Process Systems Engineering: Current & Future Contributions to Chemical Engineering

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• Roots of PSE
• Impact on ChE profession
• Research Directions
  • Energy & Sustainability
  • Product & Process Design
  • Enterprise Optimization
  • Healthcare applications
• Summary
Process Systems Engineering

The Engineering of Systems involving Physical, Chemical & Biological Processing Operations

G. Stephanopoulos & G.V. Reklaitis, CES, 2011
Processing Systems

- Produce chemicals & materials for society’s wants
- Produce & utilize fuels and energy from fossil & renewable sources
- Ensure quality of water & the environment
- Provide diagnostics & therapies for treatment of disease
- Manufacture consumer goods to enhance quality of life
Historical References


C.E. Huckaba & G. Monet (eds) CEP Symposium Series 59 (1963)
“ChE’s are primarily interested in process systems engineering in which the systems approach is employed in the design and operation of chemical processing plants”
Historical Milestones

PSE Industrial Impact

- Steady State Flowsheet Simulation
- Model Predictive Control
- Dynamic systems modeling
- Process integration /synthesis
- Process planning/scheduling
- Real time process optimization
Steady State Process Simulation
- Initiated in 50’s (Kellogg)
- Block structure / Sequential Modular
- Constraint handling
- Flowsheet Parameter Optimization
- Equation oriented alternatives

Physical Property Modeling
- Initiated in early 60’s
- Extensive experimental data
- Model libraries
- Data bases of parameters
- Pure components & mixtures
- Electrolytes
- Solubility of organics
Model Predictive Control

Process Measurement

Dynamic Process Model

Optimal Process Adjustment

“Real-time” Prediction & Optimization

Standard for refineries & petrochemicals

Problem categories

- Heat exchange & power networks
- Separation systems
- Mass exchange networks
- Reaction attainable regions
- Complete processes

Approaches

- Thermodynamic constructions (pinch)
- Heuristic methods
- Superstructure construction
- Math programming
- Systematic enumeration of configurations

Planning & Scheduling

Process planning models
- LP/MILP
- Multiperiod
- Refinery applications
- Utility systems
- Water management

Cyclic & Batch process scheduling
- State-task network
- Resource constraints
- MILP & heuristic

Objective: Set Point Optimization
- On-line measurement reconciliation methods
- Gross error detection
- Equation oriented process models
- Parameter estimation methods
- Large-scale optimization to obtain optimal setpoints

Steady State & Dynamic RTO
Applications for major petrochemical process units

PSE impact on ChE curriculum

- Capstone design course
  - *Process synthesis concepts & heuristics*
  - *Flowsheet simulation & design systems*
- Process dynamics & control course
  - *Physical experiments*
  - *Simulated applications (Matlab/Simulink)*
- Introduction to experimental design & data analysis & modeling (*Matlab, JMP*)
- Exposure to optimization & numerical analysis tools (*Excel, Matlab, GAMS*)
PSE Research Directions

- Energy & Sustainability
- Product & Process Design
- Enterprise-wide Optimization
- Healthcare applications
Energy & Sustainability

- Energy savings through process integration
- Integrated & flexible electric grids
- Community energy infrastructures
- Biofuels & Bio-derived chemical building blocks from biomass
- Integration of carbon source, land usage, CO$_2$ capture & sequestration, water subsystems
- Water resource management
- Models of Sustainable solar economy
Integration of Plant HEN with utility, refrigeration & power cycles

El-Halwagi & coworkers  *CAPE* 34 (2014)
Flexible Electric Power Grid

Smart Grids
Chem Engr Progress
August 2014

Integration of Heating Cooling Electricity CO₂ mitigation

• Demand profiles?
• Connection?

• Type?
• Size?
• Location?
• Centralized?
• Decentralized?

• Integration of
  • Local resources
  • Renewable

Marechal, Fazlollahi & coworkers, (2013)
Biomass Utilization Superstructure (BUS)

Maravelias & coworkers (2014)
Hybrid Processes: natural gas & biomass for liquid fuels

Agrawal & coworkers
Gencer et al
CACE 34 (2014)
Process & Product Design

- Process intensification (Baldea, CACE 34 (2014))
  - Hybrid separation systems
  - Micro-reaction based systems
  - Divided wall columns
- Product Design (Gani & Ng, CACE 34, (2014))
  - Molecular structures: single molecules & blends (e.g., refrigerants, solvents)
  - Formulated products (e.g., paints, cosmetics)
  - Functional Products & devices (e.g., controlled release, pharmaceuticals, barrier films)
- Integration of Product & Process Design

Multiple Dividing Wall Column
Ramapriya et al. AICHEJ (2014)
**Product Design Application: Absorbent**

**Goal:** Solvent for efficient CO$_2$ capture from flue gas

**Desired solvent properties**
- High CO$_2$ solubility
- High selectivity for CO$_2$
- Low vapor pressure
- Low energy requirement for regeneration
- Low rate of degeneration
- Moderate viscosity

**Family of Candidate Molecules: Ionic Liquids**

Organic salts that are liquid at ambient T

- Imidazolium
- Tetra alkylammonium
- Pyrrolidinium

$X = \text{selection of anions}$

Brennecke et al, 2010; Stadtherr et al, 2012; Ramdin et al, I&EC Research 2012
Integration of design of process & processing material (QM-CAMD)

- QM-based property prediction for initial set of molecules
- Generation of surrogate model to reduce burden of QM calculations
- Surrogate model imbedded in process model
- Optimization of integrated process design
- Iteration to improve surrogate

Adjiman et al at *CACE* 34 (2014)

Sequential Material Selection Approach

Gani & Ng
*CACE* 38 (2014)

Application: Find solvent maximizing reaction rate – Candidate space = 1341
QM for only 9 solvents!
Enterprise-wide Optimization

Large-scale optimization of development, design, capacity planning, supply, production & distribution to maximize enterprise performance

- Plant complex optimization
- Supply Chain management
  - Chemicals
  - Oil production
  - Shale gas
  - Biofuels
  - Pharmaceuticals
- Product development Pipeline management

Lainez-Aguirre & Puigjaner, Advances in Integrated & Sustainable Supply Chain Planning, 2014
Chemical manufacturing supply chains

Large multi-scale planning: Multiple markets, products, plant sites, multiple production trains per site, planning time periods

Shale Gas Supply Chain

Investment Planning & Operational Management

Grossmann et al 2014, Guerra et al 2014

Regional Model
Clinical Trial Supply Chain

Features

- Finite length horizon (1-2 years)
- Unused inventory at end of trial → wastage
- If right dosage unavailable on patient arrival, patient lost to trial
- Uncertainty in patient completion of treatment → demand uncertainty
- Uncertainty in manufacturing & distribution channel performance
- Multiple SKU’s for each API: dosage levels, placebo, comparator, country

Multistage stochastic decision problem balancing risks of over/under supply

Chen et al, I&EC Research (2013)
Healthcare Applications

- Systems Biology & Bioinformatics
  - Holistic modeling & analysis of cells, organisms & tissues
  - Application of systems dynamics to molecular biology
    (Foundations of Systems Biology & Engineering conferences)
- Pharmaceutical product & process optimization:
  - Product Design
    - e.g., Drug crystal engineering, Protein engineering, Drug product formulation design
  - Process Design
    - Batch Production Optimization
    - Continuous manufacture of drug substance & product
- Model-based drug development & therapy administration
  - Physiologically-based whole body PK/PD models
  - Integration of monitoring & automated drug delivery
  - Individualized patient dosing
Closed-Loop Artificial Pancreas System

Goal: Fully automated real-time management of type 1 diabetes treatment personalized to patient

Components
- Sensors: Glucose & Physiological variables
- MPC/PID controller
- Fault detection
- Dosing model
- Personalized tuning
- Patient manual input
- Insulin pump
- Computer

Status: Clinical trials

Continuous Granulation Process Automation

- Loss-in-weight Feeders
- Continuous Blender
- Roller Compactor
- Continuous Blender
- API
- Excipients

Measurements:
- Flow
- Composition
- Density
- Particle size
- Moisture
- Weight

Plant-wide Control

Ratio Control

PSD Control

Hardness Control

Abnormal Events Management

On-line sensing
Esp. Spectroscopic methods

Adverse drug reaction (U.S): 2 MM hospitalizations; 100 K deaths/y
Wide inter-patient variability in therapeutic responses to same dose

Individualized Medicine Framework

- Physiology
- Hypothesis
- Literature
- Clinical trials

PK Models

PD Models

Population Model

Building via Bayesian methods

Rich Information accumulated from patient population

Minimum Individual Patient Sampling

Integration of Patient-specific information

Individualized Patient Model

Individualized Dose Optimization

Individualized Dosage Regimen

Lainez-Aguirre & Reklaitis, AIChE J (2013);
Blau et al Pharmacotherapy (2014)
Improvements over “one-size-fits-all” dosing

**Gabapentin Case Study**

- Used to treat neuropathic pain
- Therapeutic window:
  - 2-10 µg/mL
- Data from a clinical study (Urban et al., 2008)
  - 19 individuals completed study
  - 14 serial blood collections
- Standard recommended dosing: 300 mg /three times a day

**Results**

- Use two blood draws per patient
- Individualized dosing regimen can reduce risk to 5% or less

Summary

• PSE has legacy of delivering value to industry & ChE profession and is continuing with renewed energy.
• Societal focus on renewables, CO₂ capture, shale gas, water, energy efficiency & sustainability is unique opportunity for impact and obligation to do it right!
• Enterprise-wide systems perspective provides needed context for integrating multiple corporate functions with traditional manufacturing & logistics decisions.
• Healthcare applications, including renewed emphasis by pharmaceutical industry on innovations in product design & manufacturing, are providing exciting research avenue for PSE.
• PSE has effectively entrenched its central role in ChE discipline!!