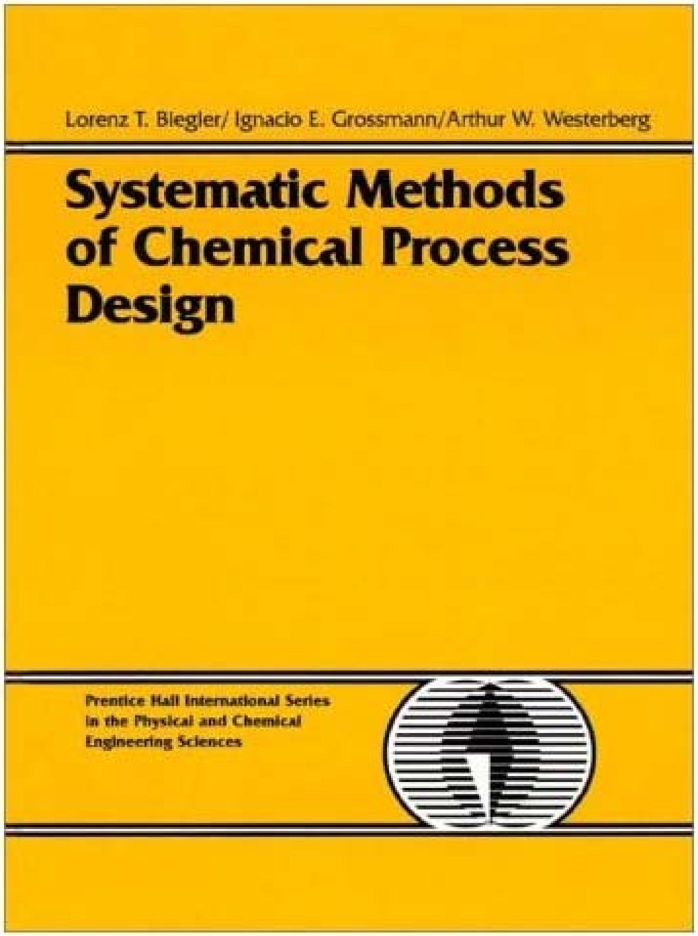
# Systematic Methods of Process Synthesis and Design

L. T. Biegler
Chemical Engineering Department
Carnegie Mellon University
Pittsburgh, PA 15213

November, 2008

# The Textbook




•Deals with decision-making concepts related to process design

•Technical and Economic Evaluation of Processes
•Material easily leveraged with capstone design project

•Conceptual and Heuristic Synthesis
•Optimization Formulations
•Background on Mathematical Programming

•Undergrad/graduate level over multi-semester sequence
•Useful research reference (widely cited in international scientific literature)

# Design Course teaches…

- Synthesis of engineering content and professional practice
- Activities that mimic the real-world workplace in process engineering
- Social process that leverages diverse personalities and skills
- Evolving to Products and New Processes
- Decision-making based on engineering experience and domain knowledge

# Issues for Decision-making

- Ill-defined problems --> well-defined formulations
- Metrics to compare alternatives
  - safety
  - environmental impact and sustainability
  - energy efficiency
  - economics
- Search among a rich set of alternatives

==> Research in PSE has focused on these issues over the past four decades

How should this be taught in a design course?

# The Basics

How should a flowsheet be constructed?

- rule-based hierarchies, based on Rudd, Powers, Siirola and Douglas
- reflect decisions that lead to state-of-the-art continuous processes

How should a flowsheet be evaluated?

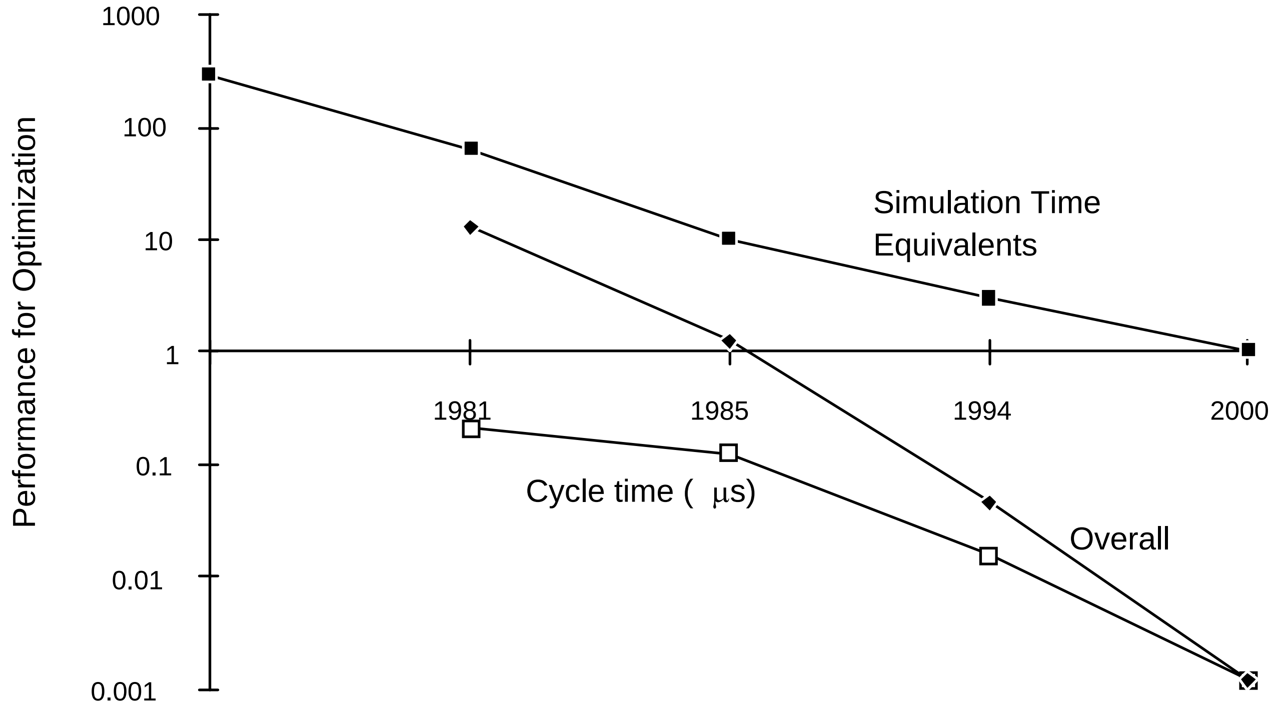
Technical Feasibility: Does it produce the desired products from given feedstocks?

- shortcut models and linear mass balances ==> flowsheet interactions
- evolve to detailed simulation models ==> what additional information is gained

Economic Feasibility: Will it be profitable for the company?

- capital and operating costs
- time value of money
- NPV vs. rates of return
- economic evaluation

# Process Simulation and Modeling Tools




- 4-6 orders of magnitude speedup in 20 years
- About three orders of magnitude due to solution algorithms
- Essential tools for process engineering education
- Ubiquitous, on everyone's laptop

# Optimization Impact on Process Simulation

- Shorter Design Cycles - 1 hr vs. up to 2 weeks of case studies to get same design
- Significantly better and more consistent performance in work processes
- Nonintuitive results
  - Increased process understanding
  - Explore limits of process model
  - Sensitivity information on process performance
- Lower level decisions of process engineering handled by optimizer
- Higher level decisions handled by process engineer, but can easily be misused – power tool analogy!
- Understand what is “under the hood”
- Diagnose problems and check answers

# Process Synthesis Concepts

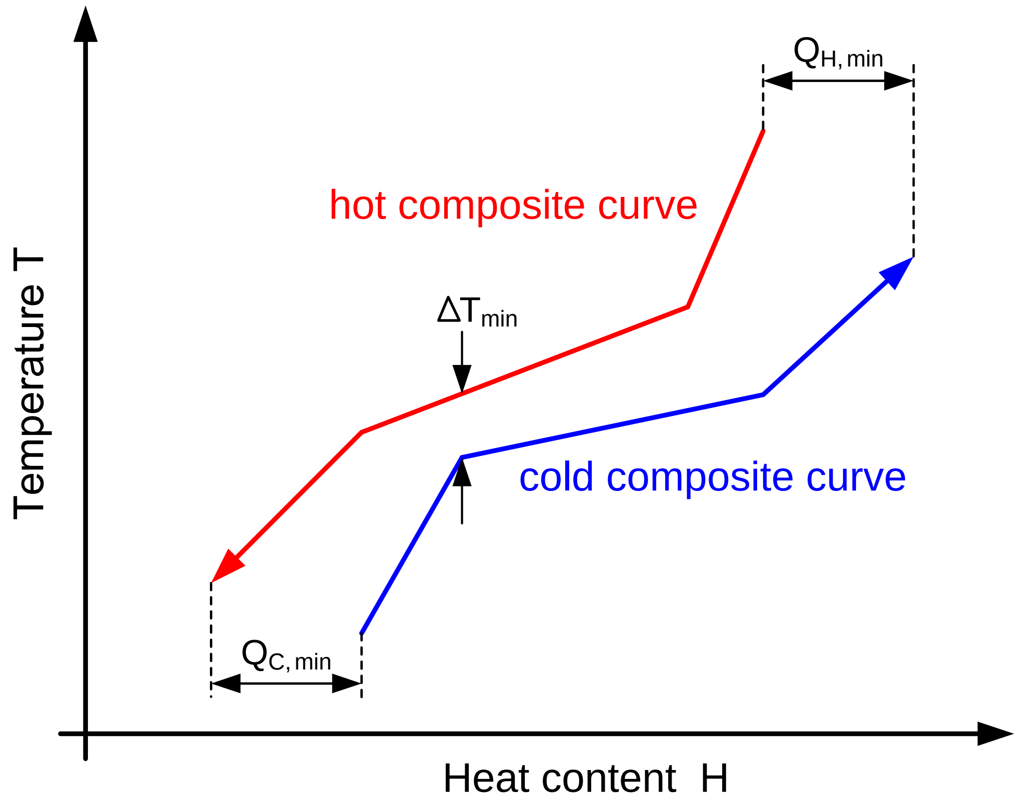
Focus on problem definition and descriptive tools to demonstrate trade-offs in design

<u>Energy Integration</u>

- pinch technology
- heat and power systems
- capital vs. energy

<u>Energy Targeting and HENS</u>

– hot/cold minimum utilities
– matching rules for HEN
– widely effective tool
– easy to teach



# Process Synthesis Concepts

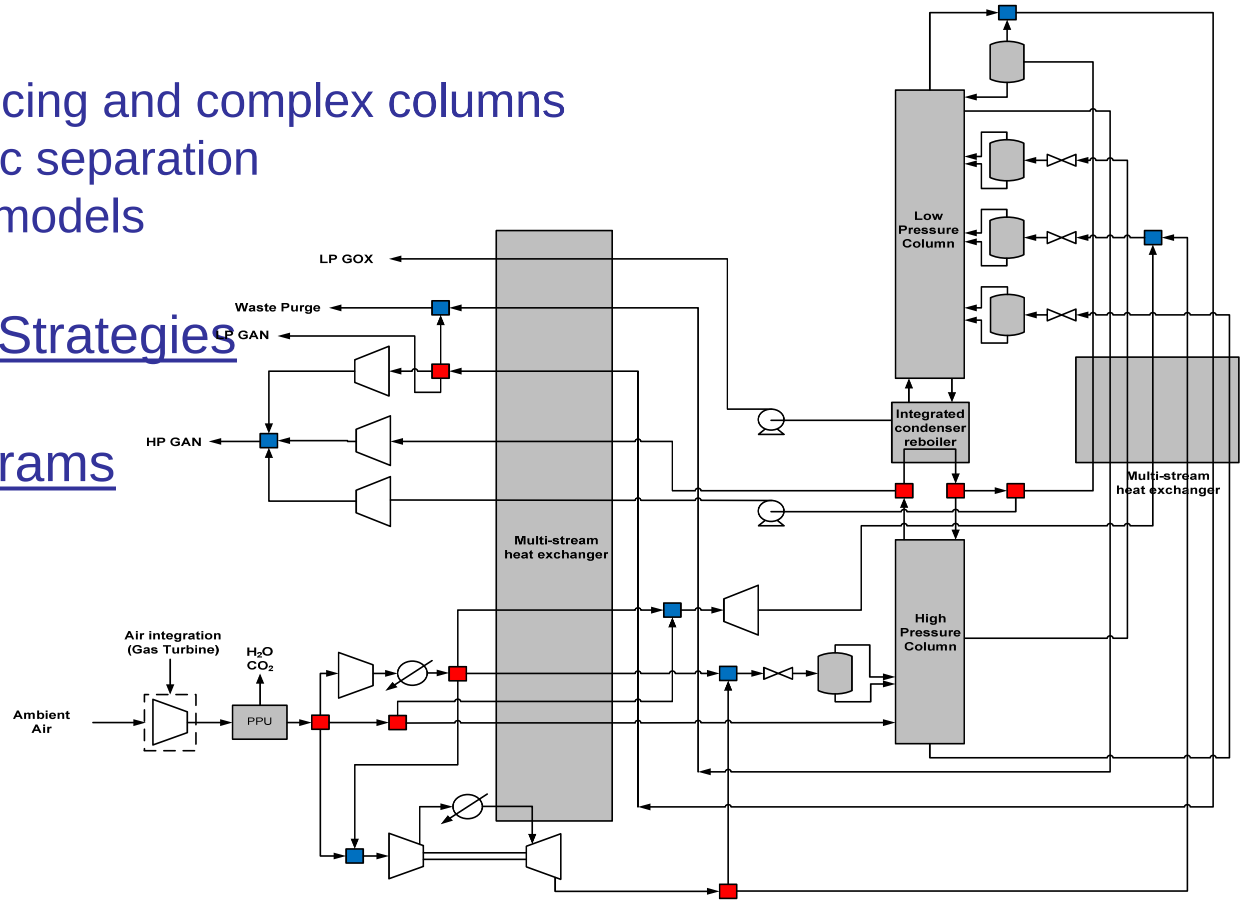
Focus on problem definition and descriptive tools to demonstrate trade-offs in design

<u>Separation Synthesis</u>

- separation sequencing and complex columns
- nonideal/azeotropic separation
- combinatorics vs. models

<u>Effective Sequencing Strategies</u>

<u>Triangular phase diagrams</u>



# Process Synthesis Concepts

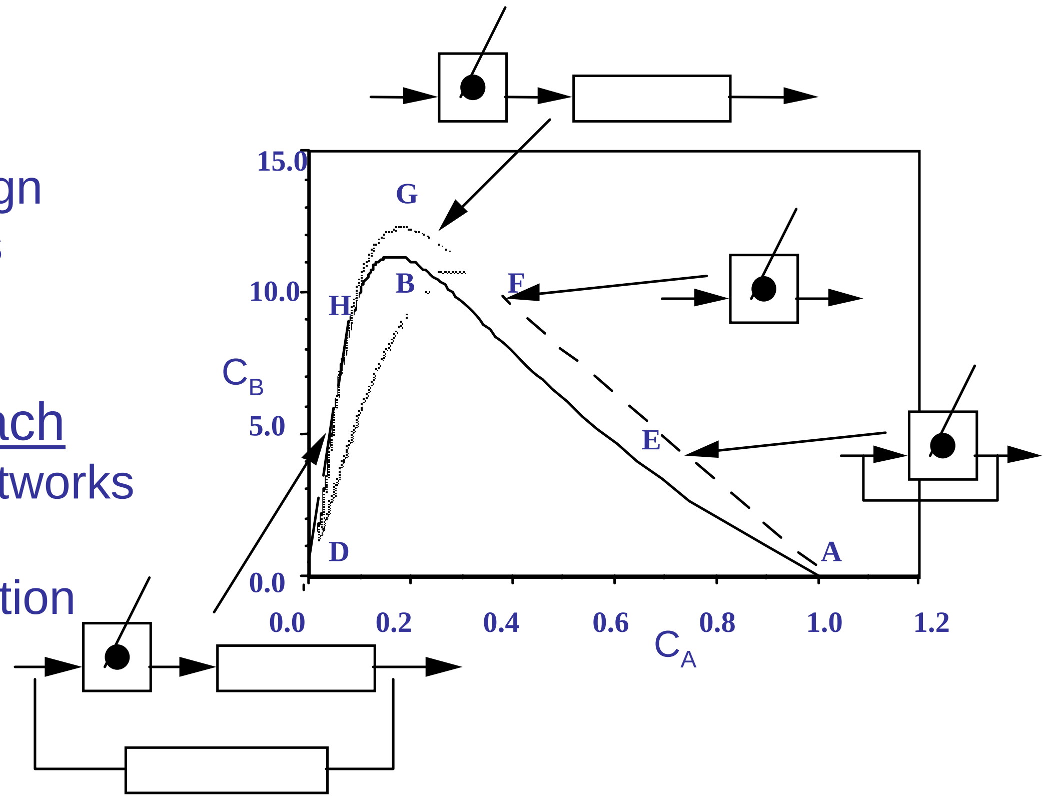
Focus on problem definition and descriptive tools to demonstrate trade-offs in design

Reactors

- beyond reactor design
- networks vs. models
- attainable regions

Novel Graphical Approach

- new insights on networks
- easy to teach
- limited by visualization



# Process Synthesis Concepts

**<u>All of these can be represented and solved as Optimization Problems</u>**

Advanced tools for evaluation of best designs, not just feasible designs

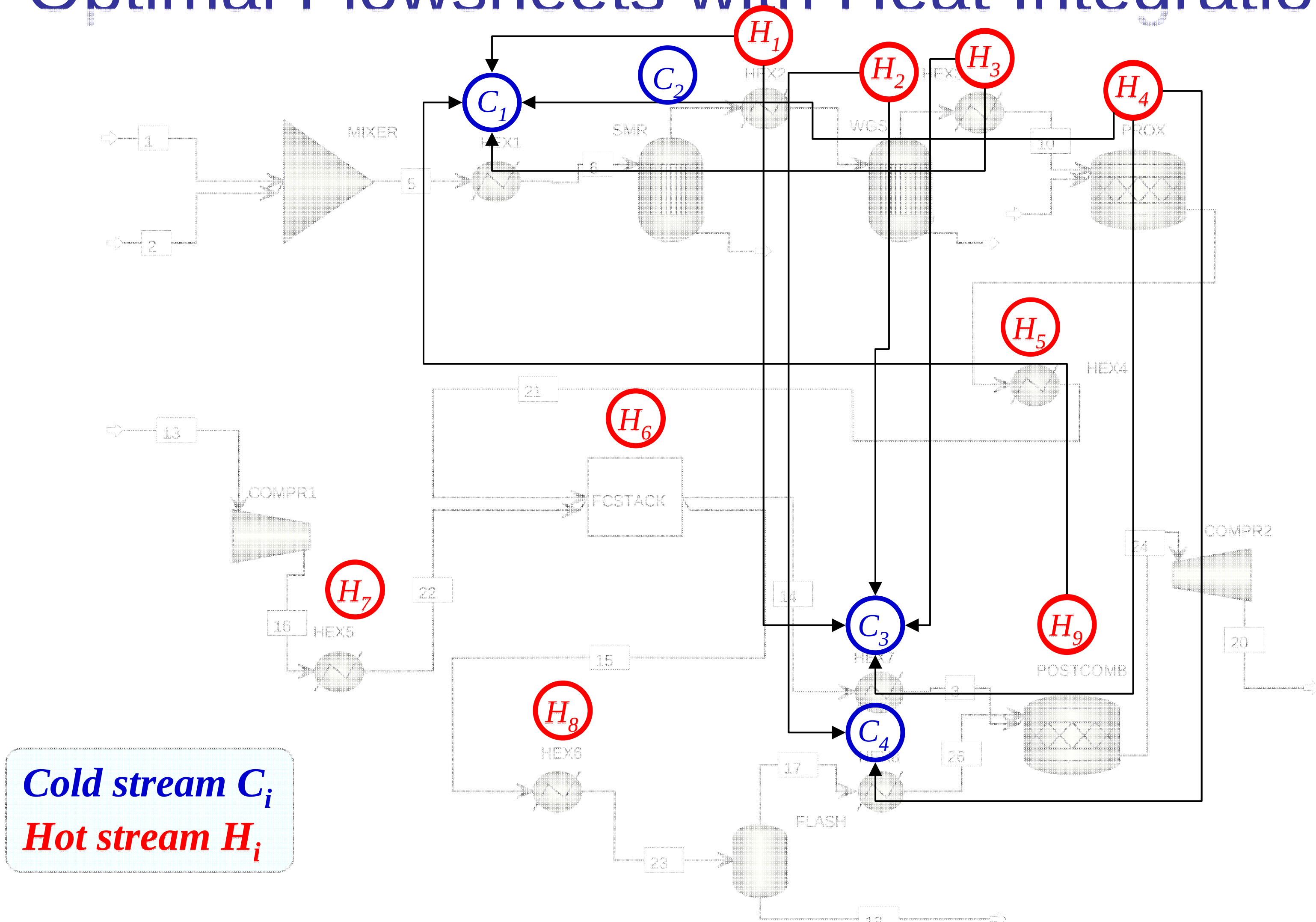
- Assess the best trade-offs
- Deal with uncertainty in the best ways

Extend beyond graphics to more advanced cases (multiple utilities, multidimensional kinetics)

Natural way to integrate design aspects

- Balance economics (capital vs. operating costs vs. environment)
- Integrate subsystems (energy, separation, reaction)

# Optimal Flowsheets with Heat Integration




Optimal trade-off: operating cost, capital, revenue for best heat integrated design

Cannot be obtained with insights and graphical methods

# Teaching Optimization in Design?

**First Semester**

Problem Representation, Graphical Insights

Alternative Generation for Flowsheets and Process Simulation

Metrics for Evaluation – Economics…

**Second Semester**

Optimization formulations and solutions

- GAMS, Aspen/Plus, Excel

Capstone Design Project

- Real-world team projects using advanced tools

# The Future

Systematic decision-making extends to:

- Further integration of multiple objectives, subsystems and modeling platforms
- New processes: energy, bio- and nano- systems
  - Development of models and need for decision-making
- Multi-scale modeling and simulation:
  - Ab Initio, Molecular Dynamics, CFD, Process simulation, Planning, Scheduling
  - Leveraging large-scale decision-making: knowledge of optimization tools and problem formulations