Process Systems Engineering and CAPE – What Next?

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What is Process Systems Engineering (PSE) & CAPE?

PSE: Use of a systematic approach to problem solving!

CAPE: Use of computer aided and systematic approach to solving process engineering problems!

Scope & Significance of PSE/CAPE is potentially very large and depends on the application range of the developed solution approaches.

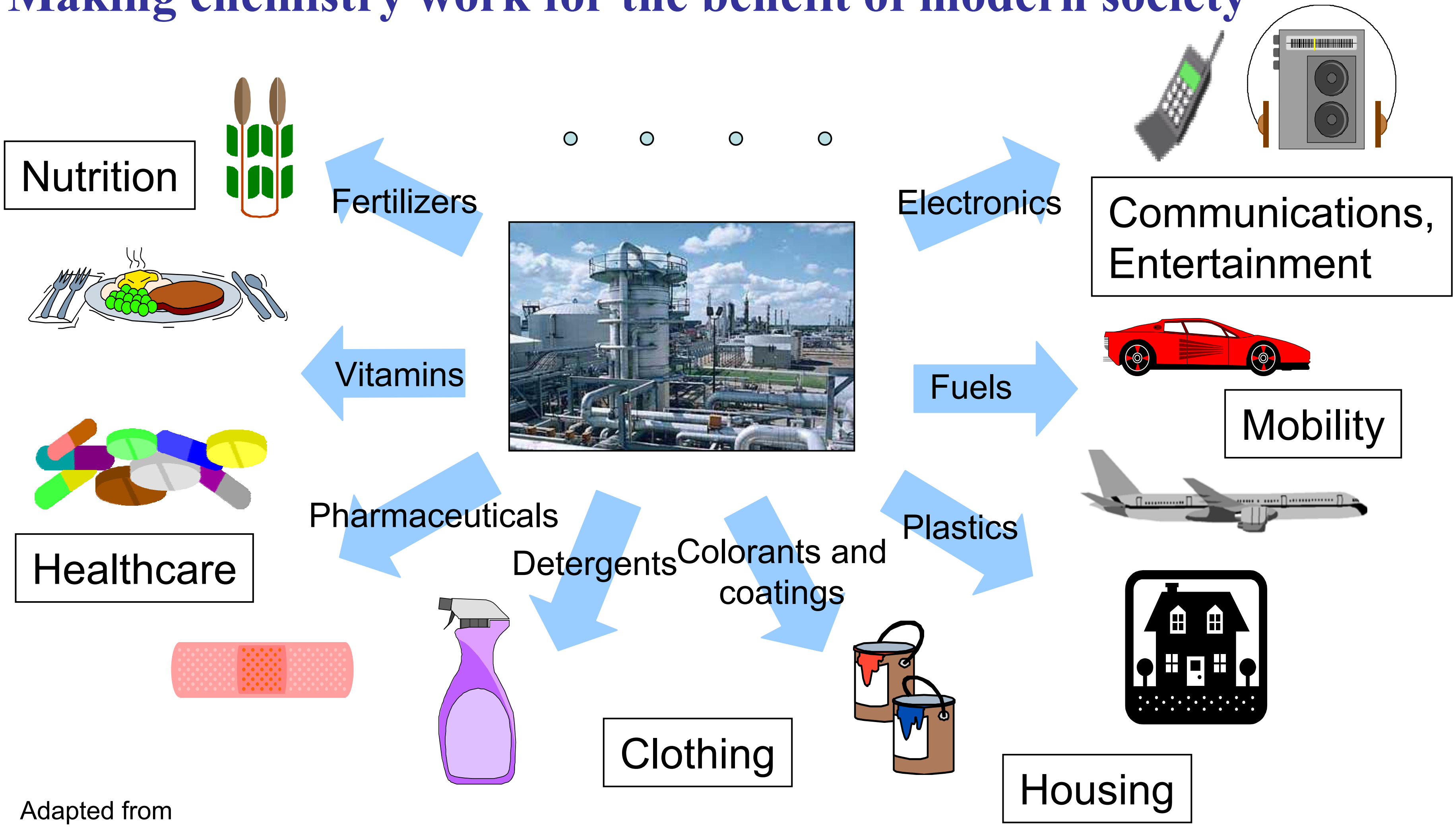
Takamatsu (1982), Sargent, …. (PSE meeting, 1982)

Outline

- **Role, scope & challenges for PSE/CAPE**
- **The ”basic” products of PSE/CAPE**
- **The framework for problem solving in PSE/CAPE**
- **Future research challenges in CAPE/PSE**
  - **Product-process synthesis, design, analysis**
  - **Energy & sustainability**
  - **Enterprise-wide optimization**
- **Remaining challenges in core PSE/CAPE**
- **Concluding remarks**

Current trends in application of Chem Eng

Making chemistry work for the benefit of modern society

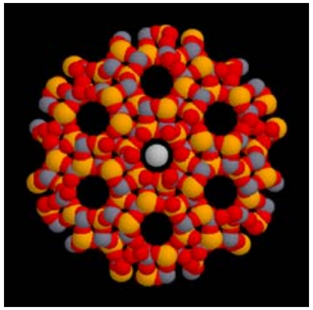


Adapted from Ploecker, 2005

Role, Future Scope & Challenges for PSE/CAPE?

1. What is the role of Process Systems Engineering in "commodity" industry vs. "new emerging" technologies?

Value preservation vs. Value creation



2. What is the future scope for fundamental contributions in Process Systems Engineering ?

Engineering vs. Science

3. What are Research Challenges in Process Systems Engineering?

Managing Complexity

Observations - 1

Trade-offs: Value preservation vs. Value growth
Chemicals/Fuels vs. Pharmaceutical/Biotechnology

Major real world challenges
Globalization, energy, environment, health

⇒Expand the scope of PSE/CAPE

Research trend away from Chemical Engineering
Science vs Engineering

⇒Maintain core of PSE research

Observations - 2

Trade offs: Value preservation versus value growth

Continuous processes versus batch operations

Low value – high rate or high value –low rate?

Wider scope of Chemical Engineering, PSE/CAPE

Chemicals: Simple/small versus large/complex

Products: Single function versus multifunction-structured

Major real world challenges

Process-product performance: single criterion versus multicriteria

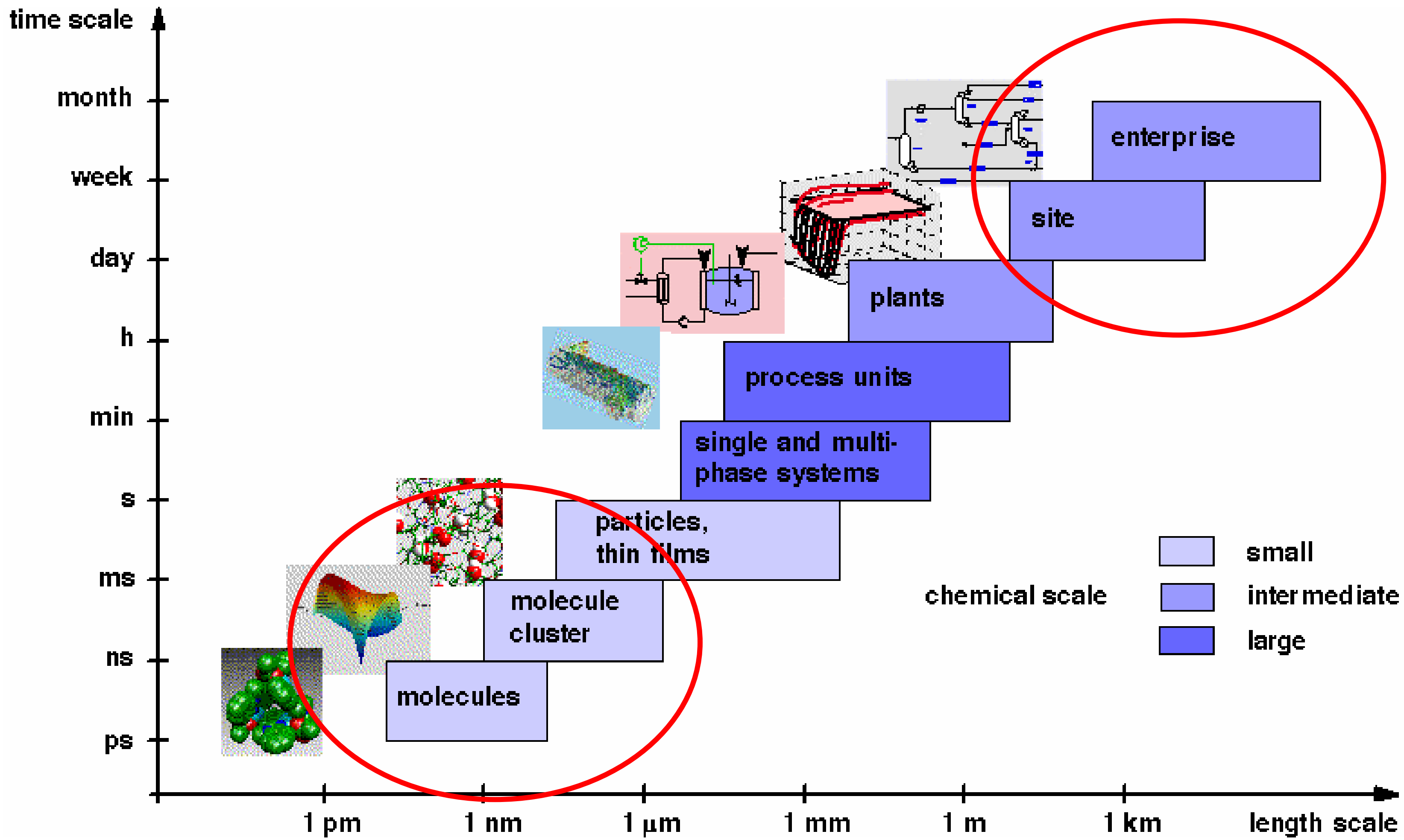
Integration: Process-product; methods; tools; …….

Sustainability: Economic versus economic-social-environmental

⇒Need to expand the scope of PSE/CAPE from a solid foundation of the core!

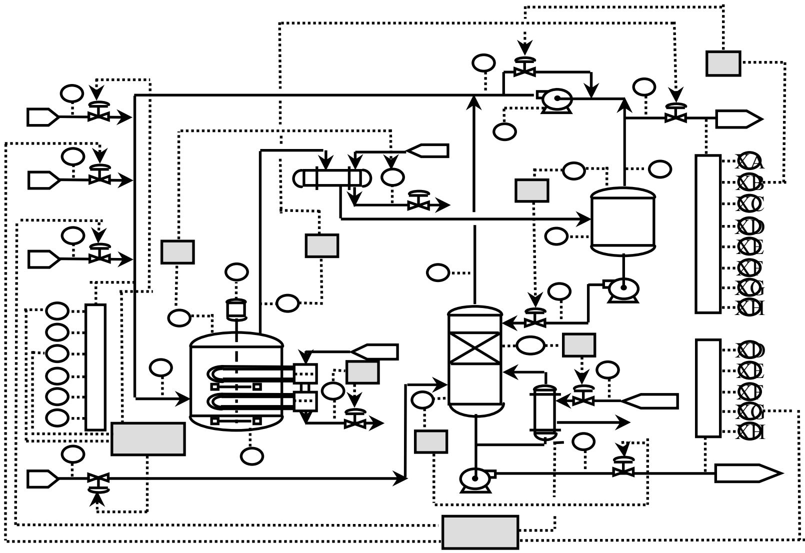
Example: Expanding the Scope in Chemical Supply Chain

(Grossmann & Westerberg, 2000; Marquardt et al, 1998)



Example of multiscale: From “Bulk” to “Molecular” Processing

George Stephanopoulos (2004)

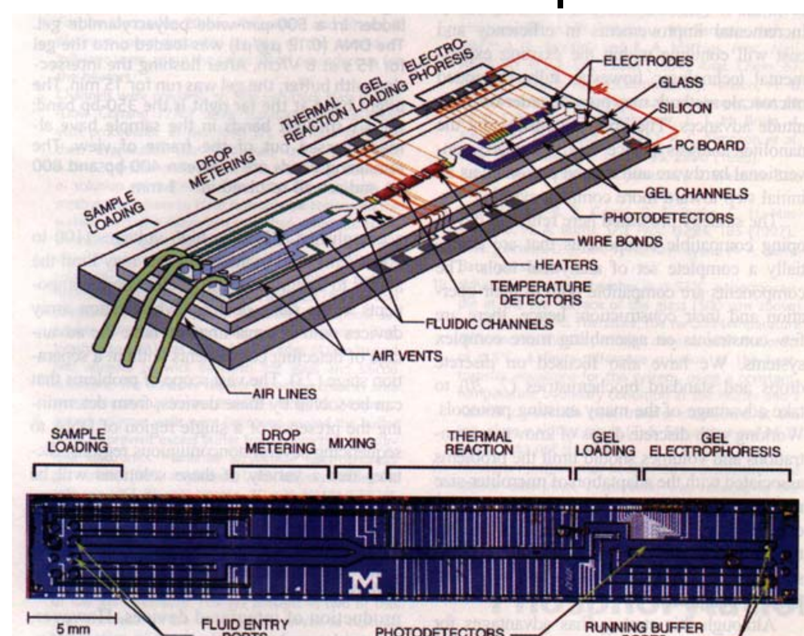


Macro-Processing:

Batch or Continuous Chemical Plants

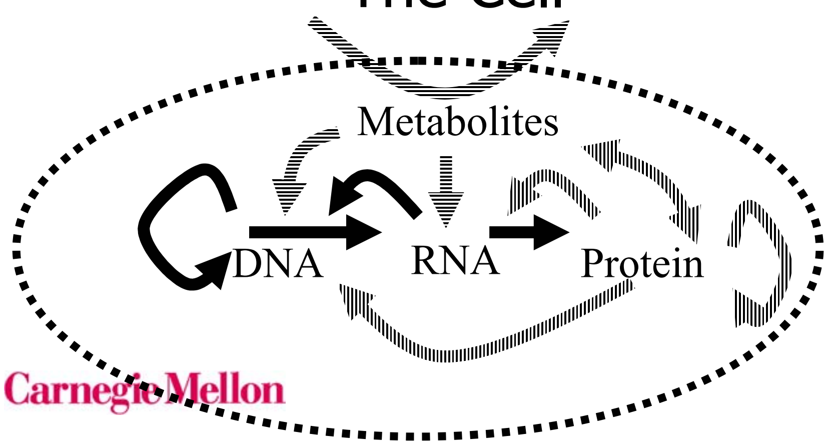
Micro-Processing:

Plant-on-a-Chip



Molecular-Processing:

The Cell



Scope of the basic "products" of PSE/CAPE

Numerical analysis => **Simulation**

Mathematical Programming => **Optimization**

Systems and Control Theory => **Process Control**

Computer Science => **Advanced Info./Computing**

Management Science => **Operations/Business**

Math Programming & Control Theory "competitive" advantage

Extend the scope of the basic "products" of PSE/CAPE

Numerical analysis => Simulation => Behavior of process-product

Mathematical Programming => Optimization => Synthesis/design

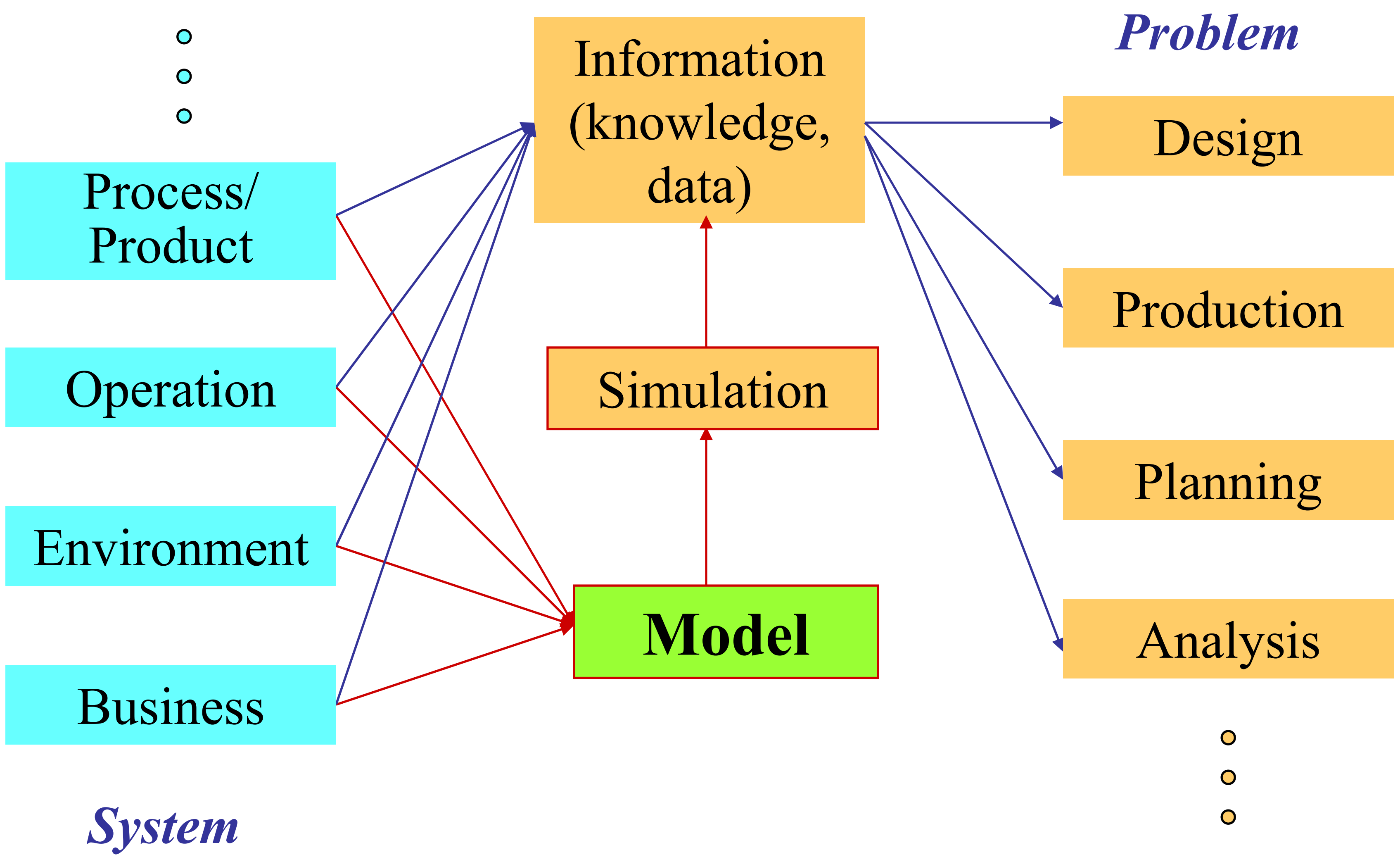
Systems and Control Theory => Process Control => Manufacture

Computer Science => Advanced Info./Computing => Efficient problem solving

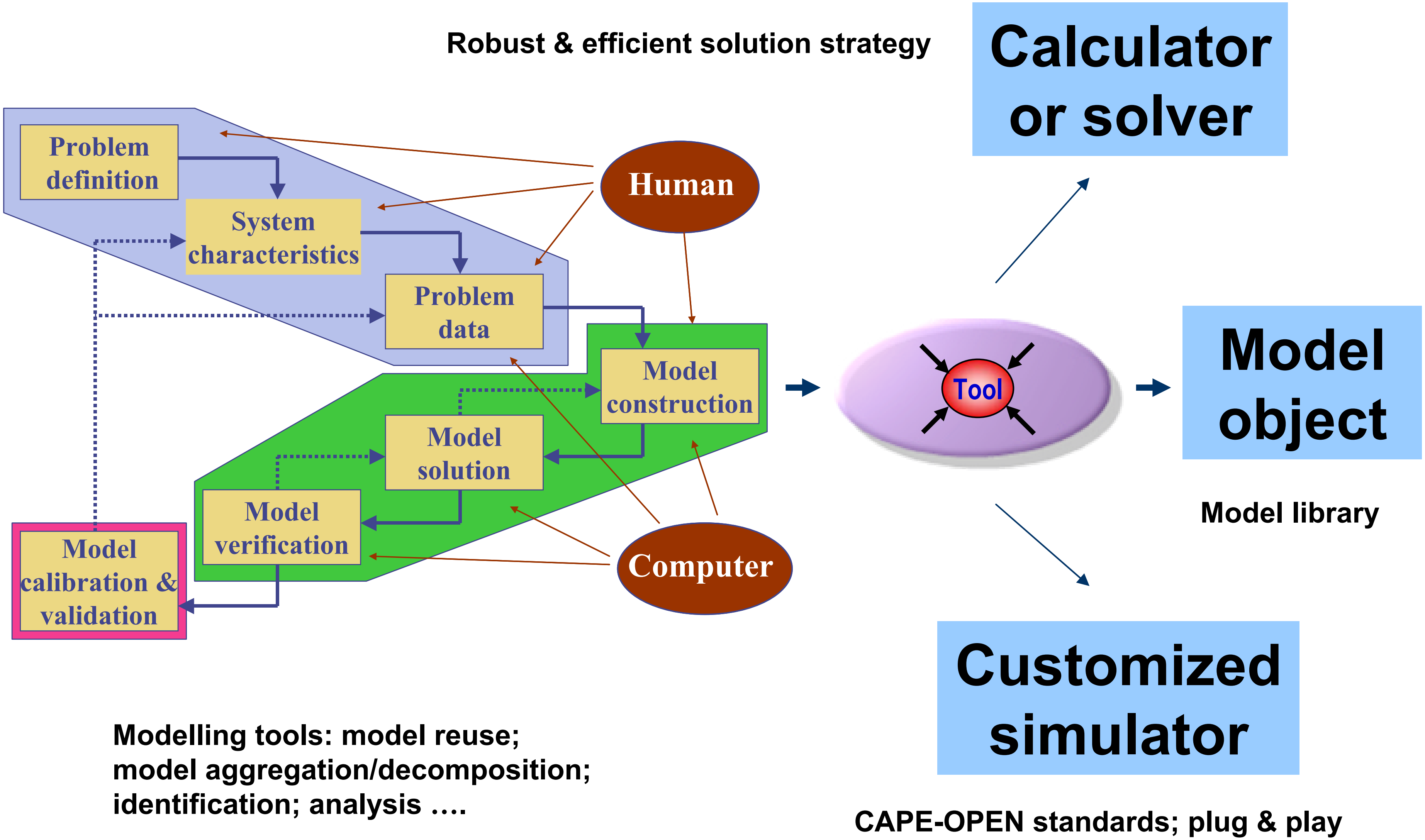
Management Science => Operations/Business => Supply chain

What is necessary is models of various types, forms and application range

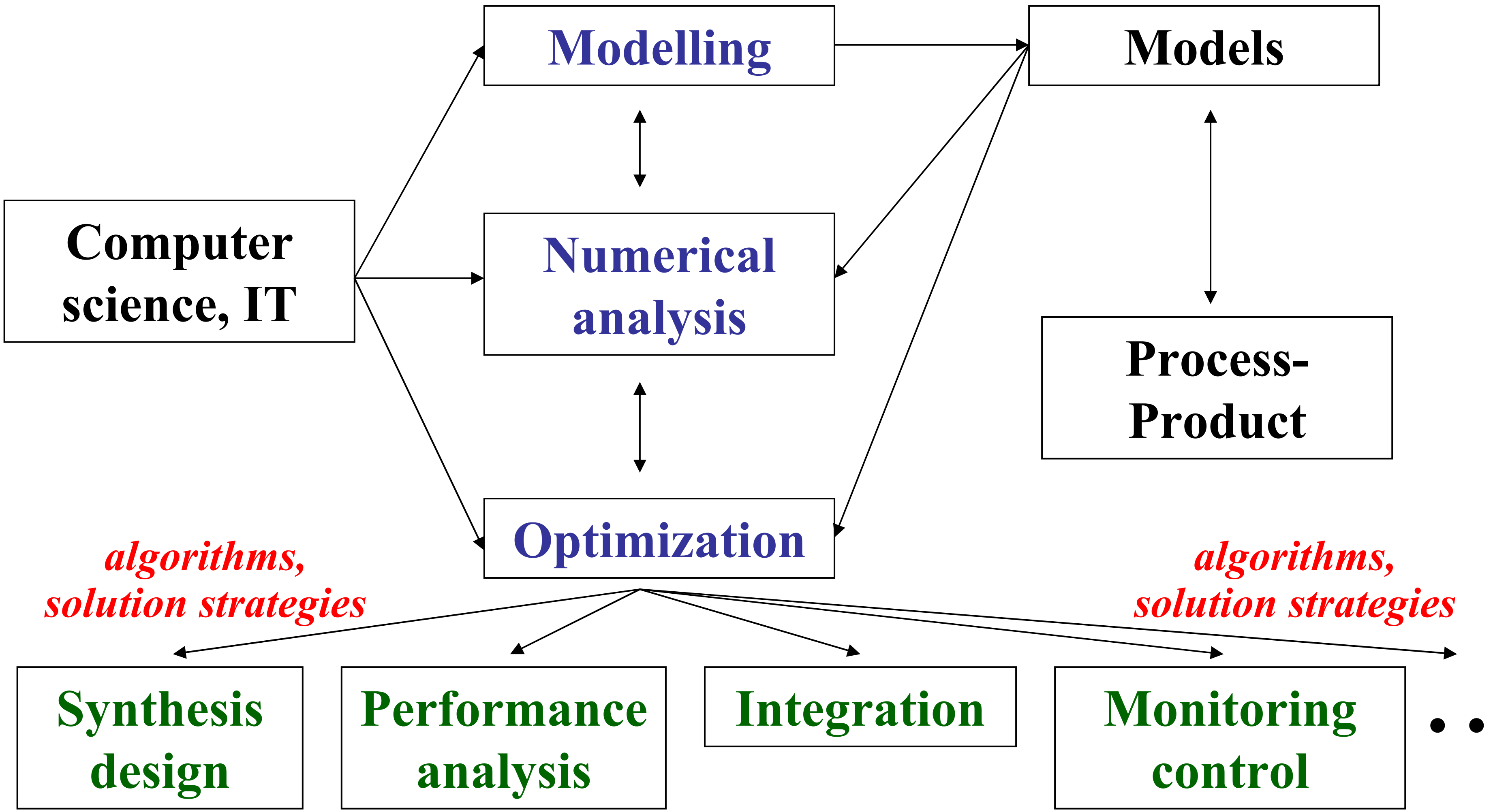
The role of models in PSE/CAPE



Computer aided modelling framework



Framework for problem solving in PSE/CAPE



Future Research Challenges in PSE

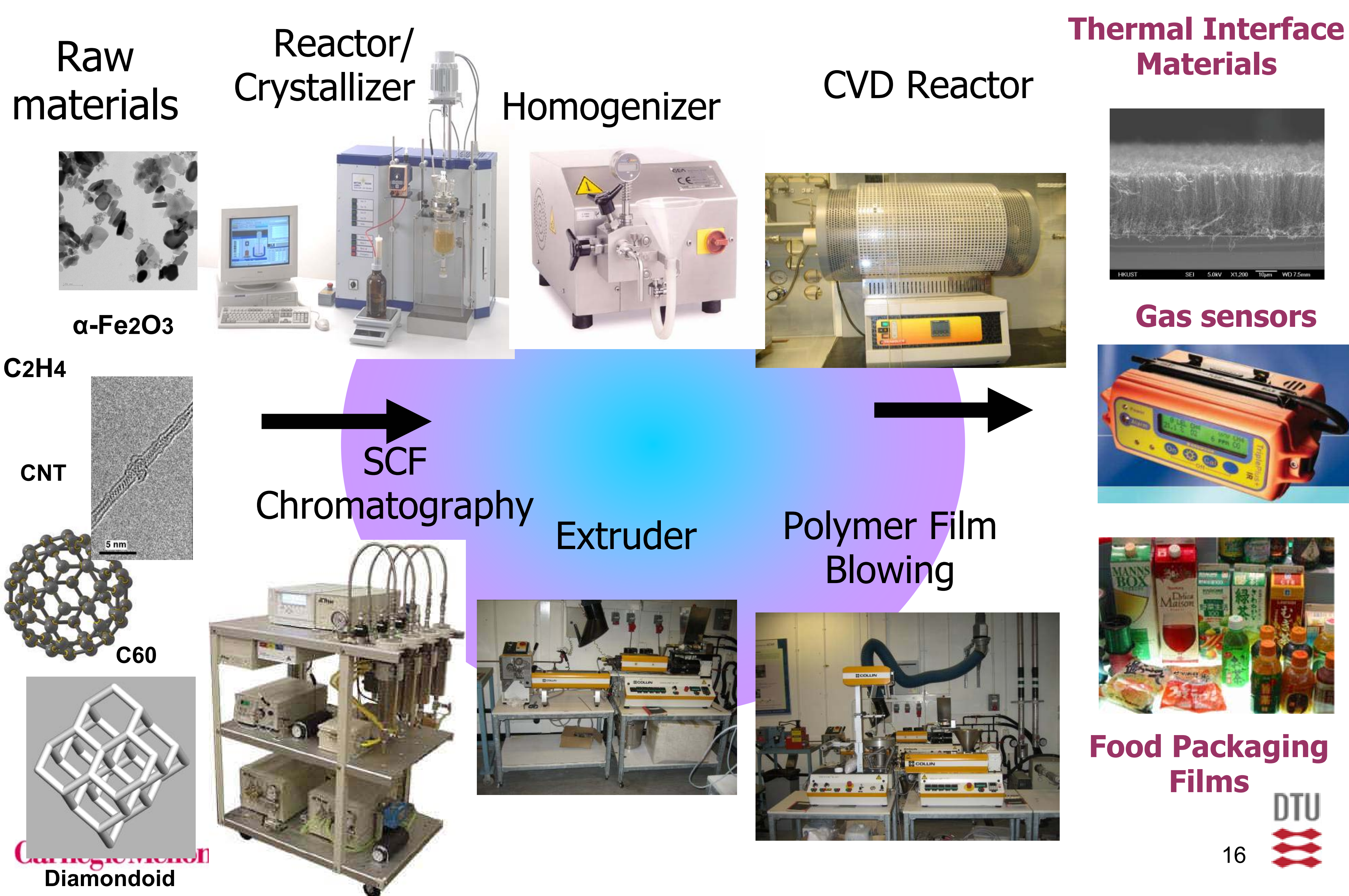
I. Product and Process Synthesis, Design, Analysis

II. Energy and Sustainability

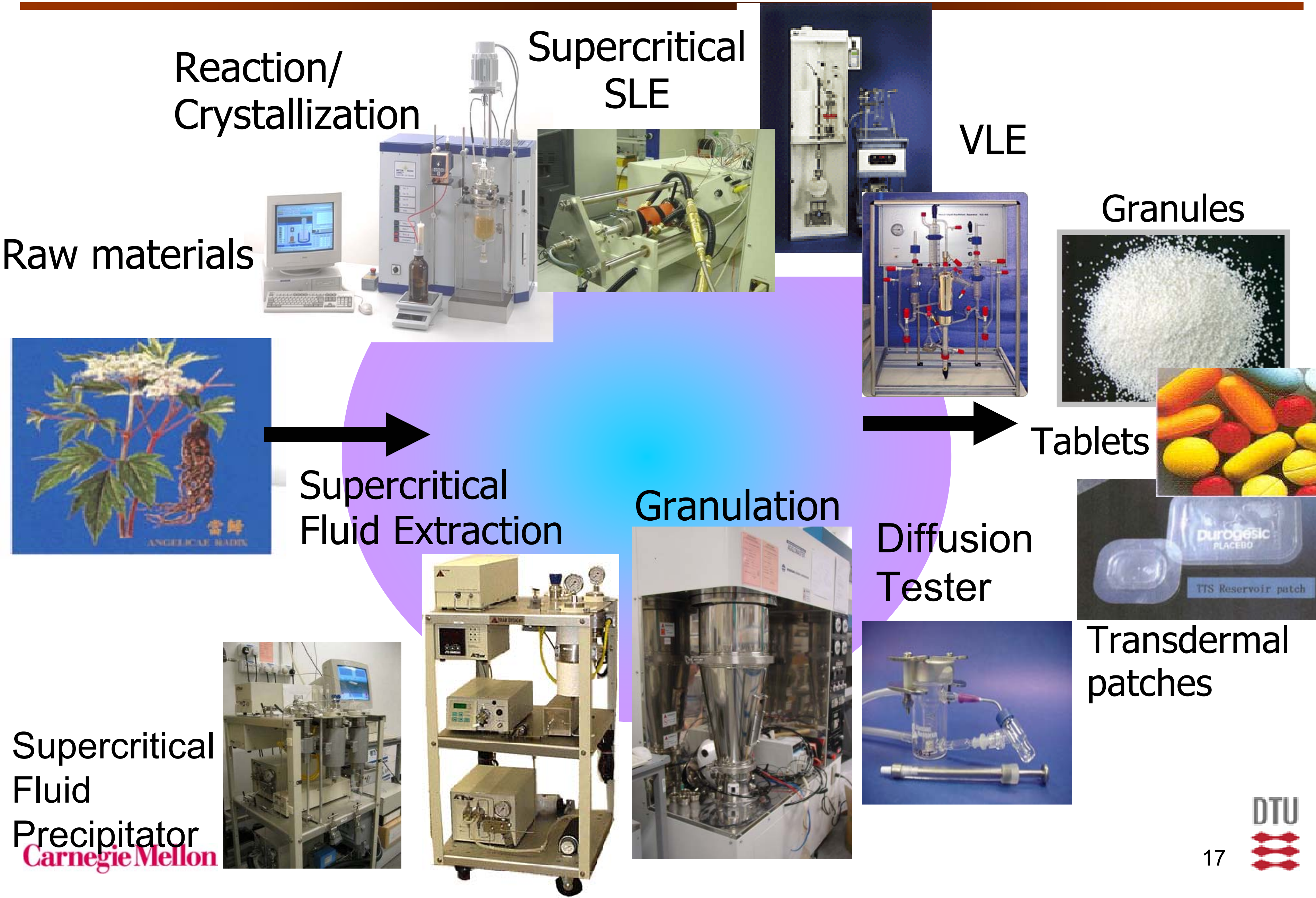
III. Enterprise-wide Optimization

Raw Materials to Consumer Products

Ka Ng (2006)

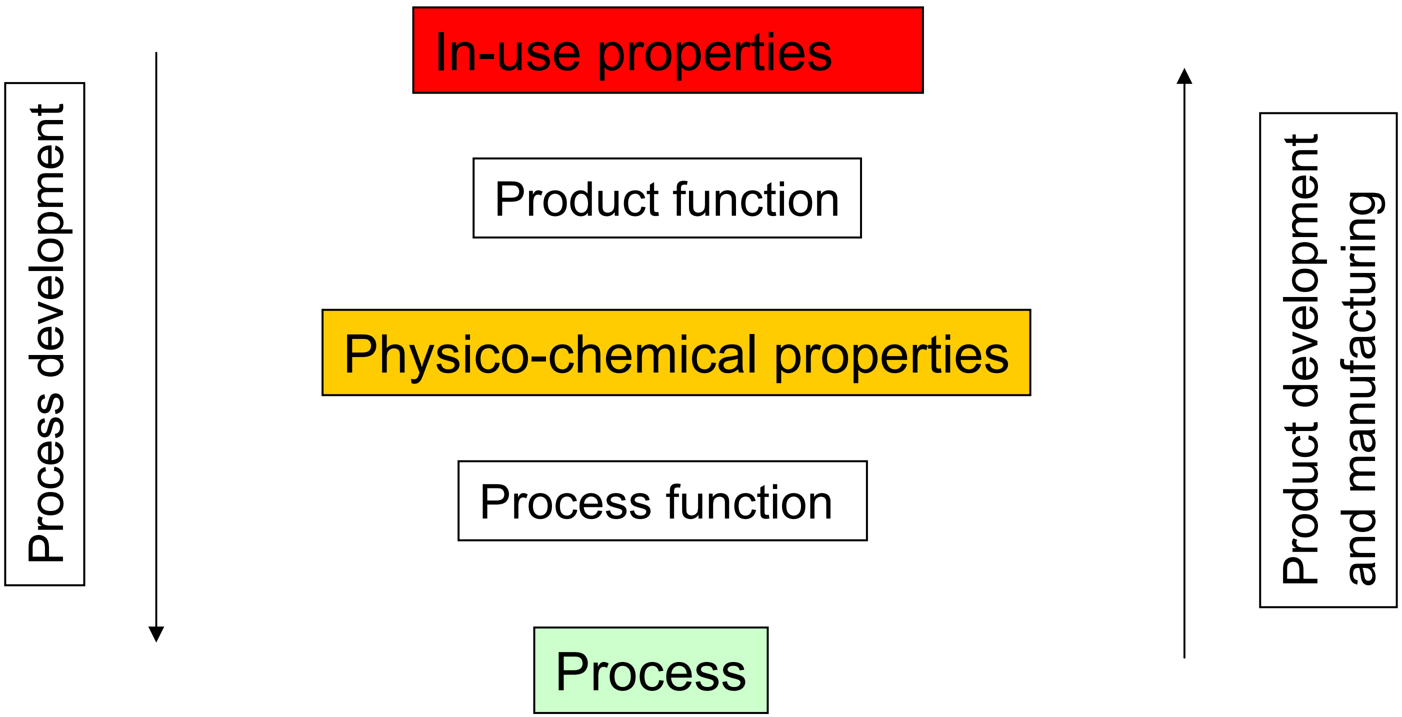


Natural Herbs to Healthcare Products *Ka Ng (2006)*



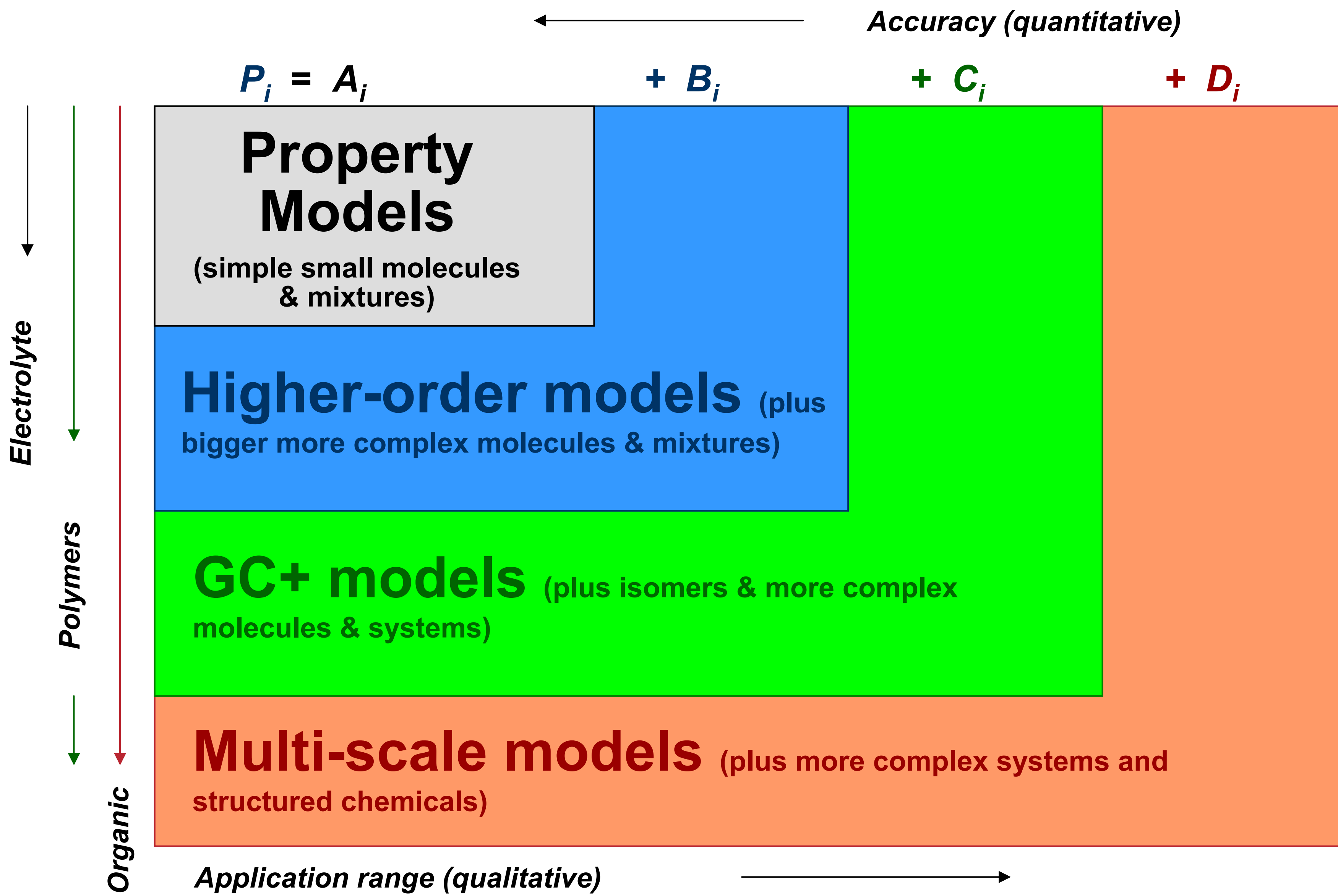
I. Product and Process Synthesis, Design, Analysis

„Nowadays, chemical products are not sold for what they are but, for what they do"

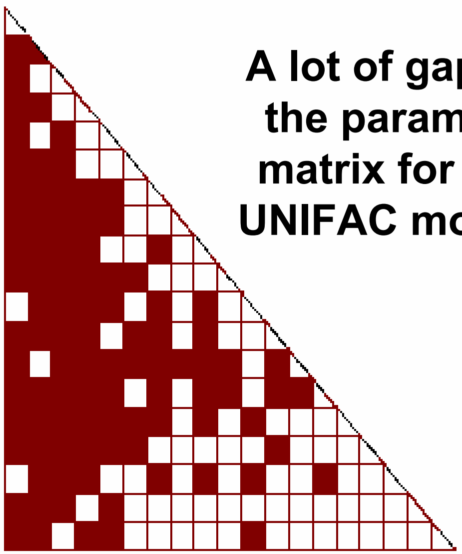


M. Kind, 2005

Extend scope through predictive constitutive models

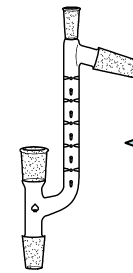


How to extend the application range without new experimental data?



A lot of gaps in the parameter matrix for the UNIFAC model!

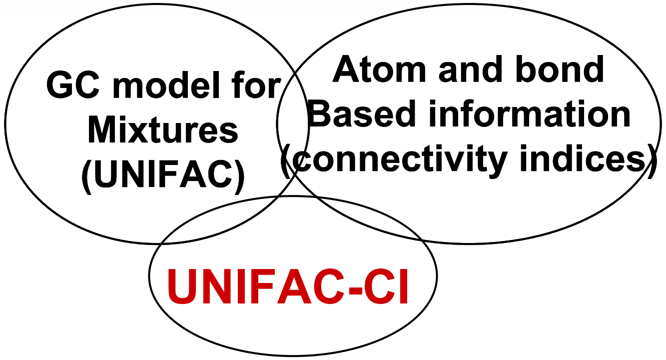
VLE, SLE, LLE experiments to collect data



Usually time consuming and expensive and may not be possible

By using only atom and bond information of the groups describing the molecules

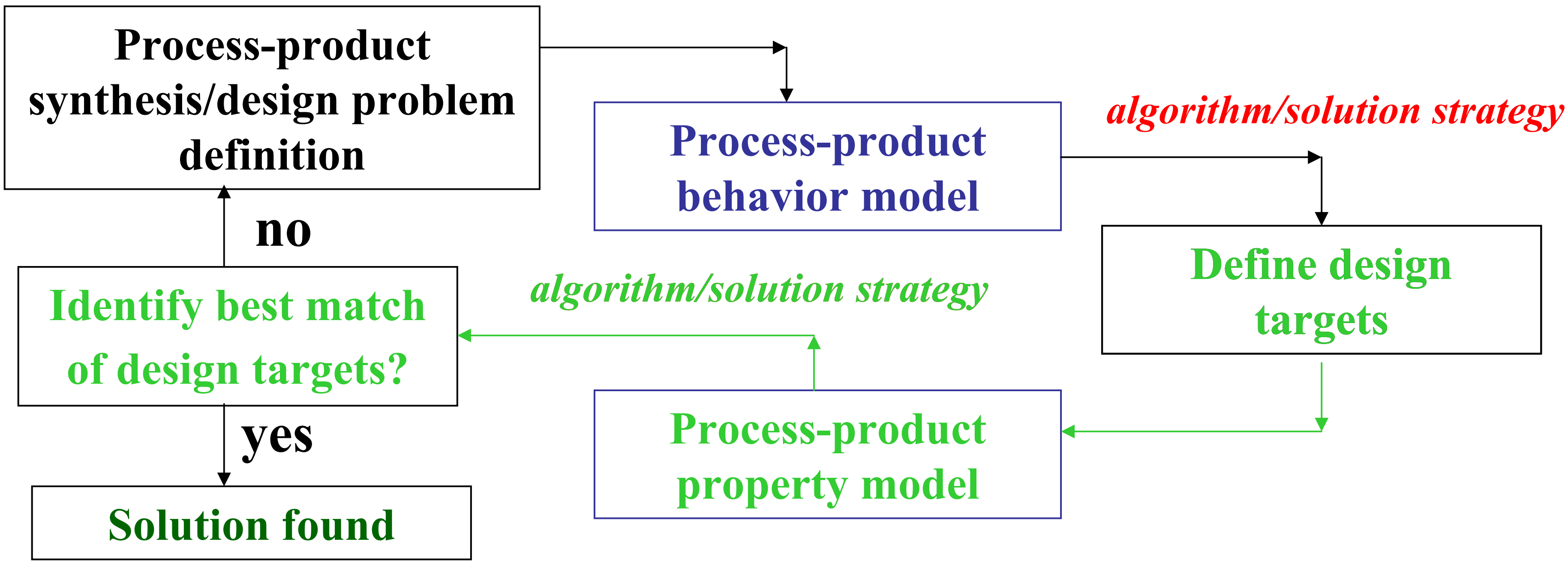
Fill the UNIFAC parameter matrix using the published VLE, SLE and LLE data



- Without any extra experimental data
- With reasonable accuracy
- Solution Approach: Modelling, IT, optimization

Gonzalez et al. A method for prediction of UNIFAC group interaction parameters, AIChE J (2007)

Use of the Model-Based Reverse/Inverse Approach



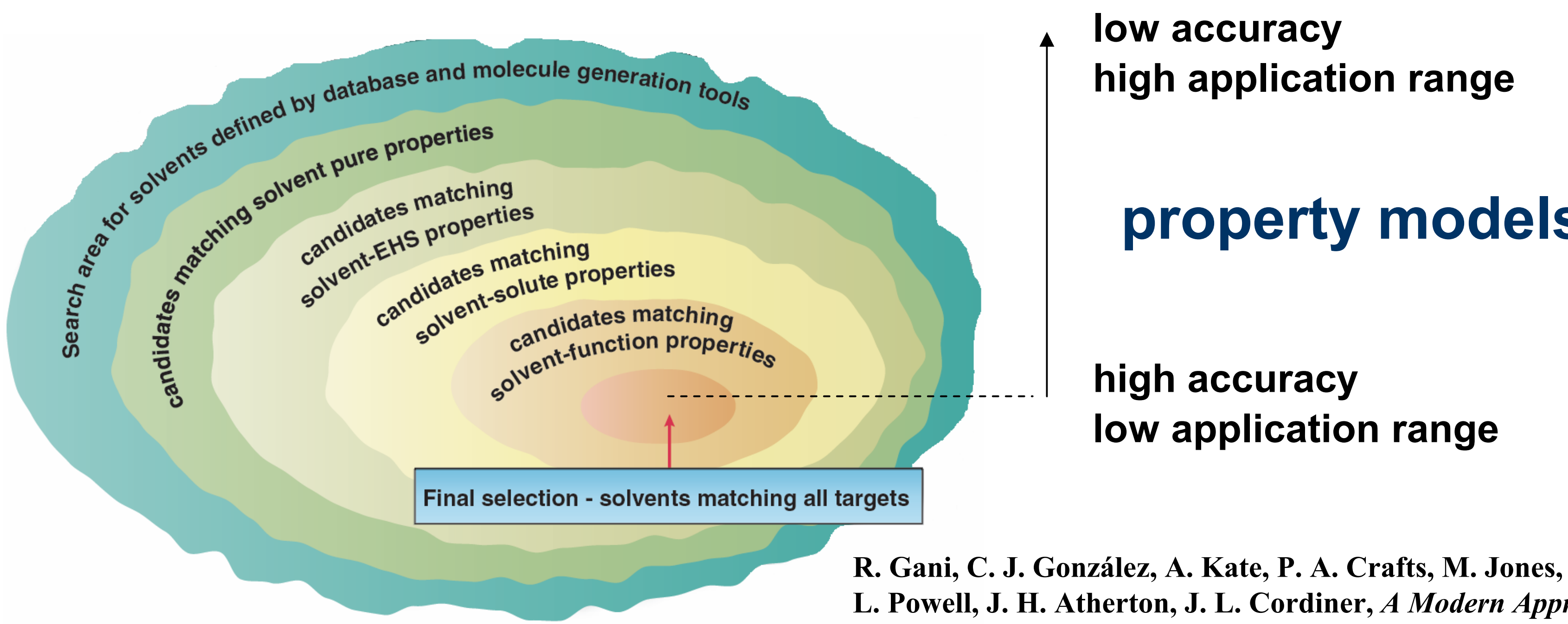
Wide range of process-product design problems can be solved:

Process design (attainable regions, heat/mass integration, ….)

Product design (solvent selection, structured chemicals, …..)

Retrofit design (sustainable process, product-process match, ...)

Example: Reverse problem with extend property models



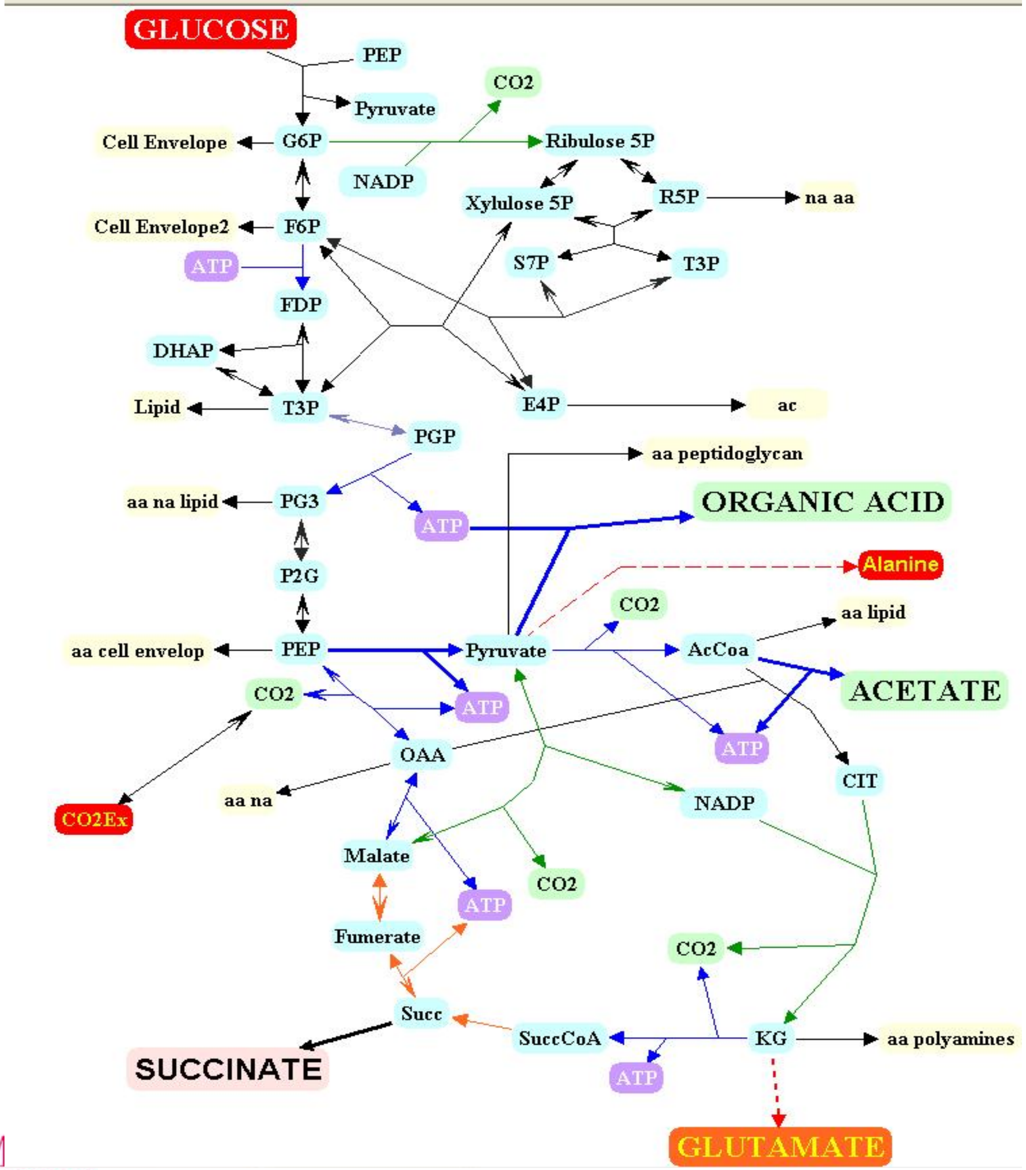
R. Gani, C. J. González, A. Kate, P. A. Crafts, M. Jones, L. Powell, J. H. Atherton, J. L. Cordiner, *A Modern Approach to Solvent Selection (March 2006), Chemical Engineering, 30-43.*

Apply CAMD techniques for solvent selection/design for separation and extraction

*(***Solution approach needs***: **Models, IT, computer science, optimization***)*

Extend to applications in pharmaceutical, agrochemical, health-care, etc. industries - organic synthesis, product recovery, process development, …, extended property models

Example: Metabolic Networks: Inverse Problem



(Ghosh, Domach, Grossmann, 2004)

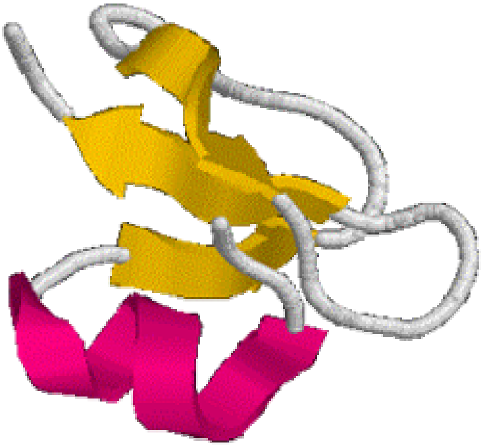
Find reaction pathway *(linear combination of extreme points for fluxes)* that minimizes squared deviation from NMR spectra for given selection of measured metabolites

MILP
Global Optimization

De Novo Protein Design *(Chris Floudas, Princeton)*

Define target template

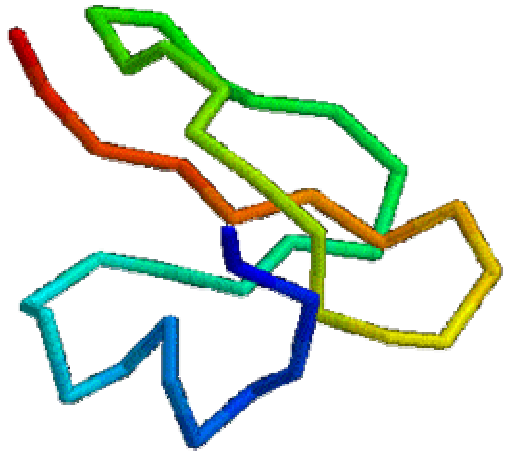
Backbone coordinates for N,Ca,C,O
and possibly Ca-Cb vectors from PDB



Human b-Defensin-2
hbd-2 (PDB: 1fqq)

Design folded protein

Which amino acid sequences will
stabilize this target structure ?



Full sequence design

Approach

In silico sequence selection => MILP

Fold specificity => Global optimization

=> New improved inhibitors

Combinatorial complexity

-Backbone length : n

-Amino acids per position : m

m^n possible sequences

(Klapeis, Floudas, Lambris, Morikis, 2004)

Product – Process: Synthesis - Design

d'Anterroches (2006)

CAMD

CAFD

Definition problem

Given a set of target properties, find the molecules or mixture that match the target properties

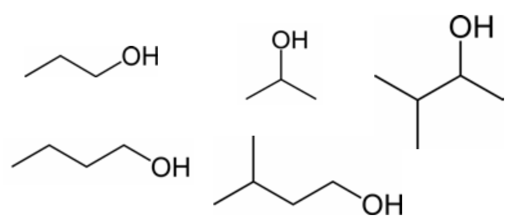
Given a multicomponent mixture, separate into a pure product streams

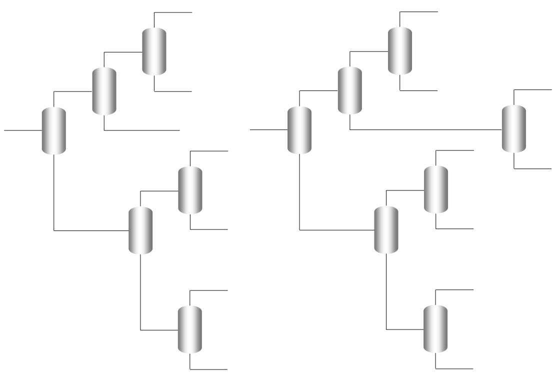
Translation into mathematical problem

A set of building blocks:
CH_2, C=C, CH_3OH, HCOO,…
+
Set of property based numerical constraints

A set of building blocks:
(A/BC), (AB/CD), (cyc G/H) …
+
Set of property based numerical constraints

Generation of alternatives & optimal design





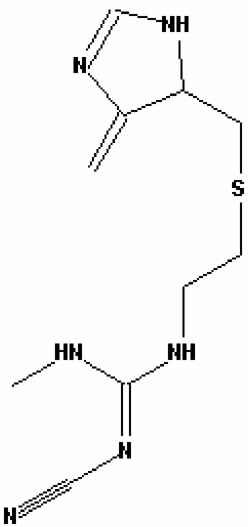
Post synthesis-design analysis

Molecular simulation
Experimentations

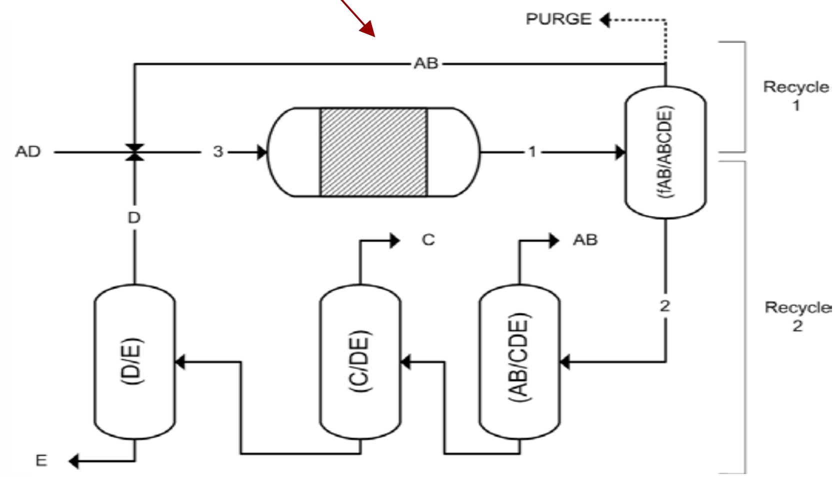
Reverse approach to get the complete design parameters
Rigorous simulation

Common Notation System for Molecule, Reaction & Flowsheet

Representation of molecule, process flowsheet or operations & reaction networks with SMILES & SFILES



(1)	$H_2 + l \rightleftharpoons H_2l$
(2)	$H_2l + l \rightleftharpoons Hl + Hl$
(3)	$N_2 + l \rightleftharpoons N_2l$
(4)	$N_2l + l \rightleftharpoons Nl + Nl$
(5)	$N_2l + H_2l \rightleftharpoons N_2H_2l + l$
(6)	$N_2H_2l + l \rightleftharpoons NHl + NHl$
(7)	$Nl + Hl \rightleftharpoons NH_2l + l$
(8)	$NHl + Hl \rightleftharpoons H_2l$
(9)	$NHl + H2l \rightleftharpoons NH_3l + l$
(10)	$NH_2l + Hl \rightleftharpoons NH_3l + l$
(11)	$NH_3l \rightleftharpoons NH_3 + l$



N#CN=C(NC)NCCSCC1NC=NC1=C

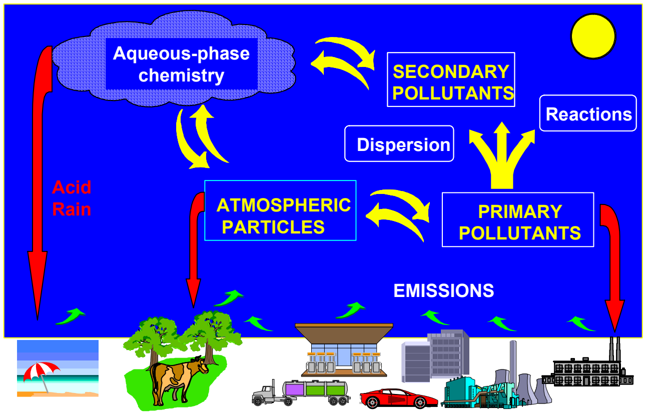
SMILES & SFILES

(H2)(1)<1(H2l)2(5)4<3(1)>1<6<5[(3)[(N2l)3]<(n2)](6)[NH1)(9)5<2(NH3l)(11)6(NH3)]<(N2H2l)<4

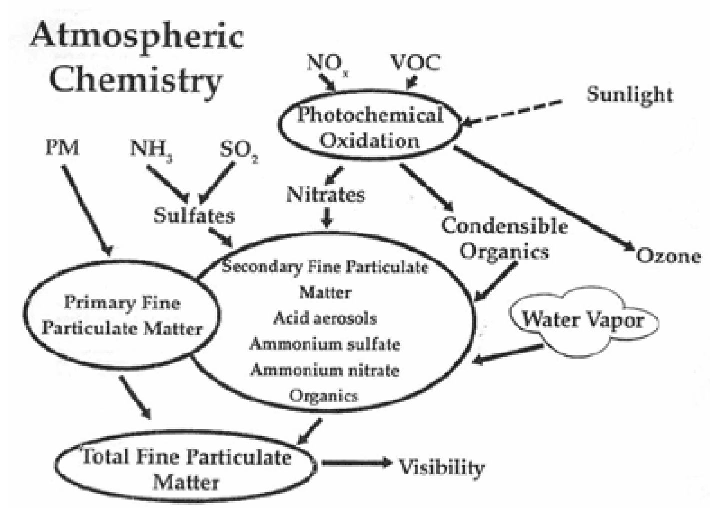
(iAD)(rAD/pABCDE)<1<2(fAB/ABCDE)1[(AB/CDE)(oAB)](C/DE)[oC)](D/E)2(oE)

II. Energy and Sustainability: Role of PSE/CAPE

The atmosphere as a chemical reactor



Spyros Pandis (Carnegie Mellon/Patras)

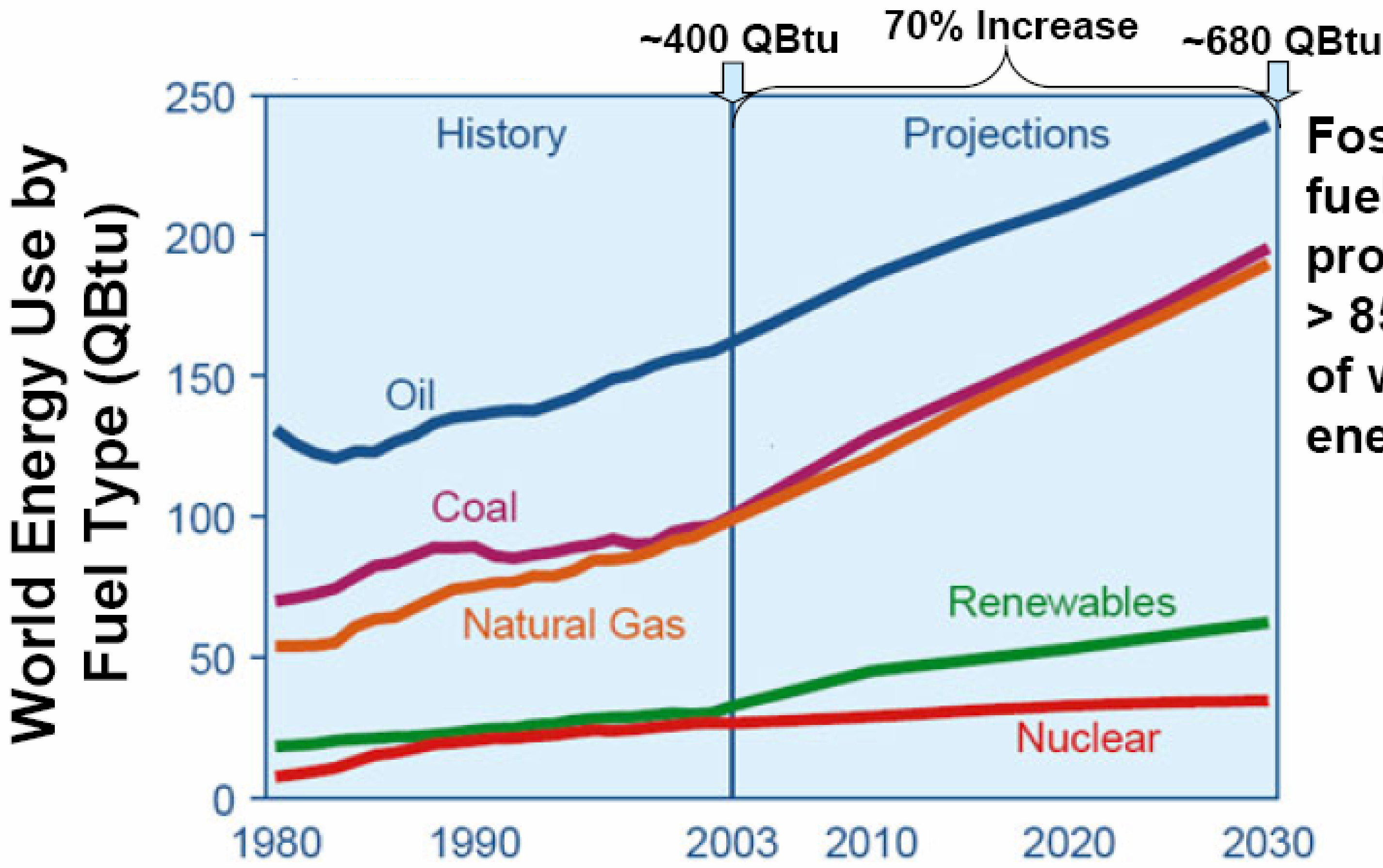


David Allen (U. Texas)

Sustainable Integrated Systems

Growing World Energy Demand

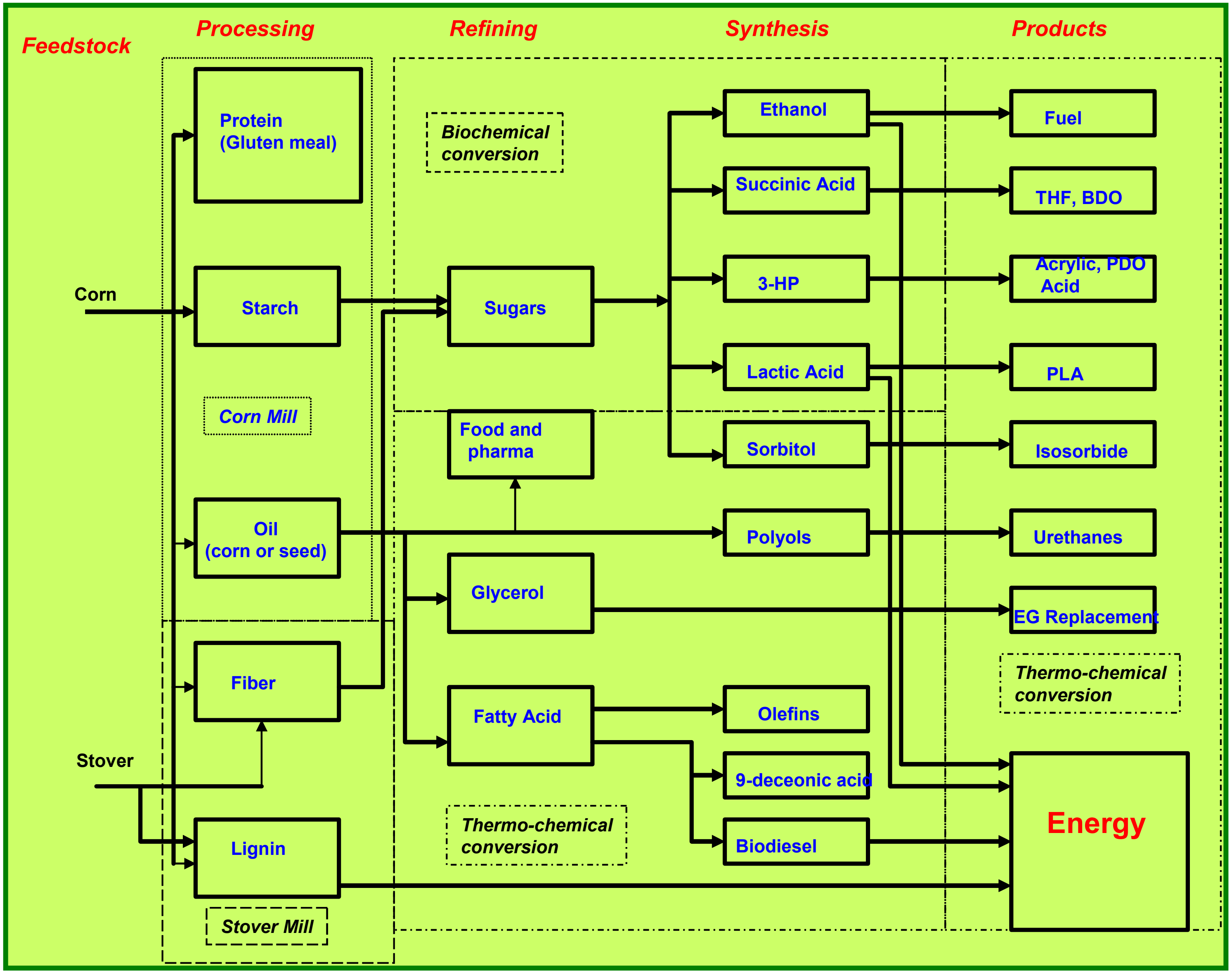
Fossil Fuels Dominate Energy Consumption



Fossil fuels provide > 85% of world energy

Courtesy: S. Zitney, NETL

Future: Biorefineries ?

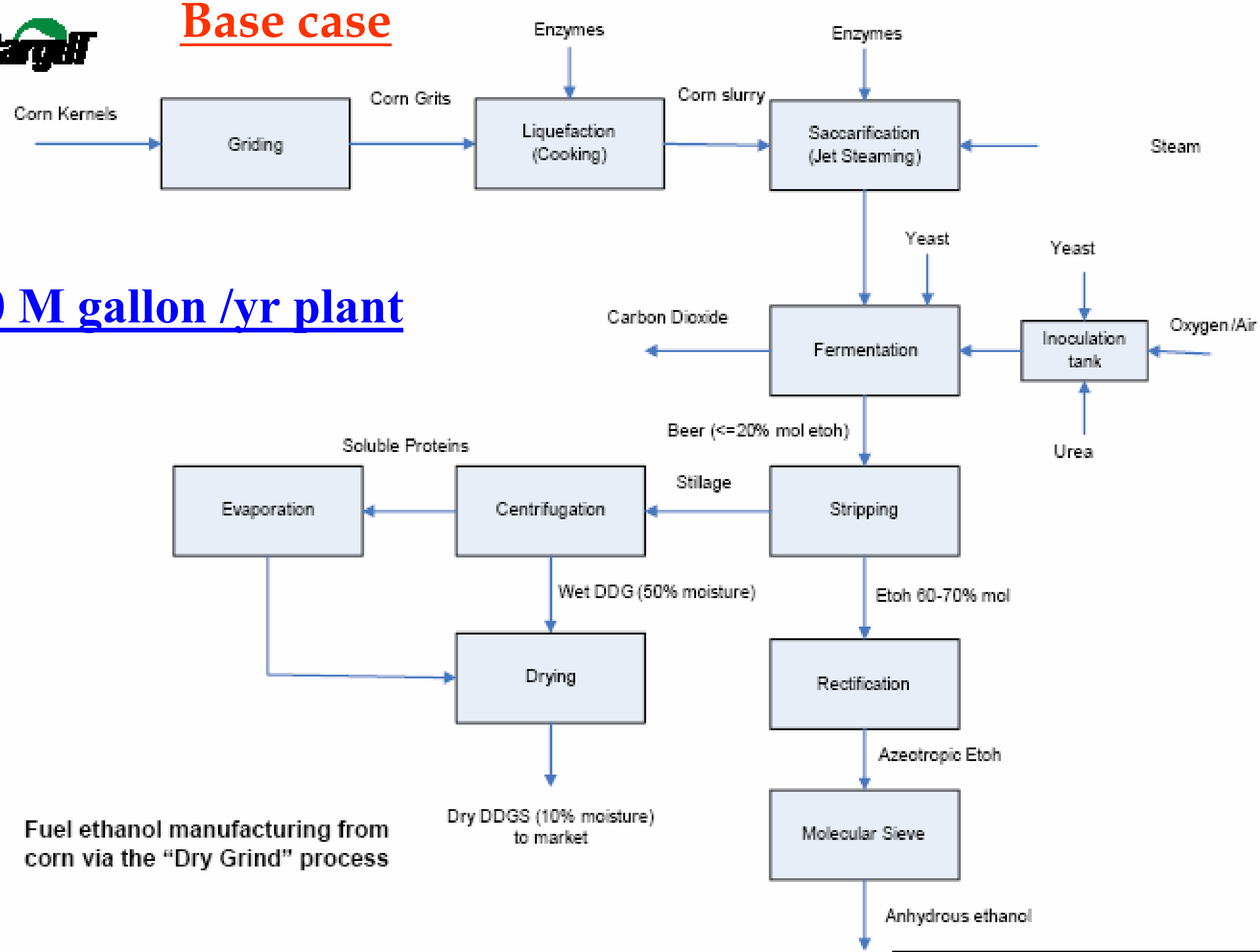


Energy Optimization of Corn-based Bioethanol

Peschel, Martin, Karuppiah, Grossmann, Zullo, Martinson (2006)

Base case

60 M gallon /yr plant

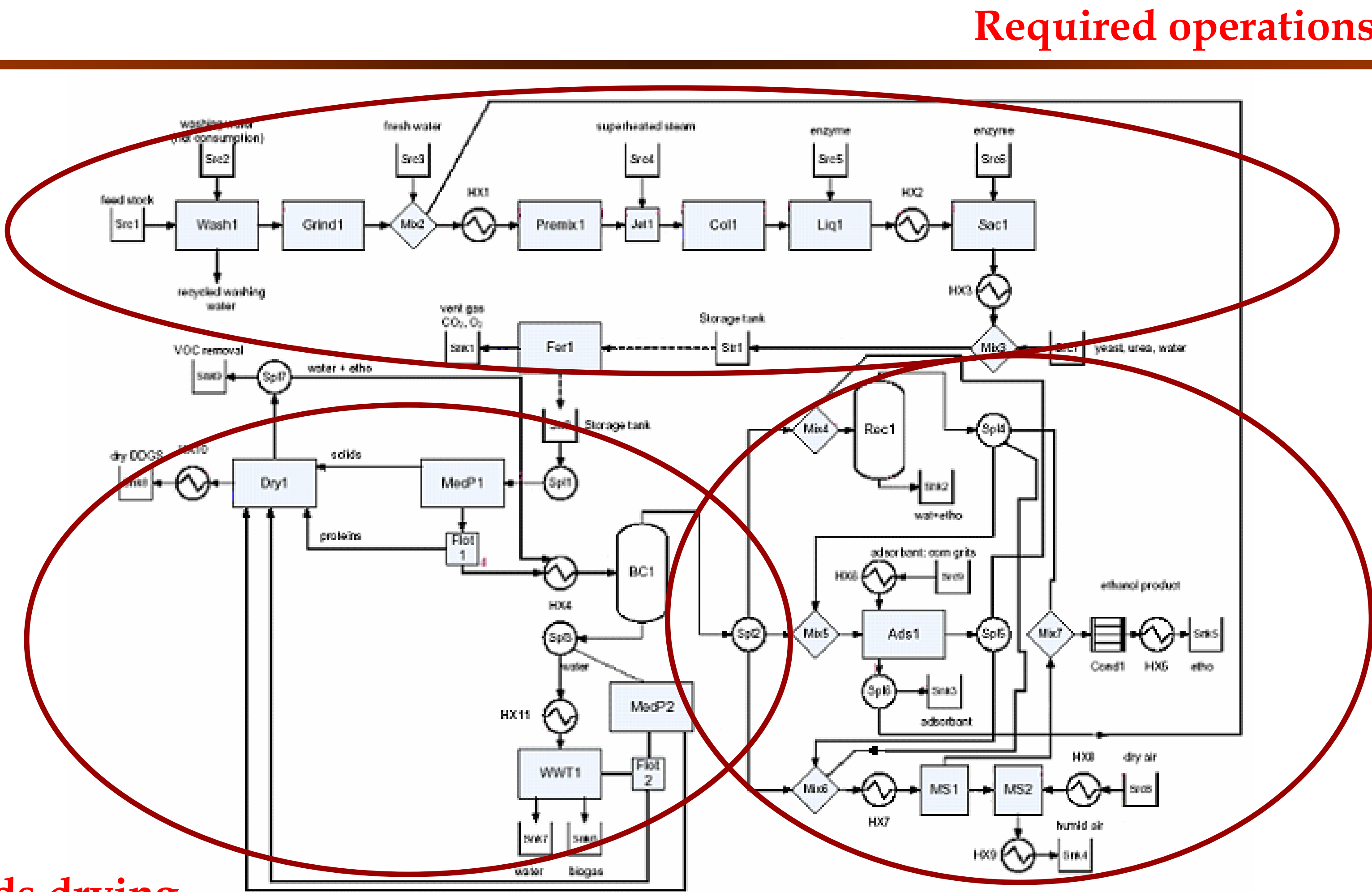


Fuel ethanol manufacturing from corn via the "Dry Grind" process

Total equipment cost = **50.3 M$** Steam cost = **15 M$ /yr**

Manuf cost = **1.61 $/gal**

Superstructure of a Bio-ethanol Plant

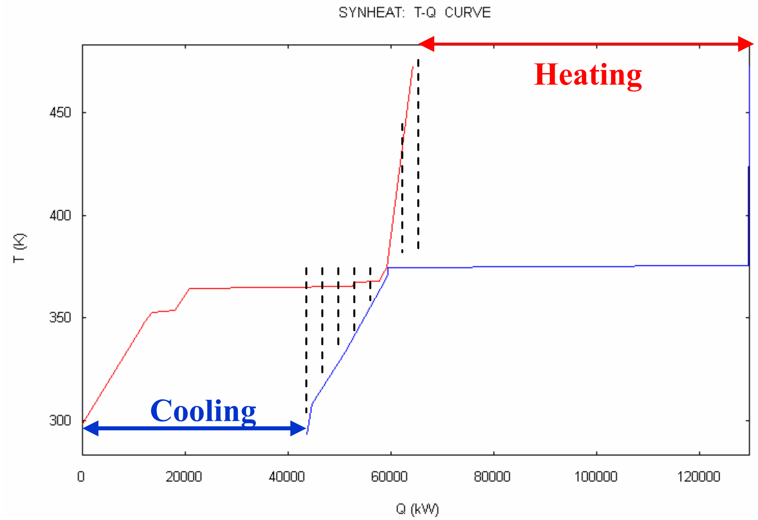


Mechanical press before/after Beer column

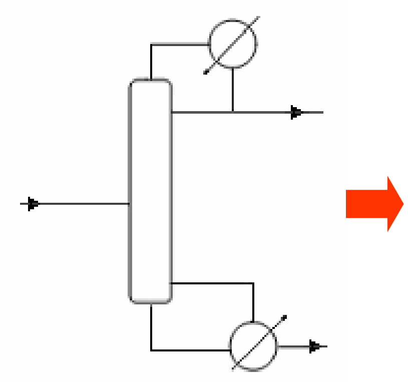
Molecular Sieves vs Corn Grits

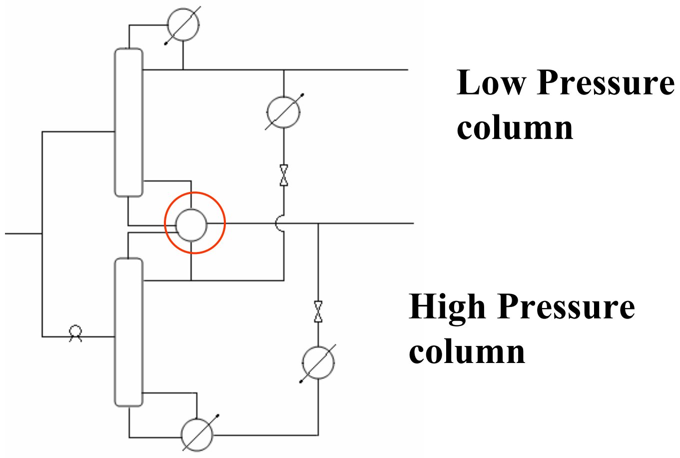
Alternatives for Energy Reduction

Heat Integration process streams:



Multieffect columns:



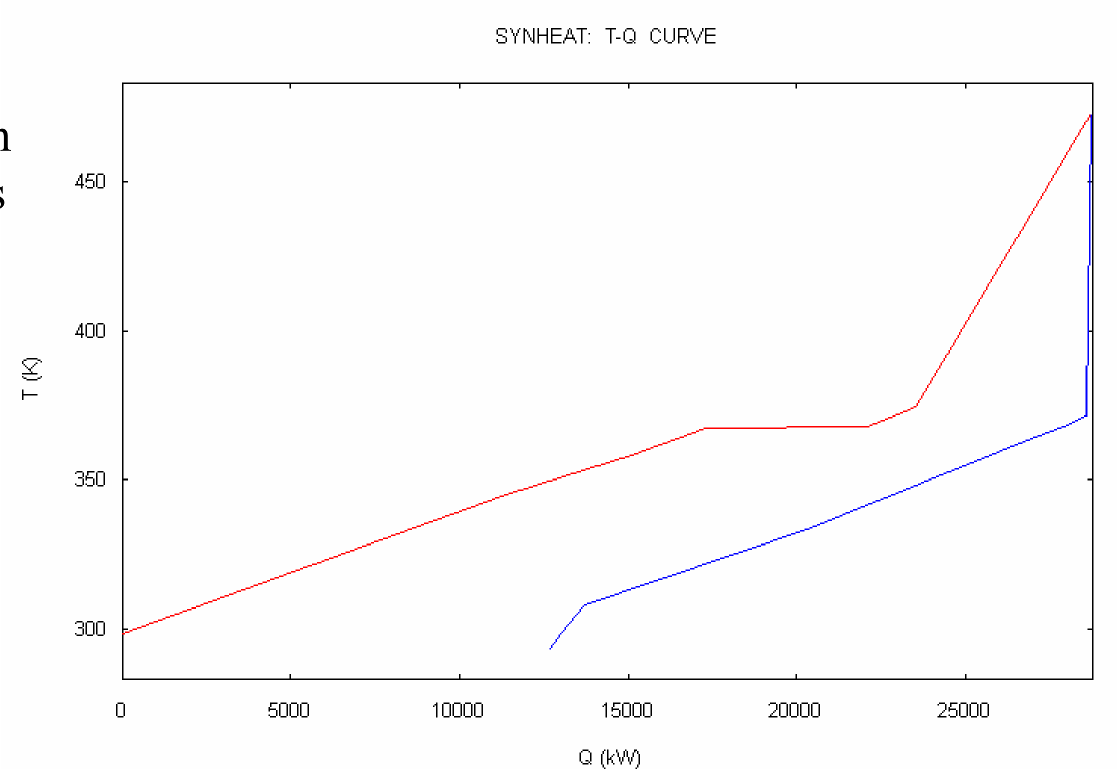


GDP model comprises mass, energy balances, design equations
2,922 variables (12 Boolean) 2,231 constraints

Simultaneous Optimization

Adsorption and Mechanical Press options plus Heat Integration and Multieffect Columns

Heat integration
Process streams



Total equipment cost = **49.7 M$**   Steam cost = **4.8 M$/yr *(-65%)***

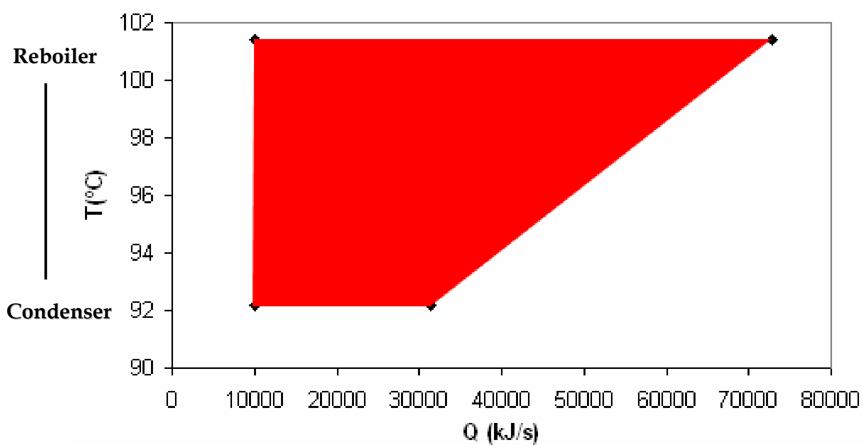
Manuf cost = **1.43 $/gal**

Reduction from $1.61/gal (base case) to $1.43/gal !

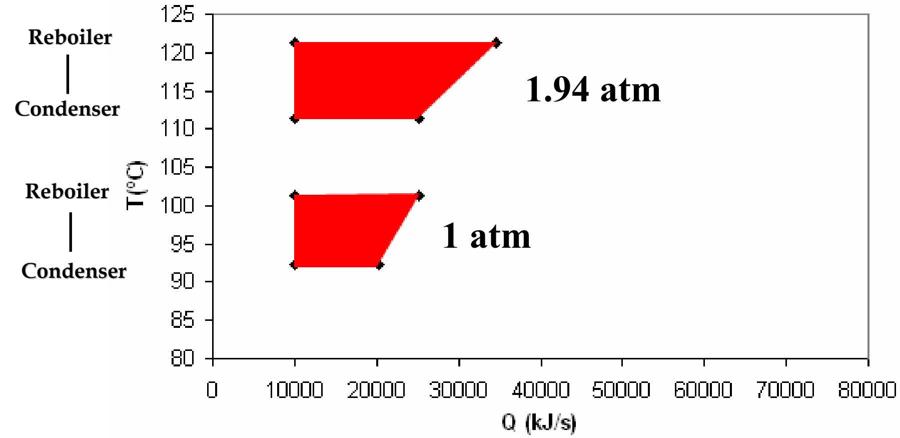
Energy Profiles in Multieffect Columns

Beer Column

Single column

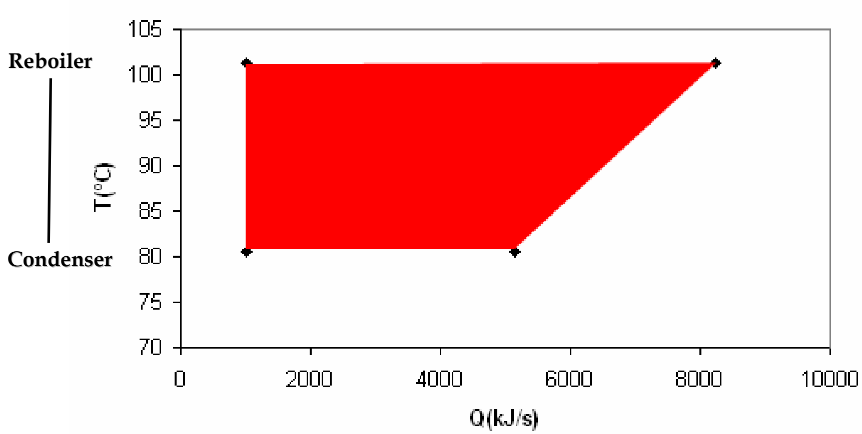


Double effect column

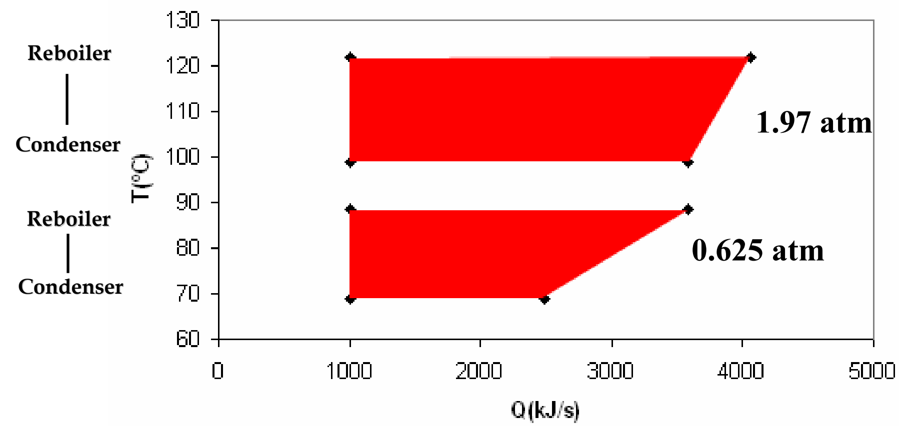


Rectification Column

Single column



Double effect column



Synthesis of Integrated Process Water Systems

Karuppiah, Grossmann (2006)

- WATER → One of MOST IMPORTANT raw materials used in process industry

- Water becoming scarce
  More stringent regulations for wastewater disposal

(Dudley, 2003)

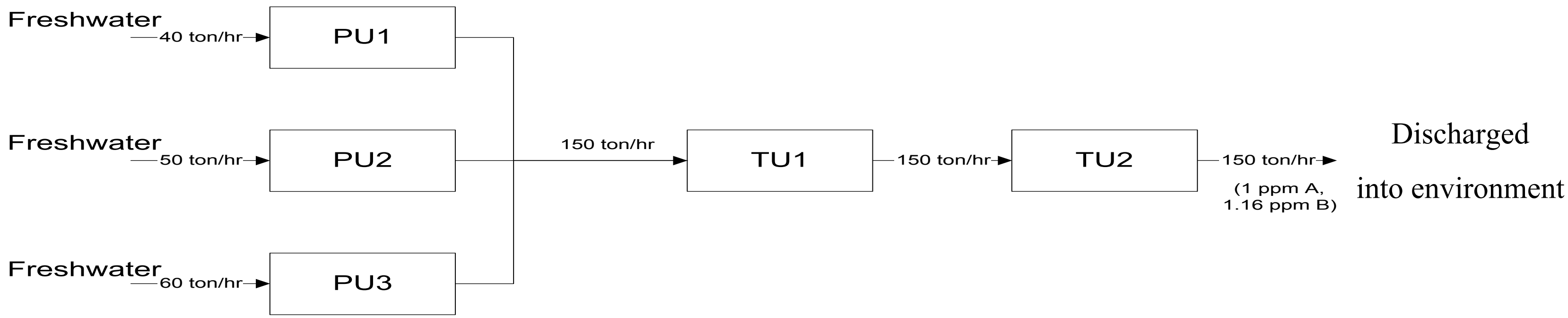
- Pressure on process industry for efficient use of water and disposal of wastewater

- Wastewater reuse, recycle → Options to reduce Freshwater consumption

GOAL:

GLOBAL OPTIMIZATION method for INTEGRATED DESIGN of Water Using and Water Treating Units

Conventional Water Network



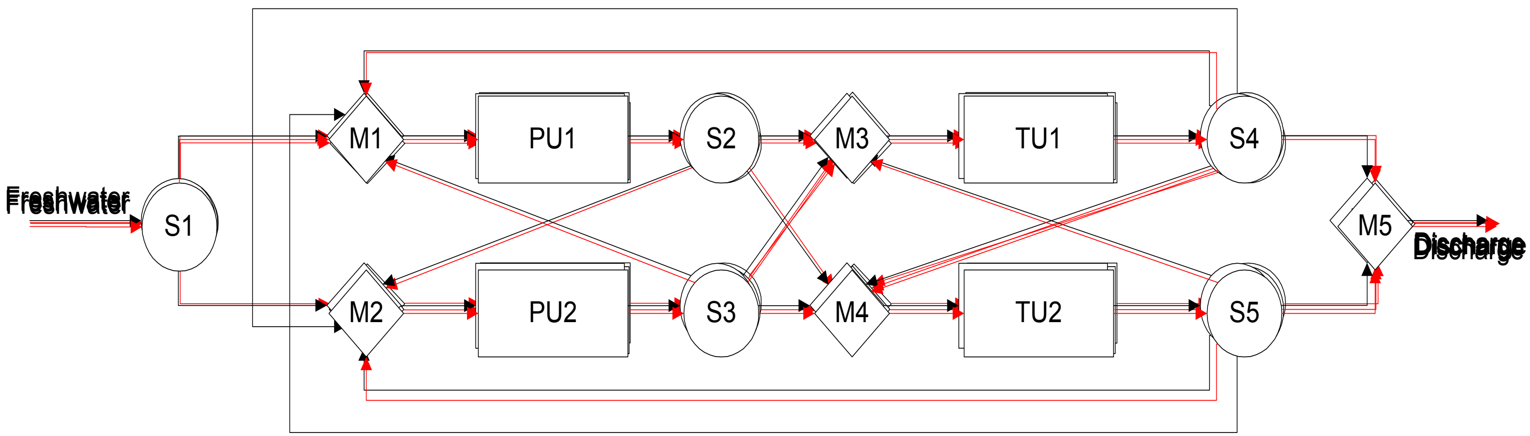
- PU1, PU2 and PU3 ⇒ Process Units using water
  - PU1 → Scrubber
  - PU2 → Washing unit
  - PU3 → Desalter

- TU1, TU2 ⇒ Water Treatment units
  - TU1 → Oil separator
  - TU2 → Centrifuges/ Filtration units

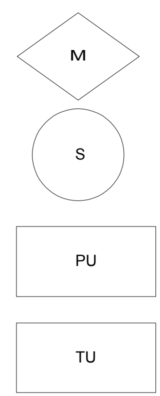
- FRESHWATER consumed = 150 ton/hr   Global minimum = 40 ton/hr

Superstructure for integrating Water Using/Treating Units

Integrated Water Network with reuse and recycle flows is proposed



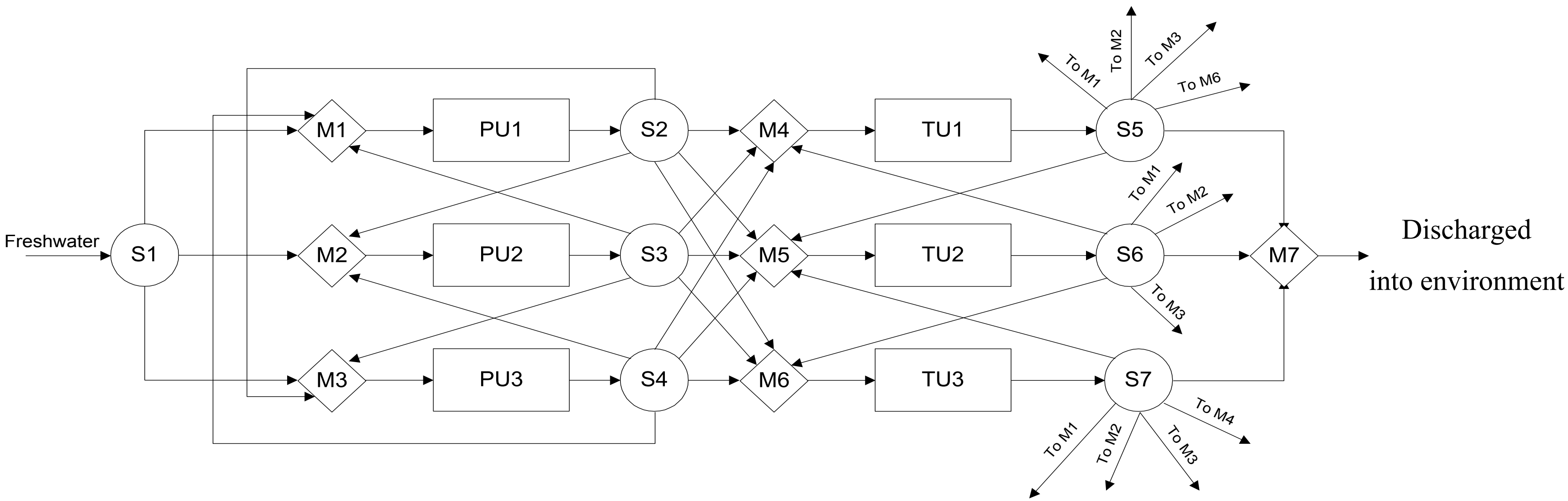
- Superstructure consists of
  1. Mixers (MU)
  2. Splitters (SU)
  3. Process Units (PU)
  4. Treatment Units (TU)



Superstructure of Integrated Water System

- Generalize superstructure development to system with arbitrary number of Process / Treatment Units

Example : 3 Process Unit - 3 Treatment Unit system



- Superstructure is formulated as a Non-Linear Programming (NLP) problem (Bilinear) and solved with novel global optimization algorithm

III. Enterprise-wide Optimization

Beyond the plant level/ Integration with business operations

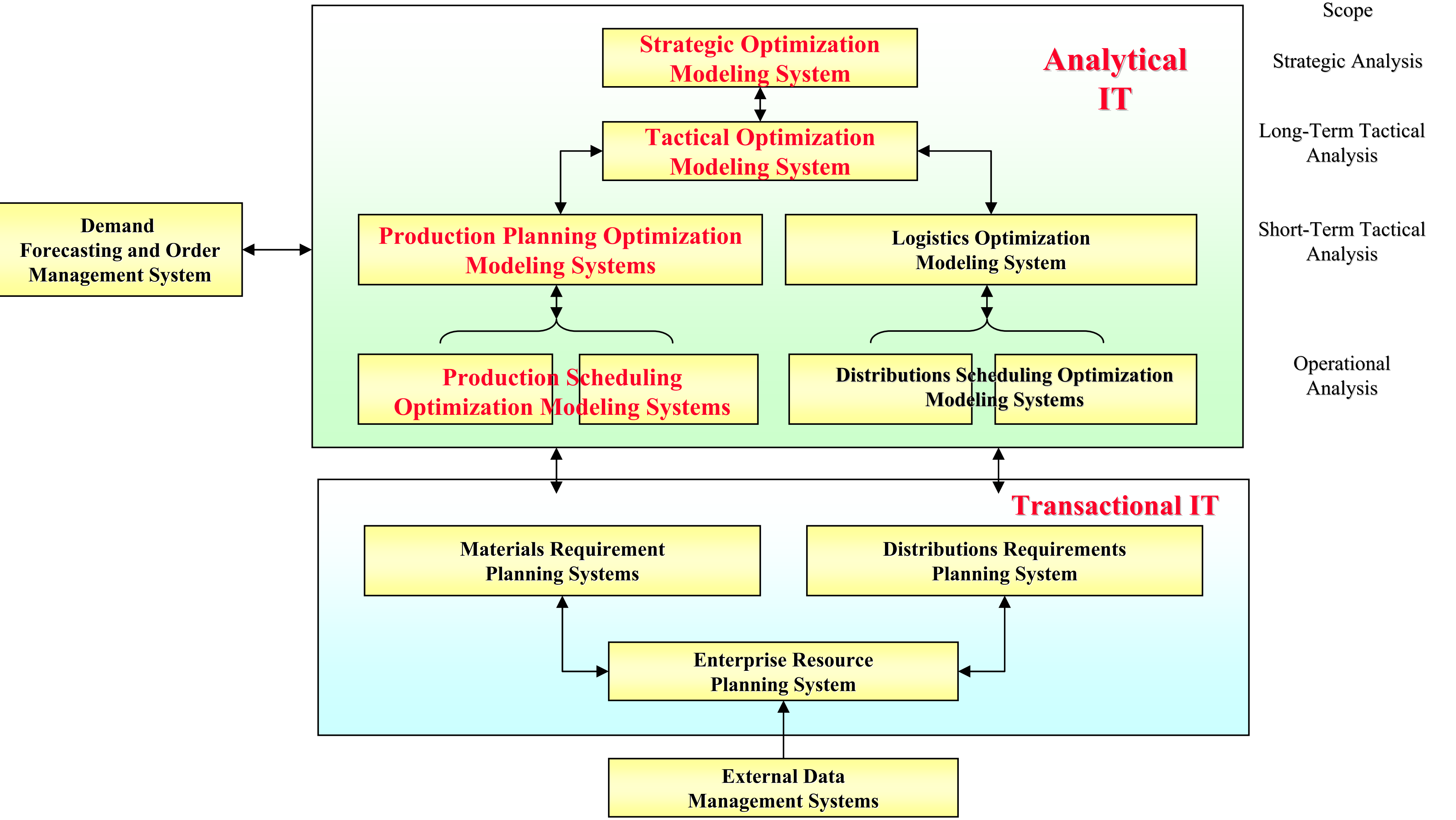
EWO involves optimizing the operations of R&D, material supply, manufacturing, distribution and financial activities of a company to reduce costs and inventories, and to maximize profits, asset utilization, responsiveness and customer satisfaction.

Key features:

-Integrate strategic, tactical and operational decision-making

-Integration of the information, modeling and solution methods

Methods/Tools for Enterprise-wide Optimization



Source: Tayur, et al. [1999]

Scope of Enterprise-wide Optimization








Wellhead	Trade & Schedule Crude and Other Feedstocks	Transfer of Crude and Feedstocks to Refinery	Refinery Optimization	Trade & Schedule Products	Transfer of Products from Refinery to Terminal	Terminal Loading	Pump

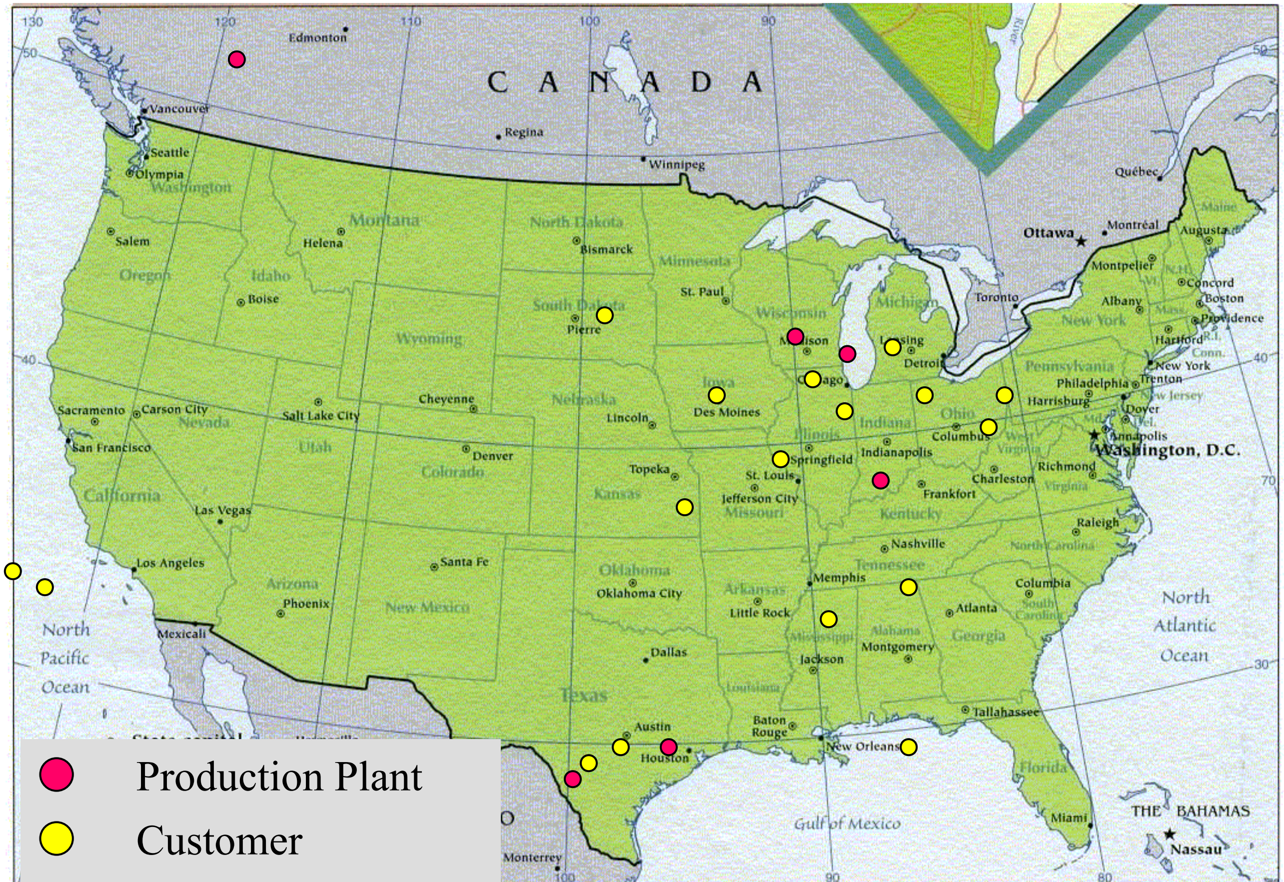
Dennis Houston (ExxonMobil)

Discovery	Development					Market
Targets Hits Leads Candidate	Pre-clinical Development	Phase 1	Phase 2a/b	Phase 3	Submission& Approval	Lifecycle Management
2-5 yrs	0.5 - 2 yrs	1 - 2 yrs	1.5 - 3.5 yrs	2.5 - 4 yrs	0.5-2 yrs	10-20 yrs

Colin Gardner (Transform Pharmaceuticals)

Simultaneous Tactical Planning and Production Scheduling

Goal: Improve the asset utilization of geographically distributed assets and reduce cost to serve by improving enterprise wide tactical production planning.



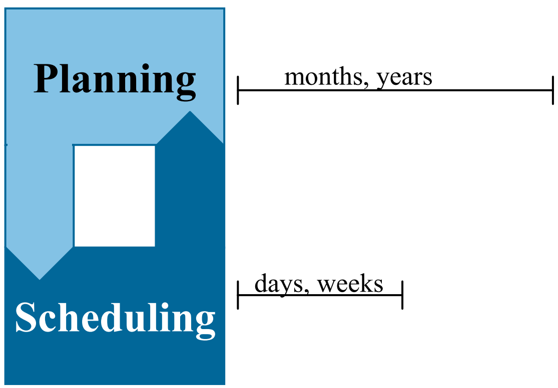
Multi-scale optimization: temporal and spatial integration

Approaches to Planning and Scheduling

Erdirik, Grossmann (2006)

Decomposition

Sequential Hierarchical Approach

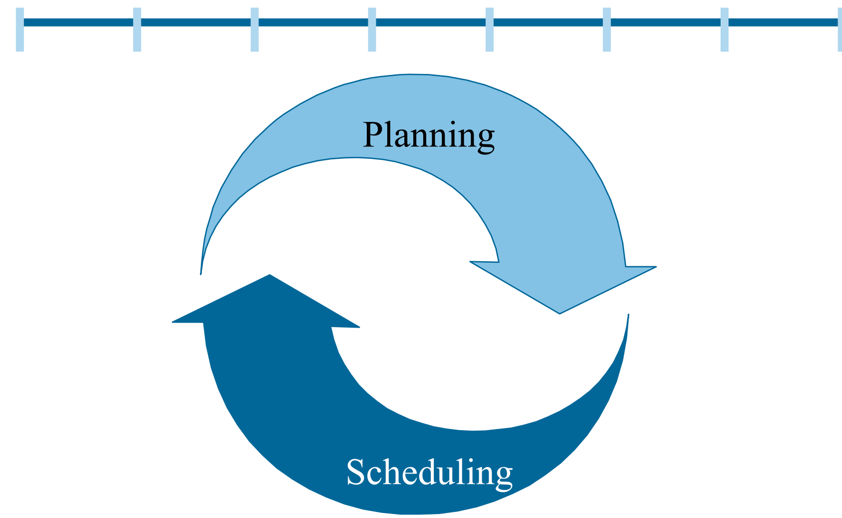


Challenges:

- Different models / different time scales
- Mismatches between the levels

Simultaneous Planning and Scheduling

Detailed scheduling over the entire horizon



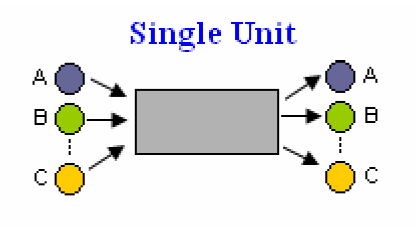
Challenges:

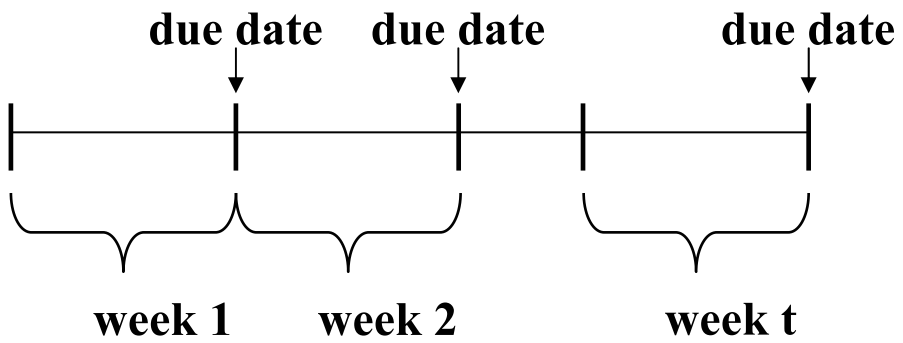
- Very Large Scale Problem
- Solution times quickly intractable

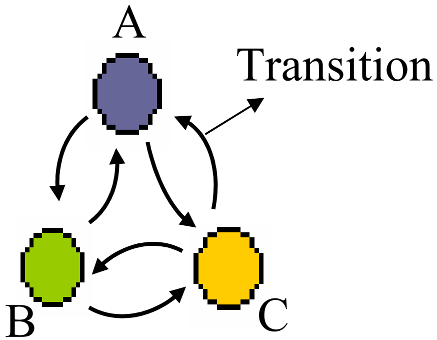
GOAL: Multi-scale decomposition algorithm to integrate planning and scheduling to ensure optimality and consistency between the two levels.

Planning and Scheduling of Continuous Plants

- **Multiproducts** to be processed in a single **continuous** unit/production line
- Time horizon subdivided into **weeks** at the end of which demands are specified.
- Transition times are **sequence dependent**
- **Continuous** time representation is used.







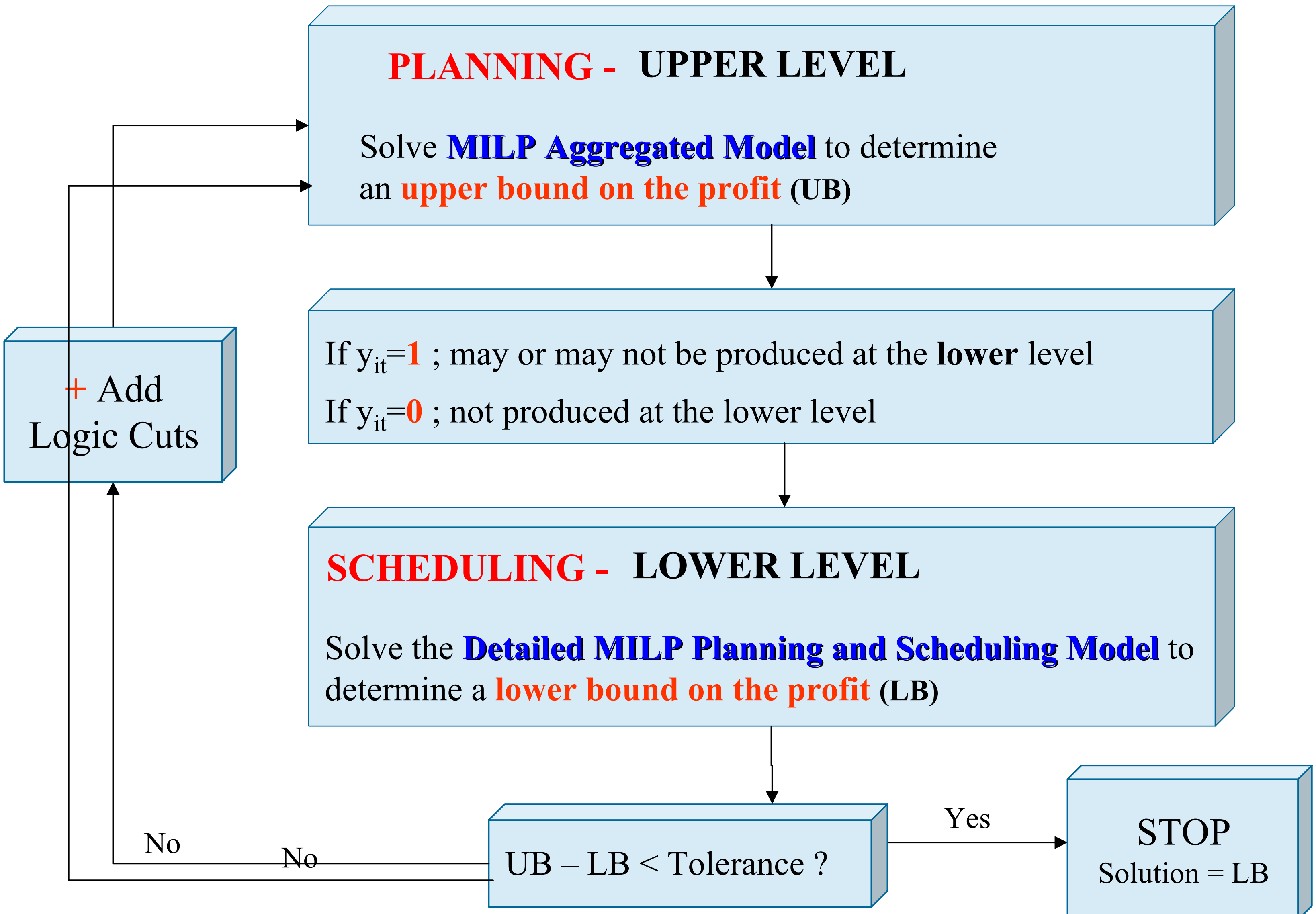
Decisions

- Amounts to be produced
- Length of processing times
- Product inventories
- Sequencing of products

Objective

- Max Profit = Sales –Operating Costs – Inventory Costs – Transition Costs

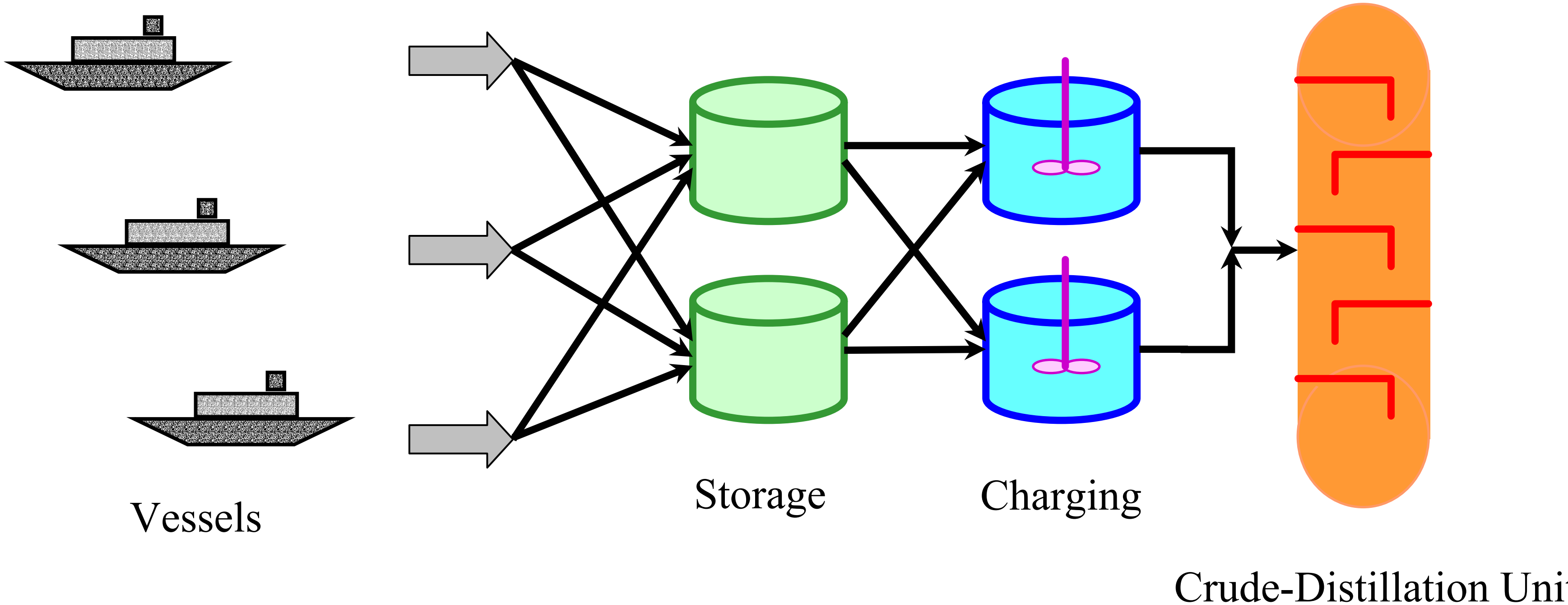
Proposed Decomposition Algorithm



Scheduling Crude Oil Movements Refinery Front-end

Karuppiah, Furman, Grossmann (2006)

- Scheduling and Planning of flow of crude oil is key problem in petrochemical refineries
- Large cost savings can be realized with an optimum schedule for the movement of crude oil



How to coordinate discharge of vessels with loading to storage?
How to synchronize charging tanks with crude-oil distillation?

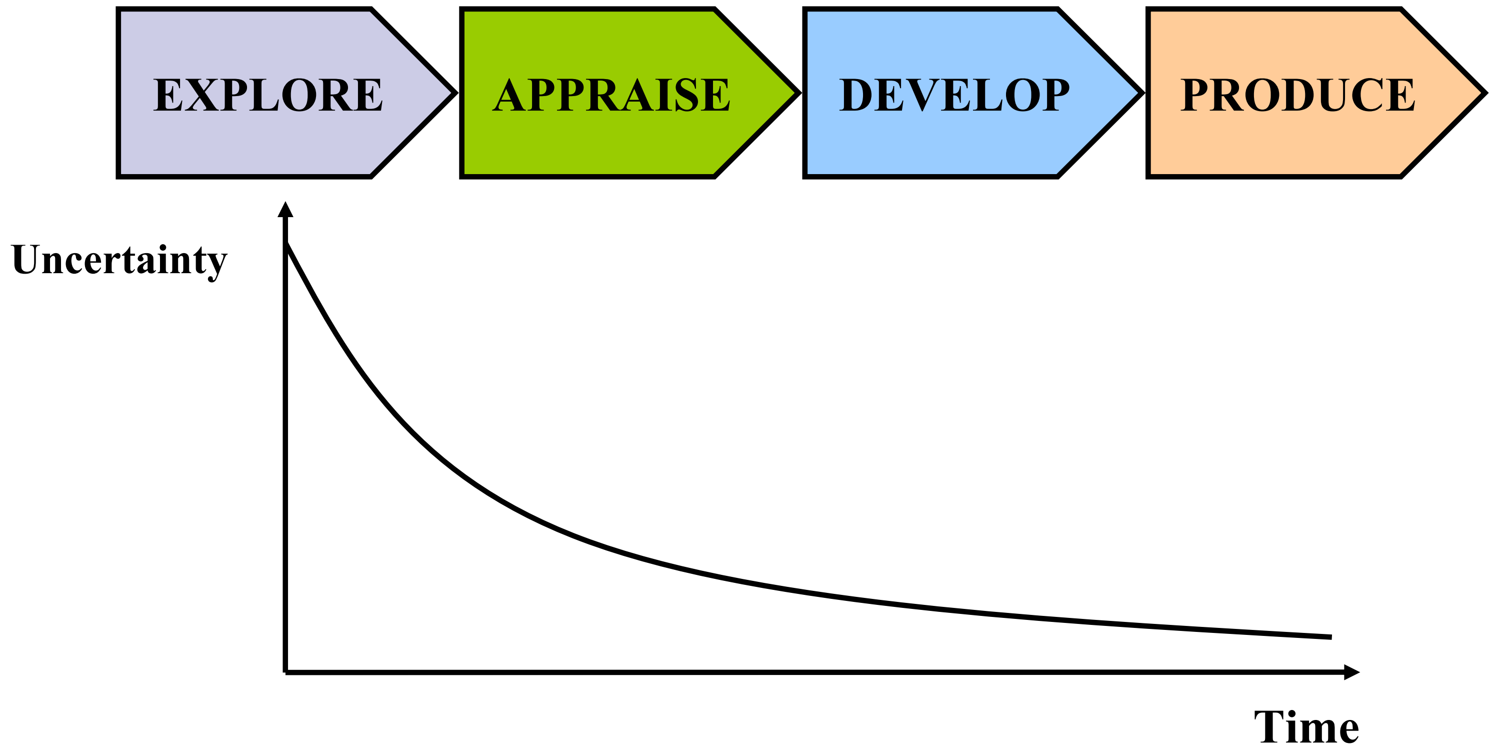
Global MINLP Optimization

Stochastic MINLP model for planning of oil fields under uncertainty

ExxonMobil

Tarhan, El-Bakry, Goel, Grossmann (2007)

Exploration & Production



<u>Goal:</u> improve the decisions about development planning under uncertainty

FPSO and TLP

 (1)

 (2)

FPSO: (Floating Production Storage Offloading)

- Small FPSO, converted from oil tanker
  - Low capacity
  - Costs less
  - Short construction time

- Large FPSO, grassroots facilities
  - High capacity
  - Costs more
  - Long construction time

TLP: (Tension-Leg Platform)

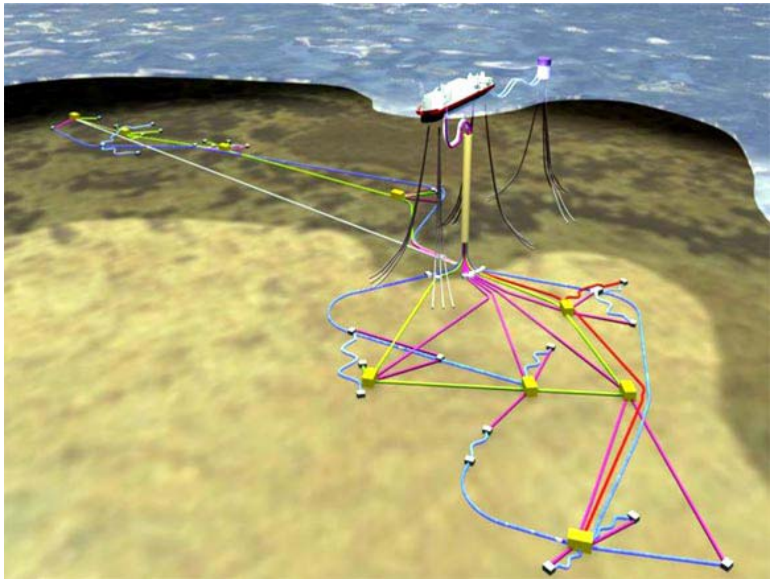
Cannot produce oil, only drilling and oil recovering capability

Pictures taken from:

(1) www.wikipedia.org

(2) www.search.com

Drilling Options



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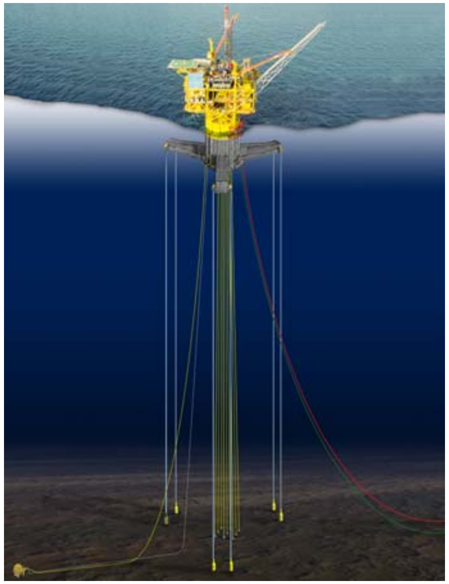


(4)

Sub-sea well:

- Can be drilled at any time
- Connect to FPSO facility

TLP well:

- Need TLP facility to drill
- Connect to TLP facility

Pictures taken from:

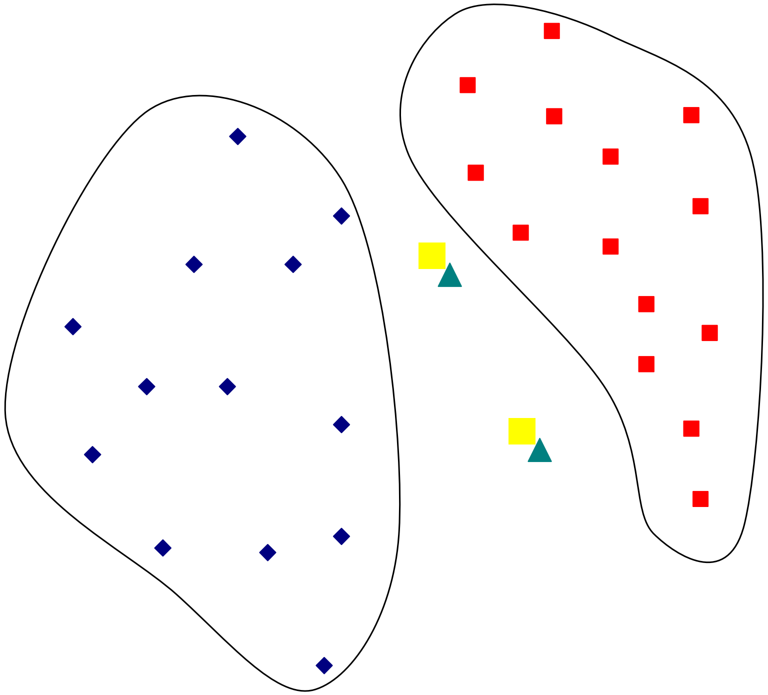
(3) www.offshore-technology.com

(4) www.aas-jakobsen.no

Model Decisions and Uncertainty

- **The aim is to simultaneously optimize the investment and operation decisions under uncertainty over the entire project horizon.**

  - **How many FPSO/TLP**
  - **Capacity of facility**
  - **Time to build**
  - **How many wells to**
  - **Sub-sea/TLP well**
  - **Production rate**



Uncertainty:

- **Sand quality (PI)**
- **Size of reservoirs**
- **Breakthrough time**

Maximize the expected net present value of the project

What about core Process Systems Engineering topics?

Are there challenges remaining in…?

Modeling*
Optimization
Process Synthesis/Design*
Process Operations
Process Control

Above areas represent core body of knowledge in PSE (*ie fundamentals*)

**** Some of the challenges in these topics pointed out in part I***

Mathematical Programming

Given a <u>space of alternatives</u> that are specified through constraints in a mathematical model <u>select decision variables</u> to optimize an objective function

$$\min Z = f(x, y)$$

$$s.t. \quad h(x, y) = 0$$

$$g(x, y) \leq 0$$

$$x \in R^n, \quad y \in \{0,1\}^m$$

MINLP- Mixed-integer Nonlinear Programming

Progress in Linear Programming

Increase in computational speed from 1987 to 2002

Bixby-ILOG (2002)

For 50,000 constraint LP model

Algorithms

Primal simplex in 1987 *(XMP) versus*

Best(primal,dual,barrier) 2002 ***(CPLEX 7.1)*** **2400x**

Machines

Sun 3/150

Pentium 4, 1.7GHz **800x**

Net increase: Algorithm * Machine ~ 1 900 000x

Two million-fold increase in speed!!

Applications of Mathematical Programming in Chemical Engineering

Process Design

Process Synthesis

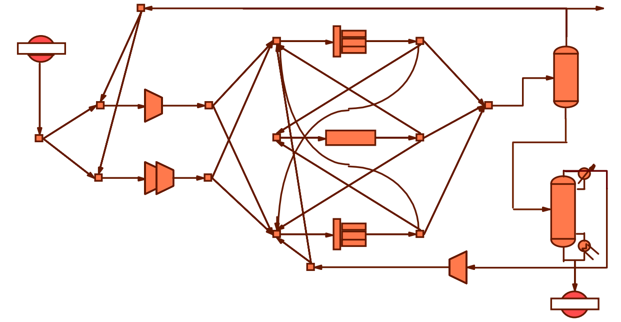
Production Planning

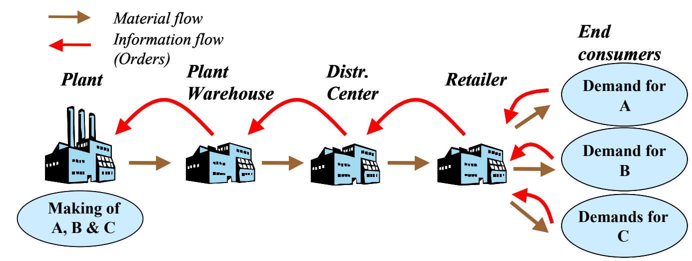
Process Scheduling

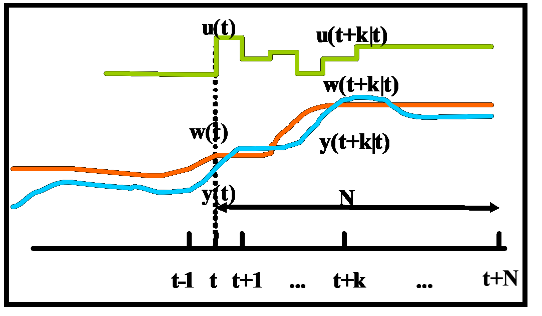
Supply Chain Management

Process Control

Parameter Estimation







LP, MILP, NLP, MINLP, Optimal Control

Major contribution:

new problem representations, models & solution strategies

Contributions by Chemical Engineers to Mathematical Programming

Large-scale nonlinear programming
SQP algorithms
Interior Point algorithms

Optimal control problems
NLP-based strategies

Mixed-integer nonlinear programming
Outer-approximation algorithm
Extended-Cutting Plane Method
Generalized Disjunctive Programming

Global optimization
α-Branch and Bound
Spatial branch and bound methods

Optimization under Uncertainty

Parametric programming

Generalized Disjunctive Programming

GDP Model: *Raman and Grossmann (1994):*

$$\min \ Z = \sum_k c_k + f(x)$$ Objective Function

$$s.t. \quad r(x) \le 0$$ Common Constraints

OR operator →

$$\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ g_{jk}(x) \le 0 \\ c_k = \gamma_{jk} \end{bmatrix}, k \in K$$

Disjunction

Constraints

Fixed Charges

$$\Omega(Y) = true$$ Logic Propositions

$$x \in R^n, c_k \in R^1$$ Continuous Variables

$$Y_{jk} \in \{ true, \ false \}$$ Boolean Variables

Concluding Remarks

Process Systems Engineering is a vibrant area of research

Theory, Models, Algorithms, Applications

Driven by Industrial Needs!!

Process Systems Engineering well-positioned to support :

Value preservation

Value growth

Process Systems Engineering requires as next step to balance:

Expanding scope

Maintaining core

Concluding Remarks

Emerging challenges in Process Systems Engineering

Product and Process Design
Energy and Sustainability
Enterprise-wide Optimization

+

Fundamental Challenges in Process Systems Engineering

Modeling
Optimization
Process Synthesis/Design
Process Operations
Process Control