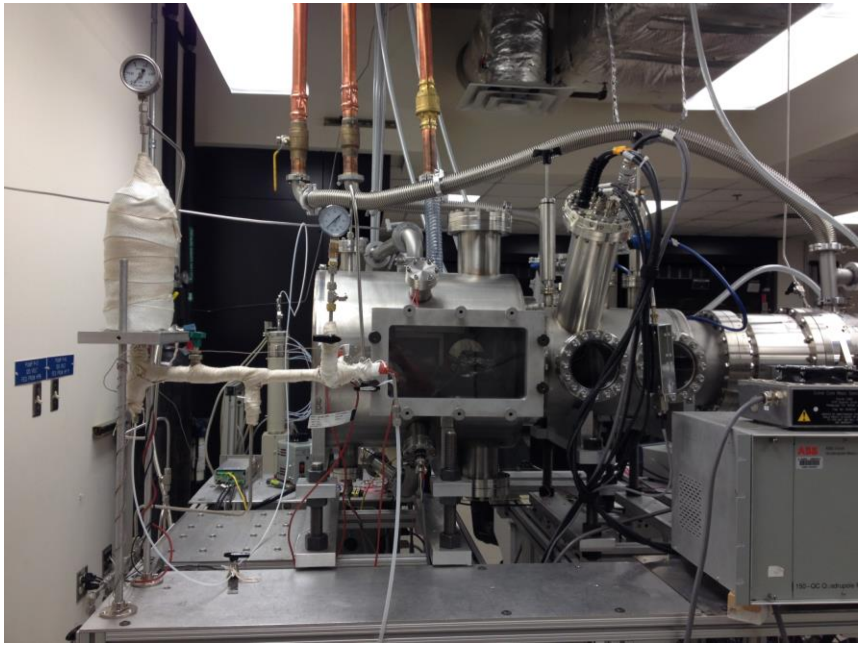


# Thermal & catalytic kinetics: Chemicals from biomass.

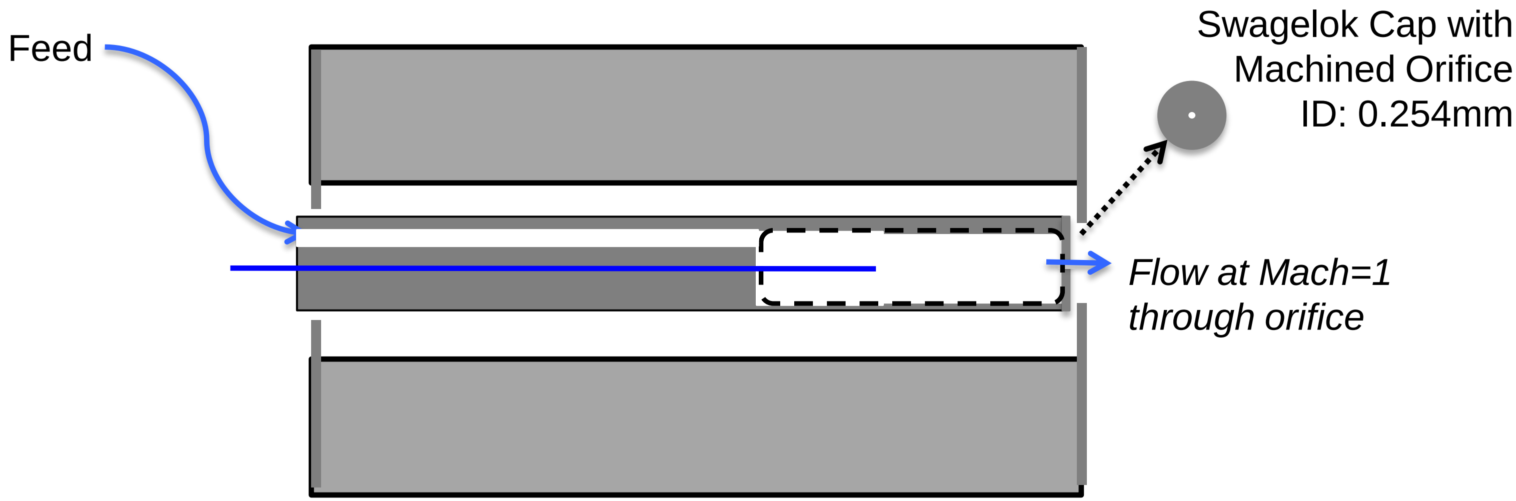
- Also: Pyrolyze or burn vaporizable intermediates and model compounds in flow reactors, CSTRs, and packed-bed reactors with exhaust analysis by molecular-beam mass spectrometry (MBMS).



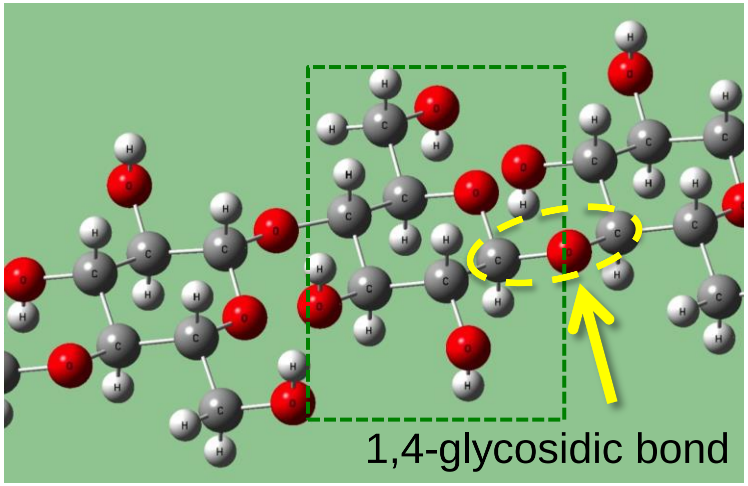


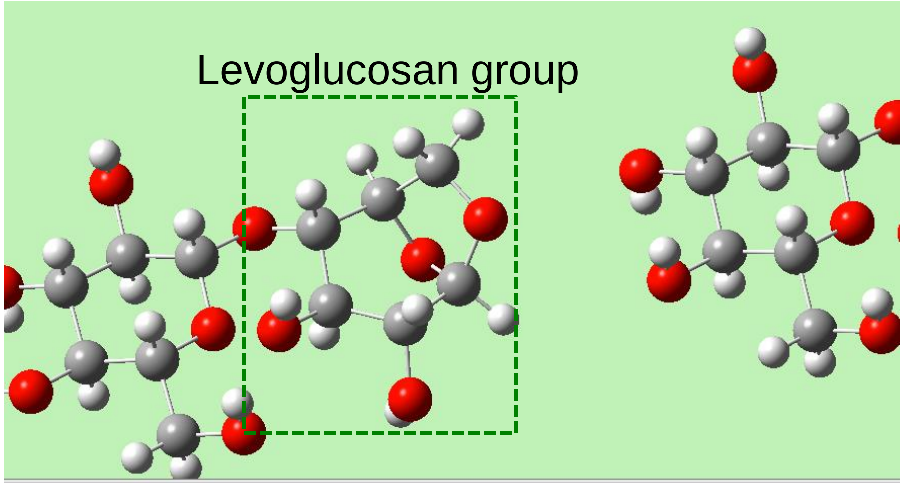
# Tubular reactor design

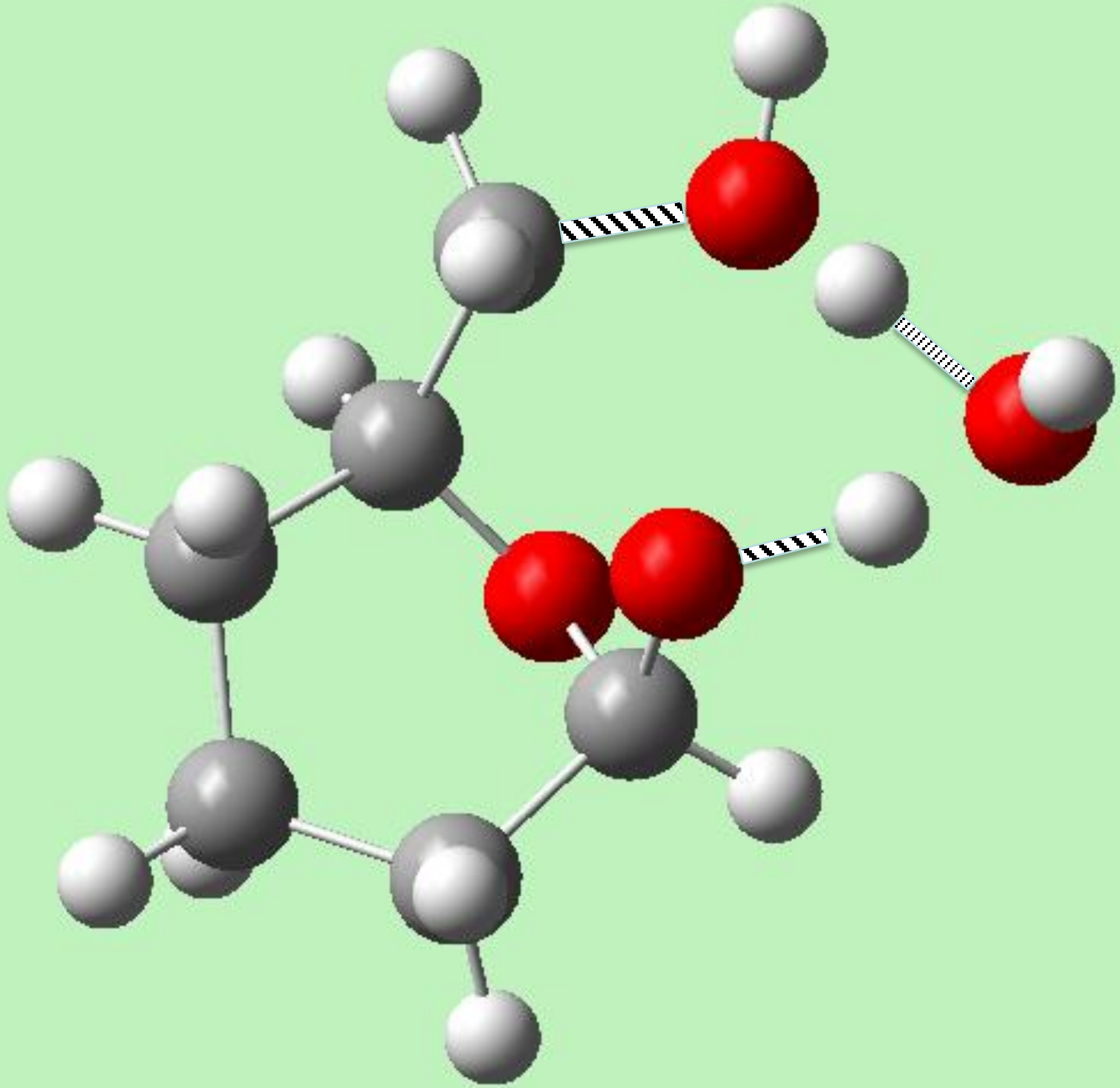


# Thermal & catalytic kinetics: Chemicals from biomass.

- 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.

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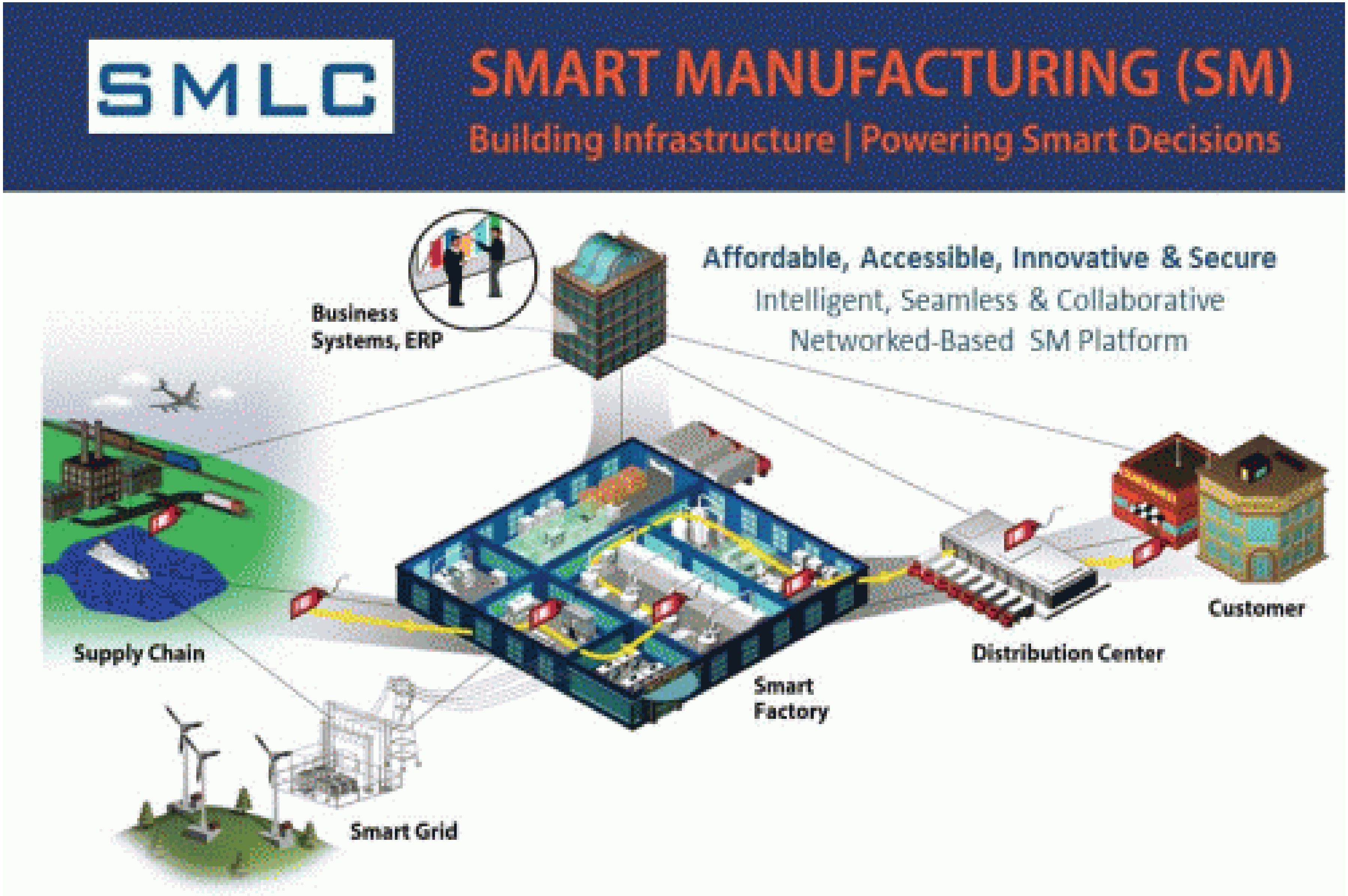
SMLC
SMART MANUFACTURING (SM)
Building Infrastructure | Powering Smart Decisions
Affordable, Accessible, Innovative & Secure
Intelligent, Seamless & Collaborative
Networked-Based SM Platform
Business Systems, ERP
Supply Chain
Smart Factory
Distribution Center
Customer
Smart Grid

# 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.

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- DOE BES (Flame MBMS).
- Eastman Chemical.
- Multi-Agency Coordinating Committee for Combustion Research and NSF (Data cyberinfrastructure).


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