Art Westerberg's Contributions to Process Systems Engineering

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Process Systems Engineering

Application of computing technology & systems engineering methodology to support technical & business decisions in design of chemical/biochemical products & processes and their operation

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Areas of PSE Accomplishments

- Steady State Process Flowsheeting
- Process synthesis
- Process/design optimization
- Dynamic systems modeling
- Process Control
- Process planning/scheduling

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

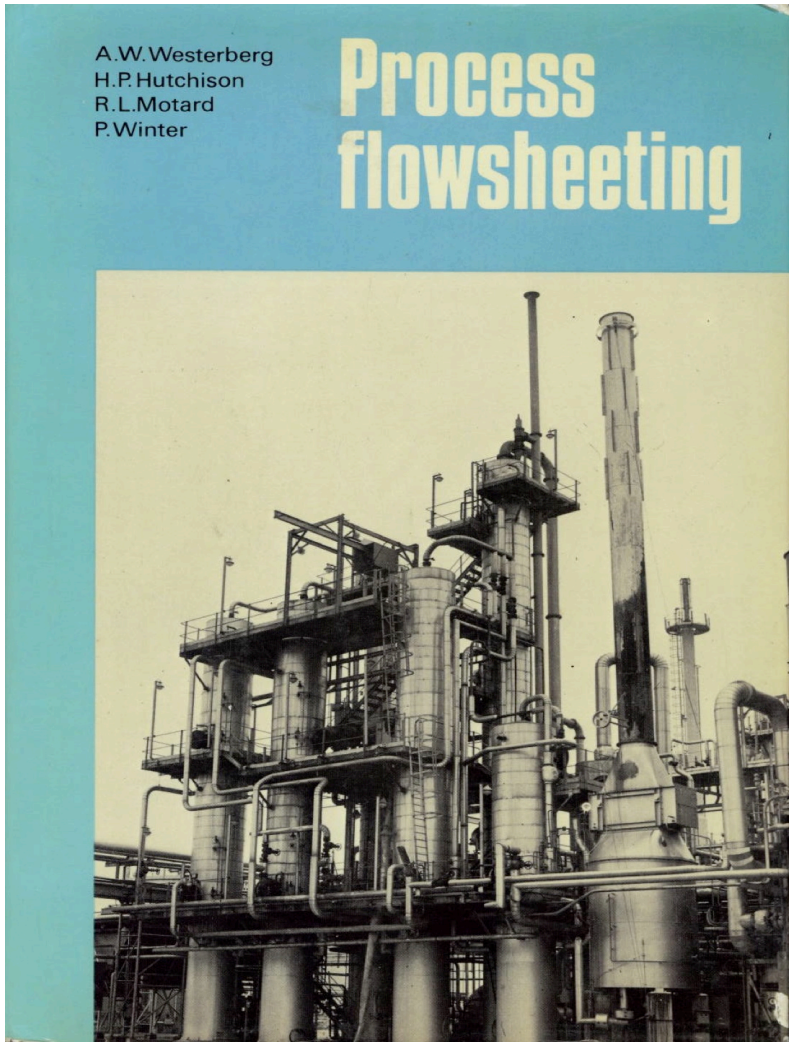
Westerberg & Flowsheeting

Steady State Flowsheeting

- Unit ops & properties models
- Approaches to model assembly
- Computational strategies for convergence/solution

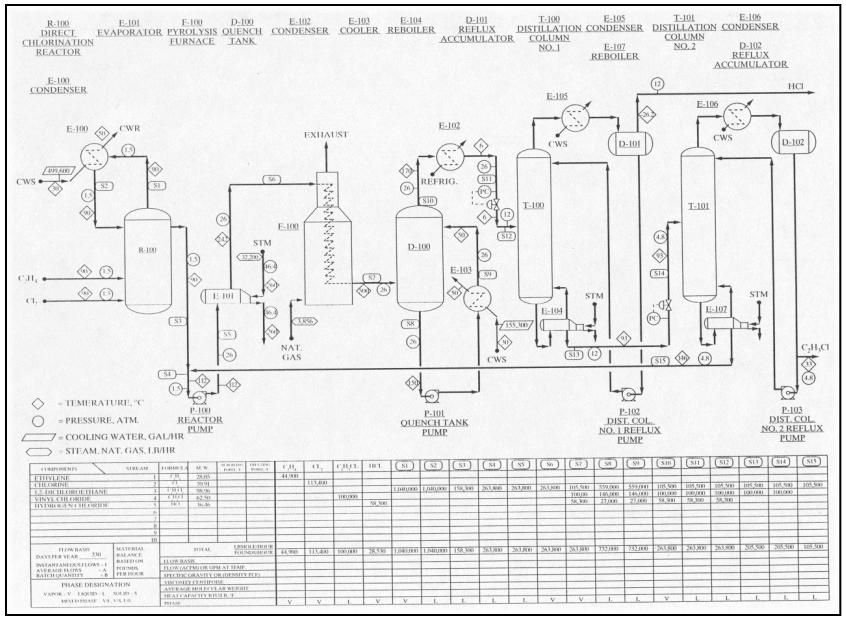
Issues pursued

- Sequential modular strategy
  - Tearing & convergence
- Equation-based simulation
  - Output assignment
  - Equation decomposition
  - Sparse matrix methods
  - Sequencing indexed equation sets
  - Newton-based computation



Cambridge University Press, 1979

Flowsheeting



Software realizations

- SPEED-UP (1964)
- ASCEND-II

Westerberg & Benjamin

"Thoughts on a Future Equation-Oriented Flowsheeting System"

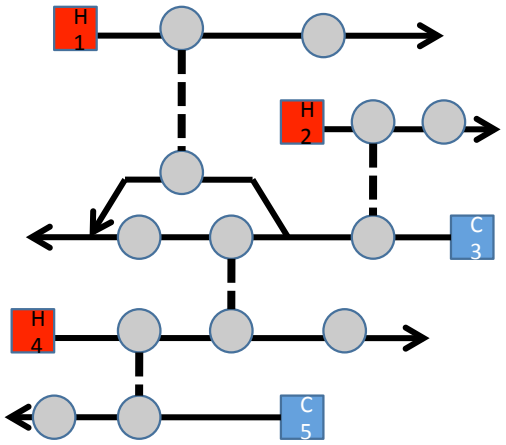
Comp Chem Eng 9(5) 1985

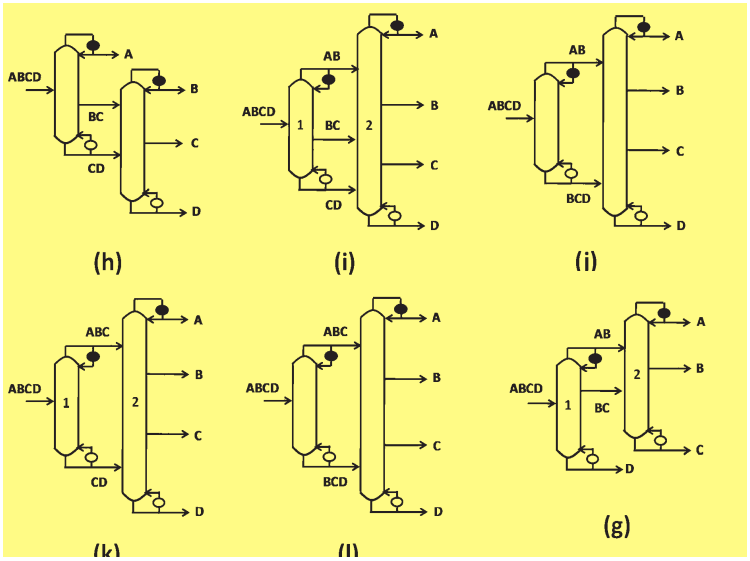
Important Issues

- Storage, retrieval, reuse & repurposing of models
- Language for model building
- Treatment of procedures
- Hierarchical models
- Decomposition/ordering
- Initialization/scaling
- Convergence
- Intelligent user interaction

Westerberg & Process Synthesis

- Systematization of the Invention of Process Flowsheets
- Problem categories
  - General process flowsheets
  - Retrofit designs
  - Heat & power exchange networks
  - Distillation sequences
  - Evaporator sequences





Nishida, Stephanopoulos, Westerberg
"Review of Process Synthesis"
AIChE Journal 27(3) 1981

Process Synthesis

Specific contributions

- Heat exchange
  - Min No of units; Min utilities
  - Restricted matches
  - Heat integrated batch processes
- Distillation sequences
  - Conventional non-sharp/ sharp
  - Heat integrated distillation
  - Azeotropic distillation
  - Reactive distillation
  - Batch distillation sequences

Approaches

- Evolutionary
- Branch & bound enumeration
- Expert systems / Knowledge based
- Systematic enumeration of configurations

Implementation

EROS, SPLIT I & II

Westerberg
"A retrospective on design and process synthesis"
Comp Chem Eng 28(4) 2004

Westerberg & Process Optimization

Large scale NLP

- Projected gradient & Active constraint strategies
- Method of Multipliers & duality gaps*
- Reduced space form of Powell's/ SQP approach

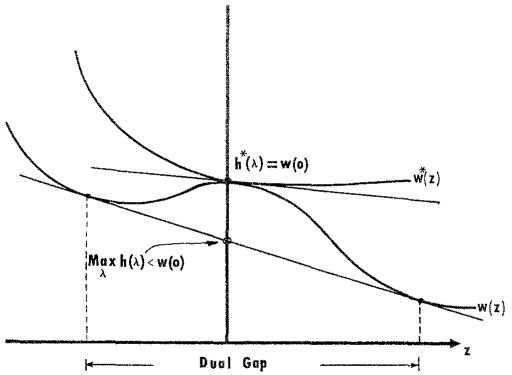
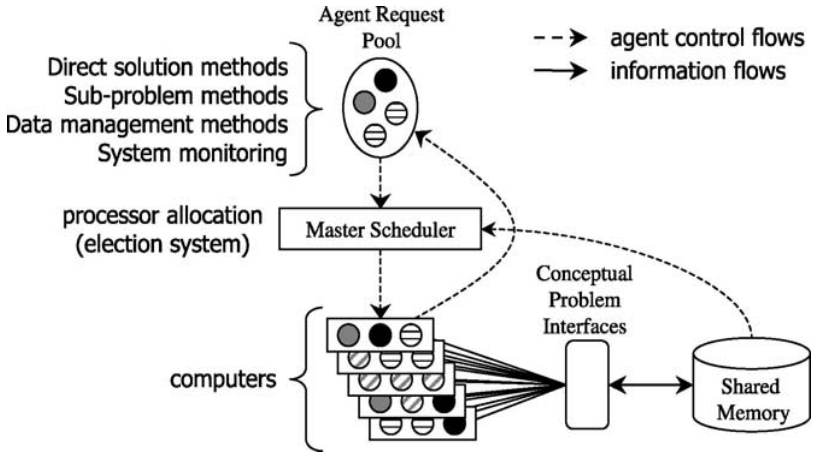


Fig. 2. Failure of the dual approach to yield the primal solution.

*Stephanopoulos & Westerberg, J. Opt.Thry Appl. 15(3) 1975

Alternative objectives

- Global optimization
- Multi-objective optimization
- Bilevel optimization
- Use of distributed agents**



**Siirola et al, "Towards agent-based process systems engineeering", Comp Chem Eng 27 (12) 2003

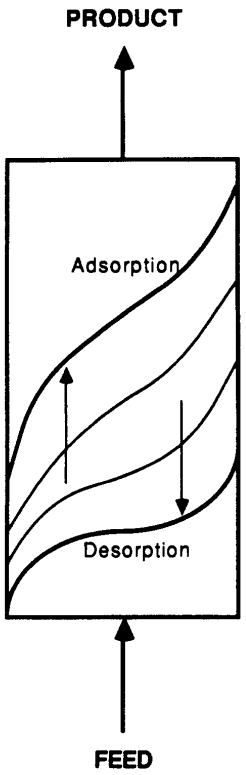
Westerberg & Dynamic simulation

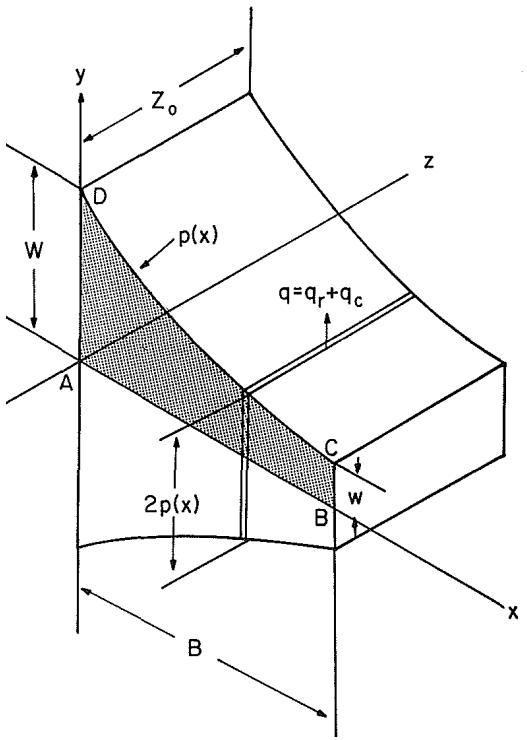
Numerical issues

- Latency in flowsheet simulation
- High index DAE models
- Near index / stiff models
- Moving grid finite element methods

Applications

- Pressure swing adsorption
- Extended heat transfer surfaces





Chung & Westerberg, "A proposed numerical algorithm for solving nonlinear index problems", Ind Eng Chem Res 29(7) 1990

Hrymak et al, "An implementation of a moving finite element method", J Comp Phys 63(1) 1986

PSE areas for 21st Century

- Computer-aided environments for PSE practice
- Product centric design & development
- Enterprise-wide optimization
- Risk Management

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

Westerberg & CA design environments

Model management

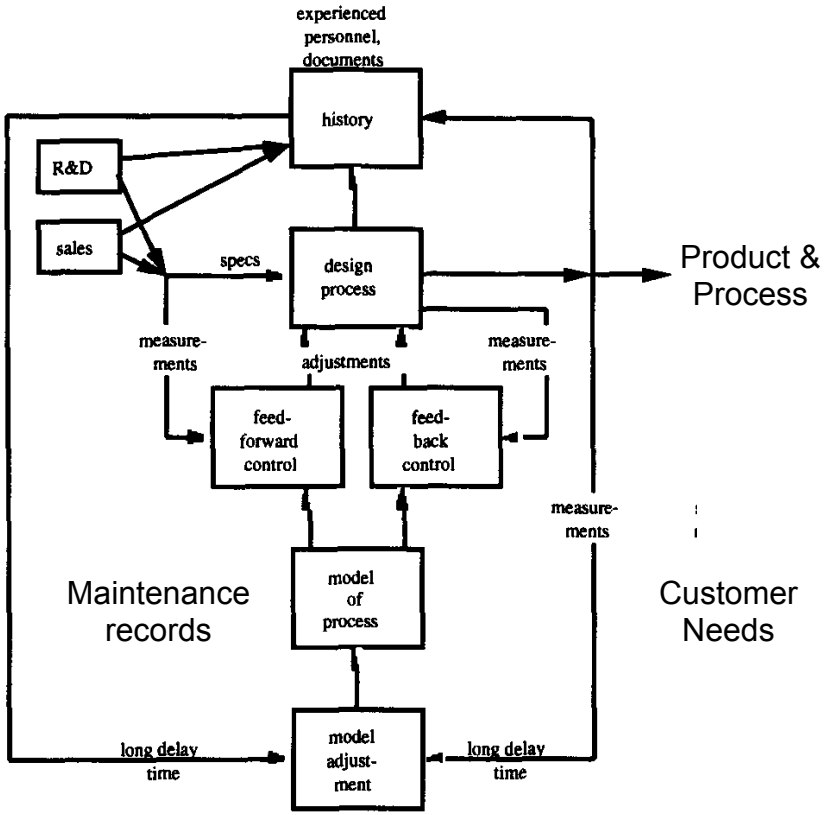
- Modeling language
- Robust solution processes
- Model reuse & repurposing
- Version management

Collaboration environments

- Formalize work flows
- Model information
- Retain history
- Manage access & ownership
- Capture knowledge

Software Implementations

- SOAR, ASCEND, n-dim



Piela et al, "ASCEND: An O O Computer Environment for Modeling & Analysis: Part 1", Comp.Chem Eng 16(1)1991

Westerberg et al, 'Designing the Process Design Process", Comp Chem Eng 21 (S) 1997

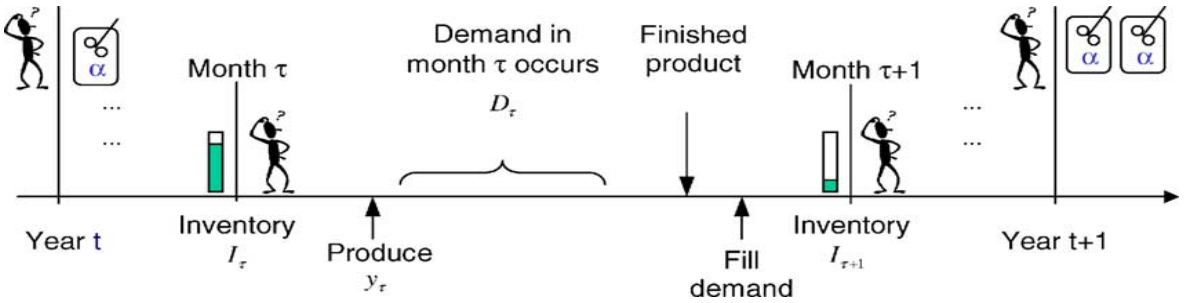
PSE areas for 21st Century

- Computer-aided environments for PSE practice
- Product centric design & development
  - Westerberg & Subrahmanian, “Product Design” (FOCAPO 2000)
  - Banares-Alcantara et al, “Decade: A Hybrid Expert System for Catalyst selection”, Comp Chem Eng (1987,1988)
- Enterprise-wide optimization
- Risk Management

Westerberg & Enterprise Optimization

Capacity planning & production scheduling under uncertainty

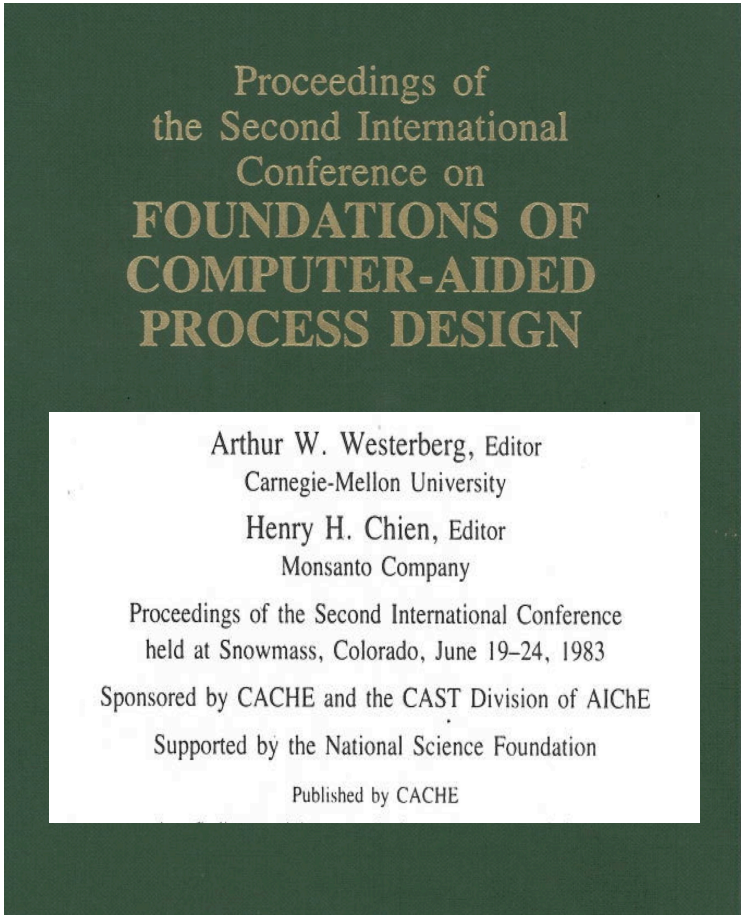
- Sequential decision making under uncertainty
- Select capacity, technology, inventory & production level
- Maximize profit & minimize downside risk
- Strategies
  - Multistage stochastic programming problem
  - Multi-objective Markov decision problem
  - Stochastic optimal control approach
  - Simulation-based optimization



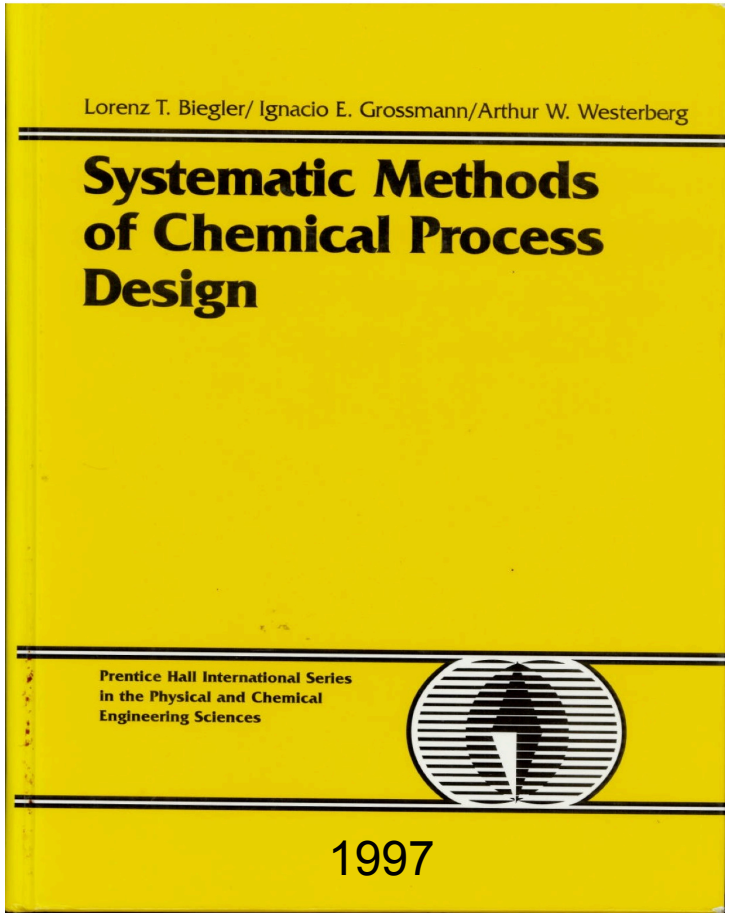
Cheng et al, "Design & planning under uncertainty", *Comp Chem Eng* 27(6) 2003
Cheng et al, "Multiobjective decision processes under uncertainty", *Ind Eng Chem Res* 44(8) 2005

Contributions to PSE Community

Major Symposium



Education



Summary

- AWW major contributions to PSE technology
  - Steady state & dynamic flowsheet simulation
  - Process synthesis: problem formulation & synthesis methodologies
  - Optimization: algorithms & problem structure
  - CA Environments to support design process
  - Conceptualization of stochastic decision problems of enterprise-wide perspective
- AWW major contributions to PSE community
  - Dissemination, education & training

Happy & Healthy 75th !

Art