Model based methods and tools for process systems engineering

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***Sustainable Product-Process Engineering, Evaluation & Design**

What is Process Systems Engineering?

Takamatsu, Sargent, …. PSE-series (1982), PSE-China(1979)

Sargent (1988): Process systems engineering is all about the development of systematic techniques for process modelling, design and control…..

Some formulate their problem, or some useful simplification of it, in precise mathematical terms, then seek to exploit the mathematical structure to obtain an effective algorithm, while others seek insight on the problem structure from physical intuition.

What is Process Systems Engineering?

Takamatsu, Sargent, …. PSE-series (1982), PSE-China(1979)

PSE: Use of a systematic approach to problem solving! Also, 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.

Basic products (disciplines-themes) of PSE

Numerical analysis => **Modelling & Simulation**

Mathematical Programming => **Optimization**

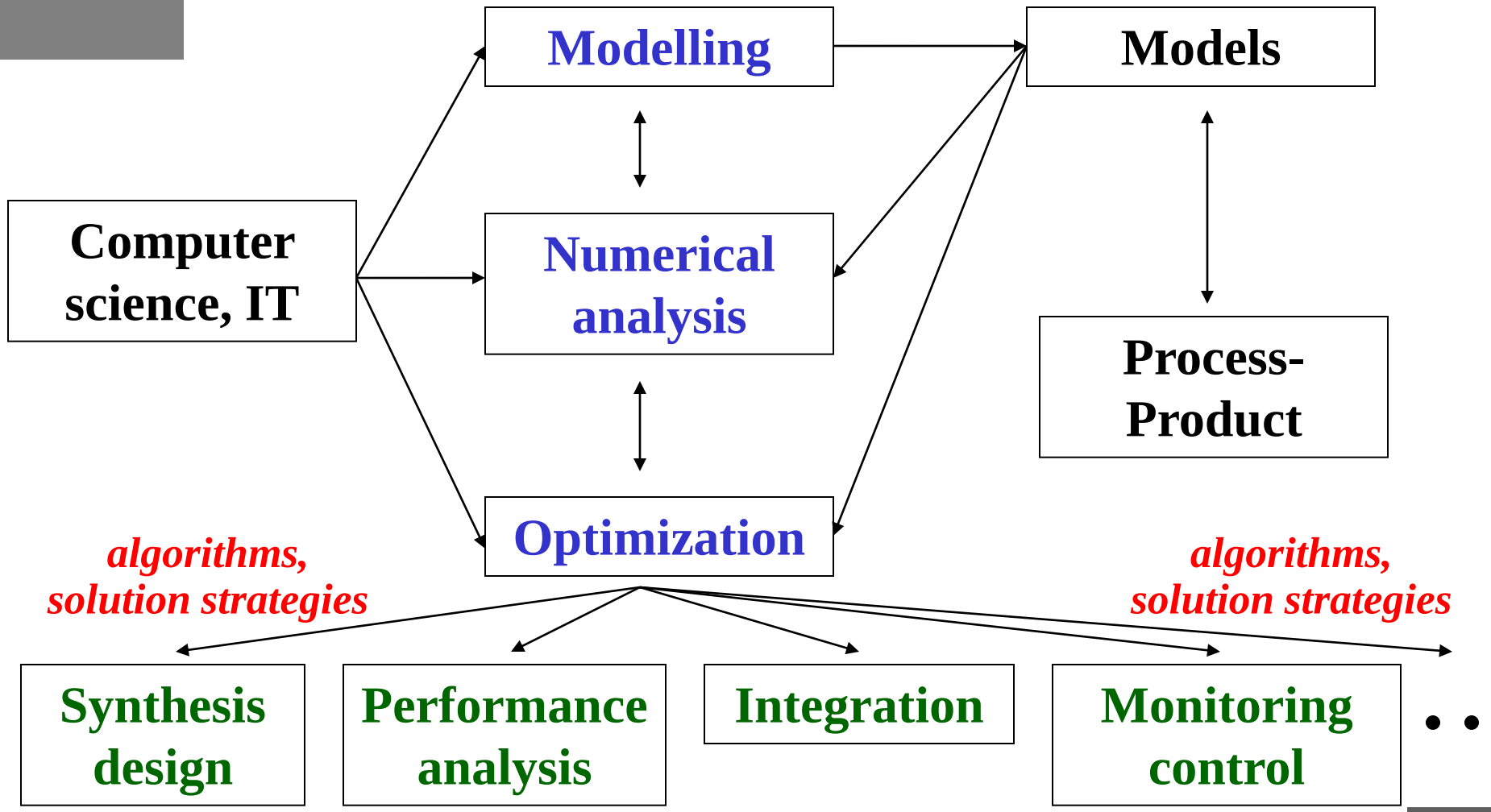
Systems and Control Theory => **Process Control**

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

Management Science => **Operations/Business**

Math Programming & Control Theory "competitive" advantage

Framework for problem solving in PSE



Scope of the basic products of PSE

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

Mathematical Programming => Optimization => Synthesis/design

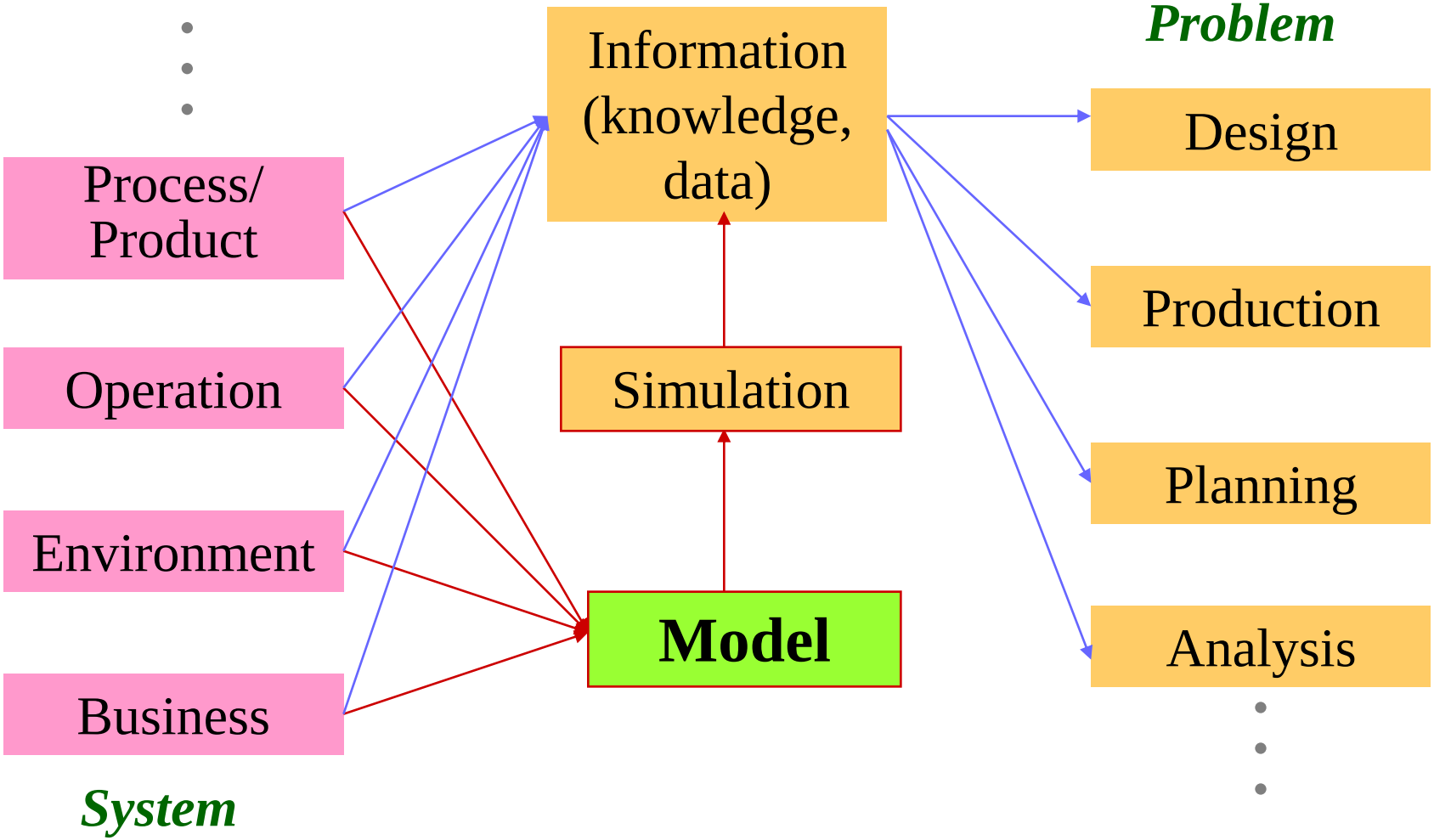
Systems and Control Theory => Process Control => Manufacture

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

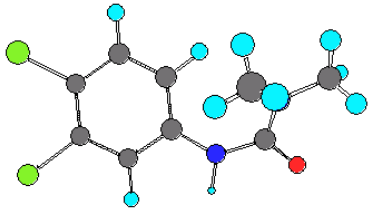
Management Science => Operations/Business => Supply chain

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

Models have an important role in PSE

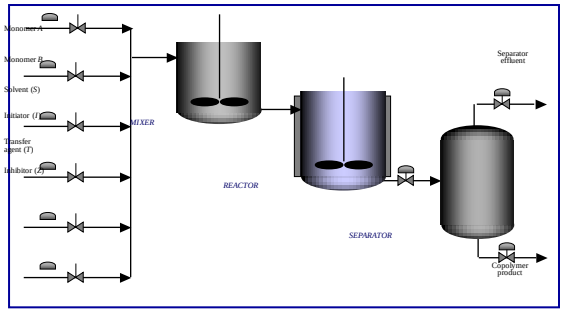


Example: Problem formulation & solution



Property models

$$Log\ P_i = A_i + [B_i/(C_i + T)]$$



Process models

$$\frac{dm_i}{dt} = f_{in,i} - f_{out,i} - r(m,T,P)V; i = 1, NC$$

Models for environmental impact

Operation models

Process models

Property-kinetics models

Cost models

Models for sustainability metrics

Formulation process model

Product evaluation model

Example: Problem formulation & solution

Fobj = min {$C^T y$ + f(x, y, u, d, θ) + S_e + S_i + S_s + H_c + H_p}

Process-product model

P = P(f, x, y, d, u, θ)

Process-product

0 = $h_1(x, y)$

Equipment-material

0 ≥ $g_1(x, u, d)$

0 ≥ $g_2(x, y)$

Flowhseet-chemical alternatives

B x + $C^T y$ ≥ D

Problems:

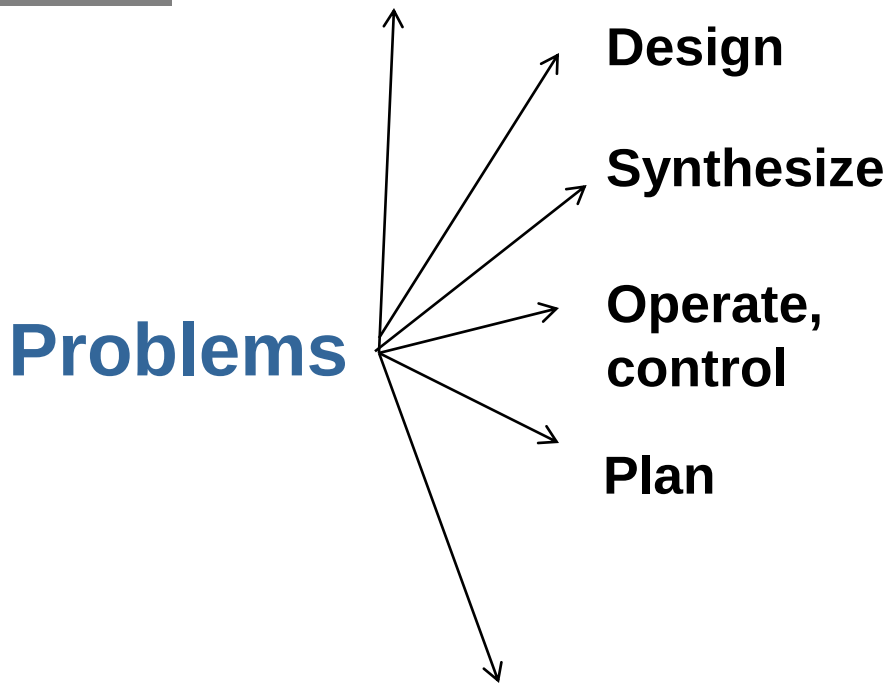
LP, NLP, MILP, MINLP, process simulation, ...

Solution strategies:

Direct, Decomposition based

x: real-process variables; y integer-decision variables

Managing the complexity through PSE



Problem defined by

- System boundary
- Models (of different types, sources, ...)
- Data (from different sources,)
- Multi-objectives & multi-disciplines
- .....

PSE = *systematic solution of problems by efficient management of the complexity*

Most used methods & tools in PSE

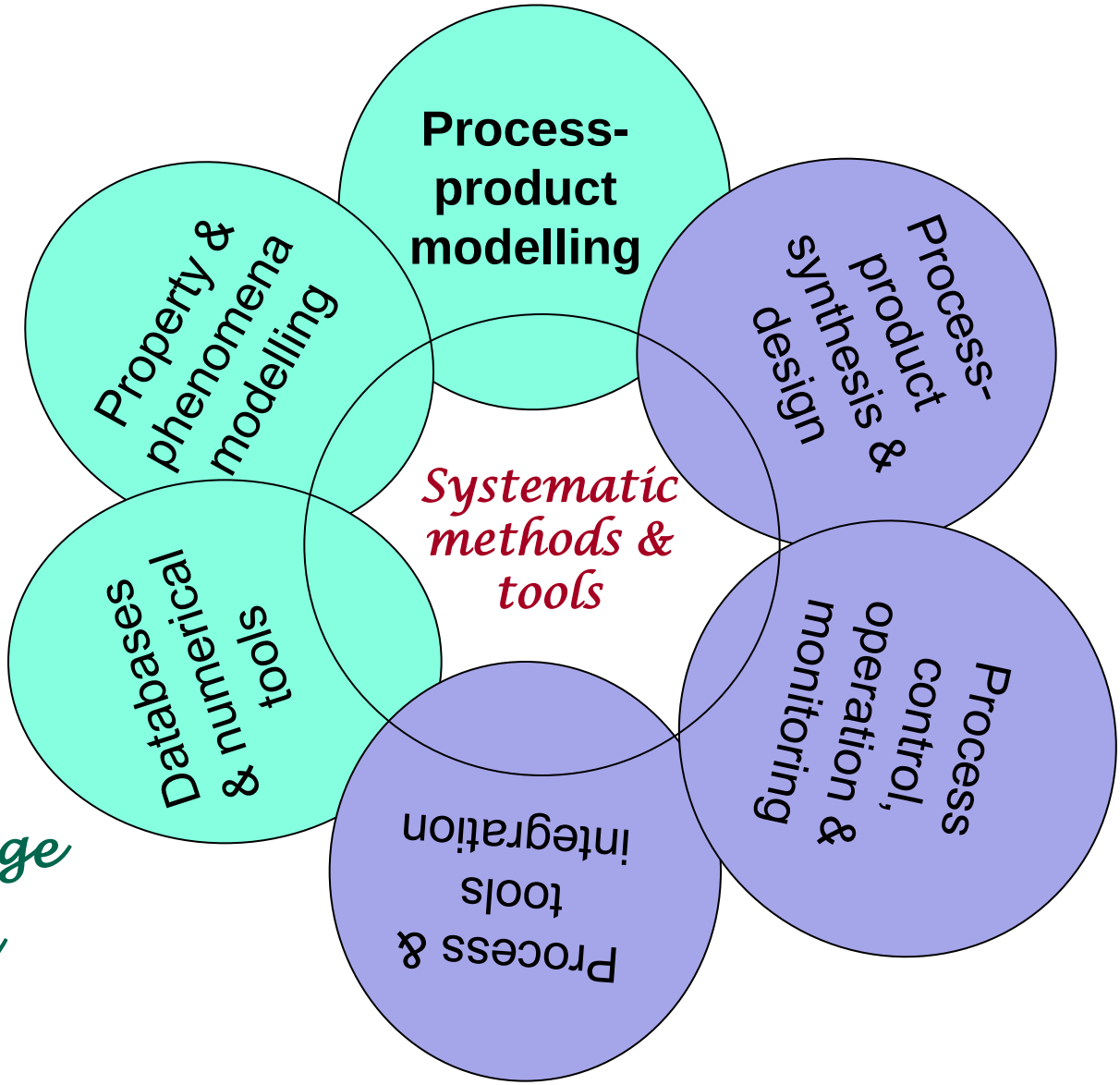
- **Process simulators (mainly commercial)**
- **Solvers (GAMS, Matlab, …)**
- **Specialized software**
  - **Control**
  - **Planning & scheduling**
  - **Fault diagnosis**
  - **……**

Managing the complexity: Framework

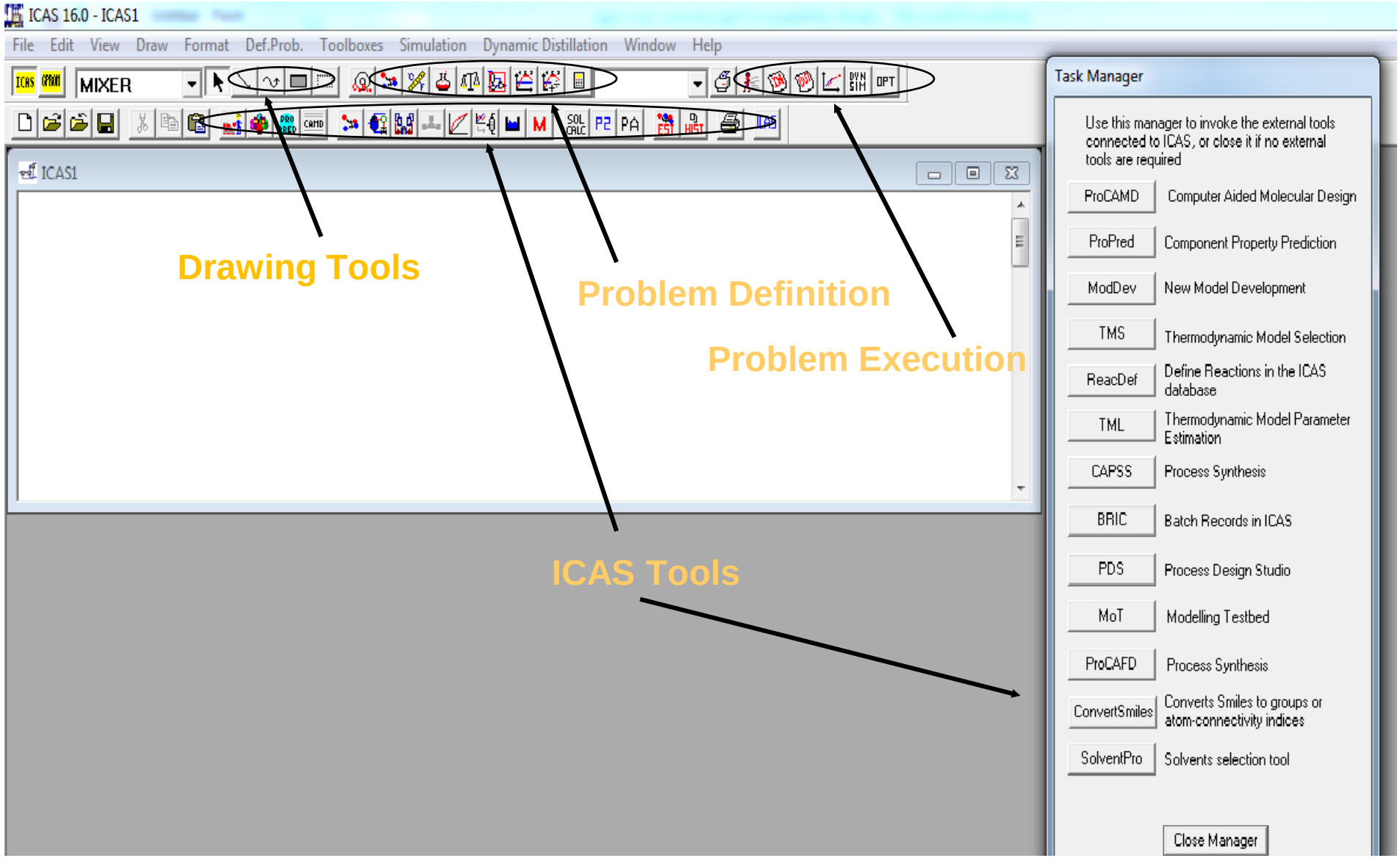
- **Define the problem**
- **Analyze the problem**
- ***Determine an appropriate solution strategy***
- **Solve & verify**

Defines application range

Defines solution approach

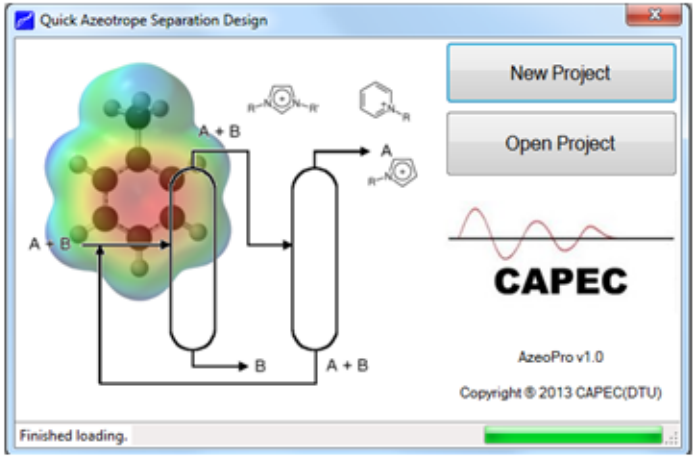


Manage the complexity: Tools integration

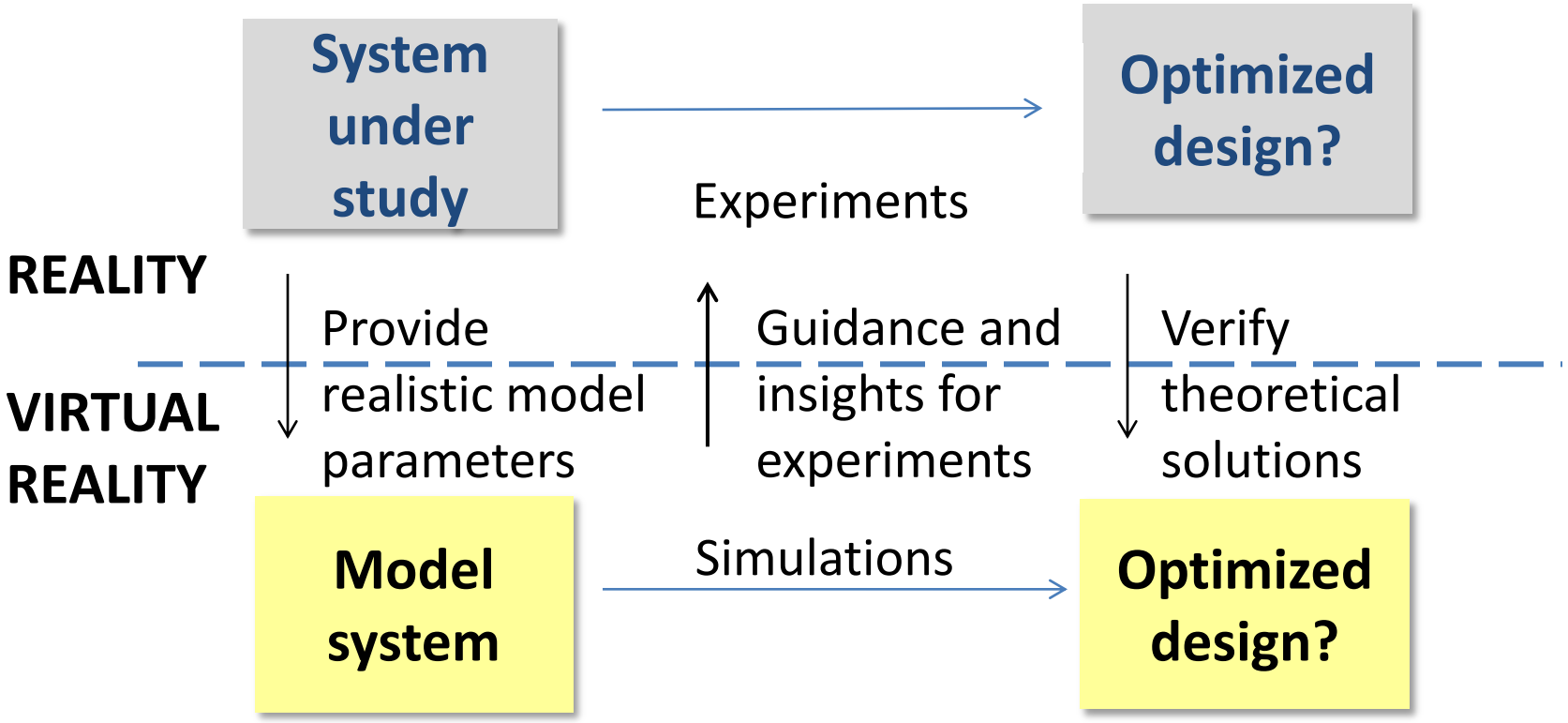


ICAS & Associated Tools

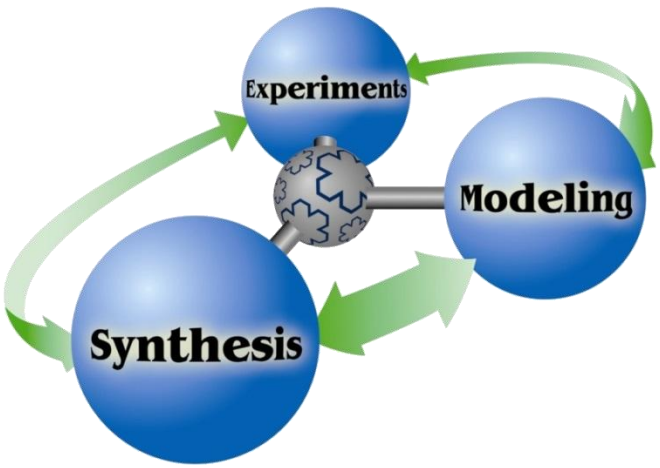
ICAS-Tools	New Software	EXCEL-based Macro
Database Manager	**AzeoPro**	**SustainPro** Sustainable process design
ProCAMD		**LCSoft** Life cycle analysis
ProPred		**ECON** Economic analysis
MoT		**ICAS-PAT** PAT system design
SolventPro SolventPro Solvent Selection tool		**Run-PC-SAFT** Use of PC-SAFT equation of state for pure component properties



The Role of Models & Experiments



- Approaches
  - Integrated modeling, experiments and synthesis
  - Ability to find predictive-innovative solutions

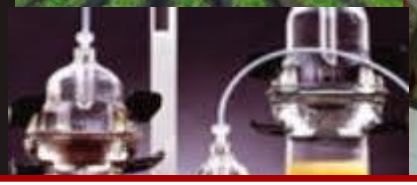
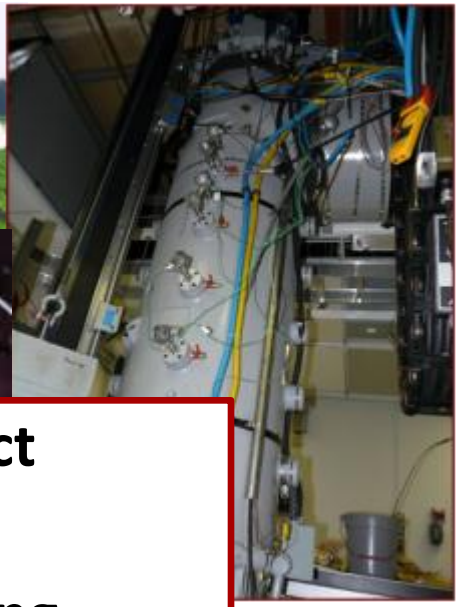


Computer Aided Modelling

Goal: Development of a computer-aided modelling framework

Computer-aided modelling of increasing importance to face current and future challenges product-process engineering.



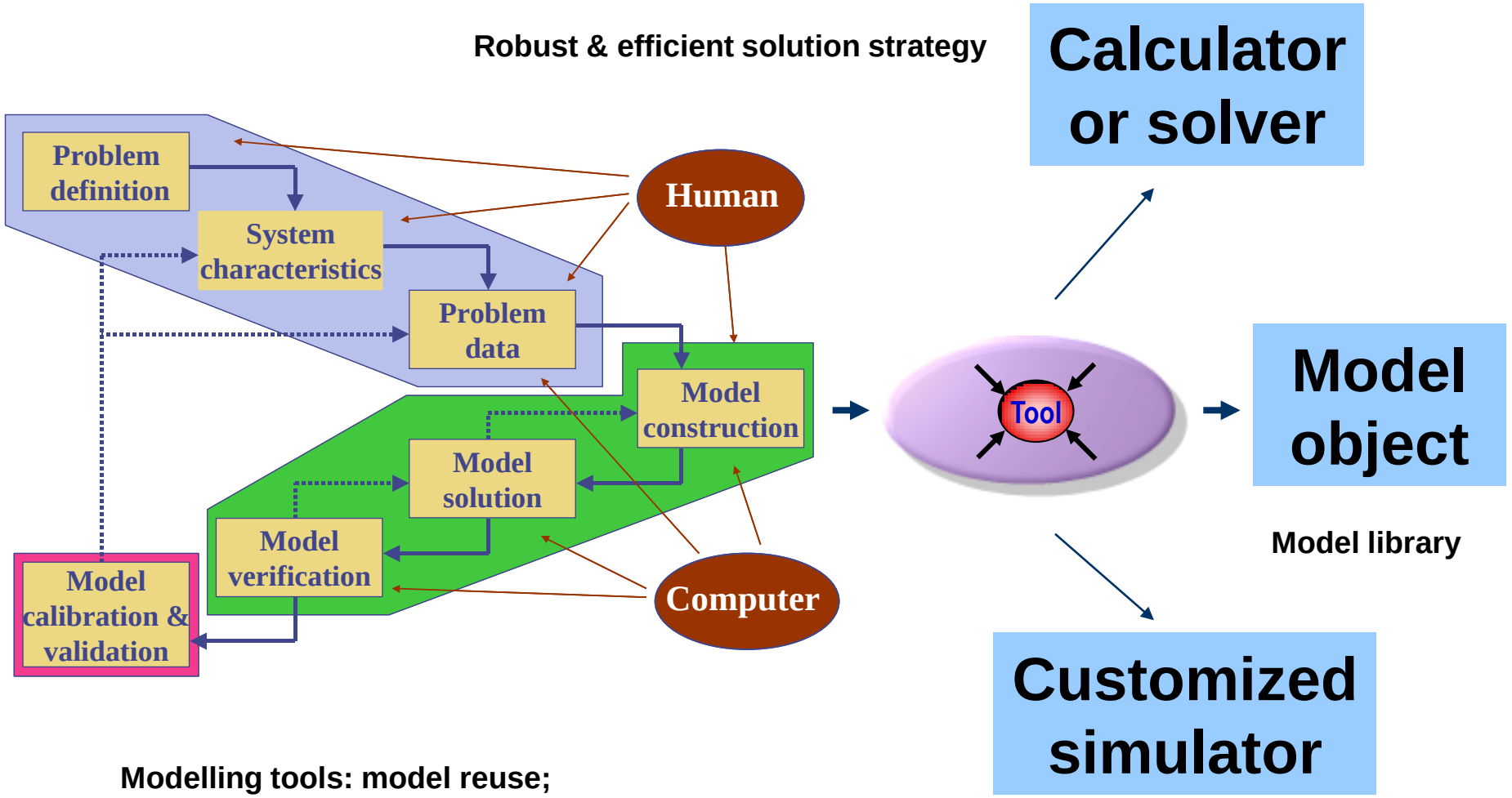
-> Prediction and optimization of product process behaviour

-> Reduce number of resource-demanding experiments

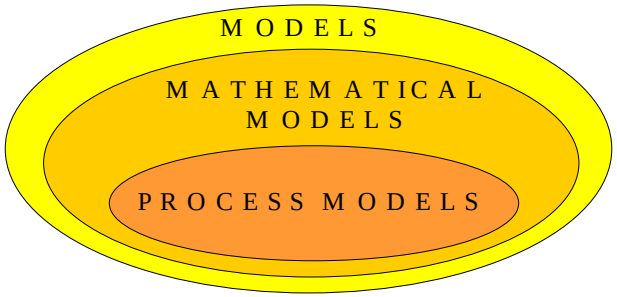
-> Deliver truly innovative solutions

-> Improved understanding of domain system

Computer aided modelling framework



Idea of computer aided modelling system

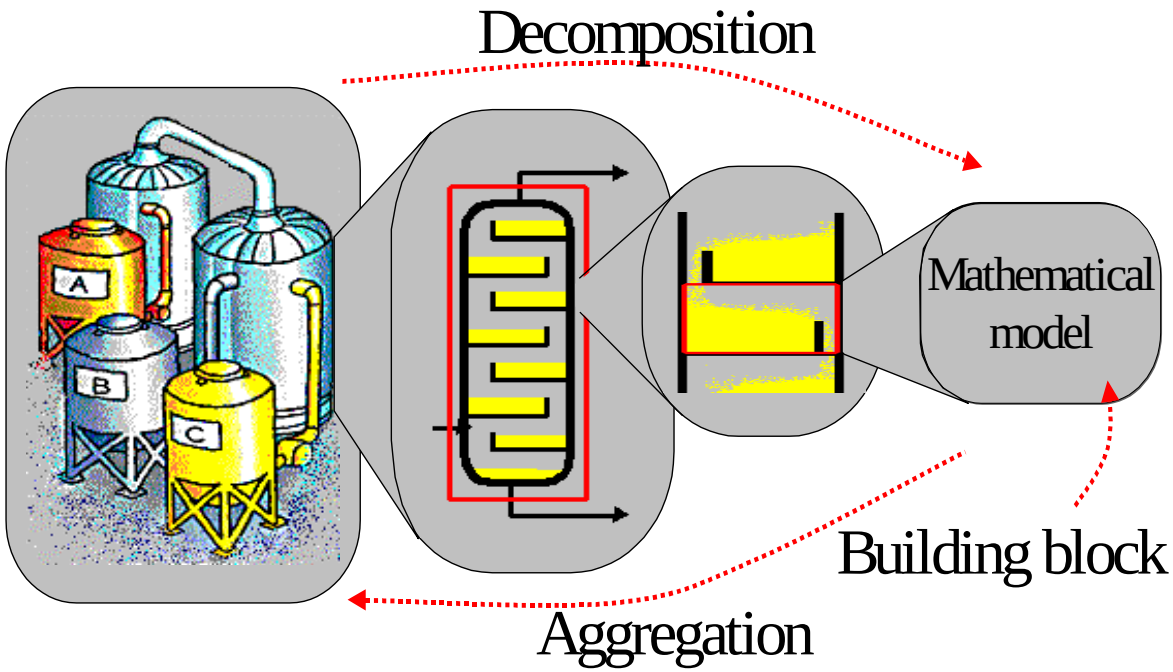


Model domain

- **Derive the model equations (model generation)**
- **Translate & Analyze model equations (model translation)**
- **Solve model equations & generate model "object"(also, create library for use with a simulator or for on-line solution)**

A computer aided system assists the user in performing the above tasks

Examples of Model construction & solution



Three Classes of Equations

*** Balance Equations**

***Constraint Equations**

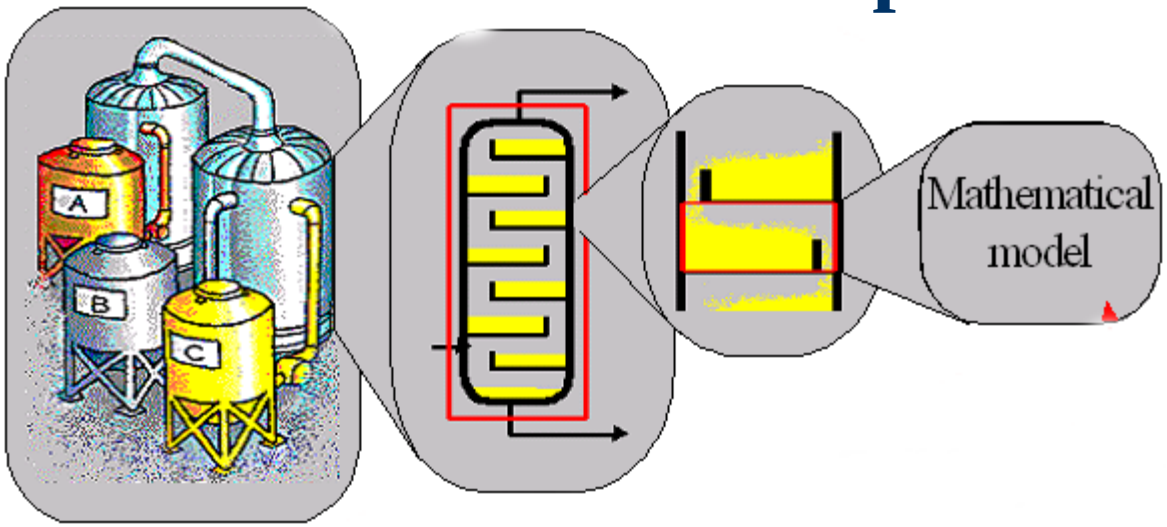
***Constitutive Equations**

Define Boundary → Describe System → Identify Building Block

Allows model construction, generation & reuse

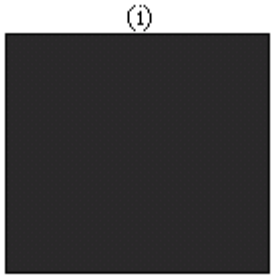
Generate & use models at various scales

Examples of Process Models

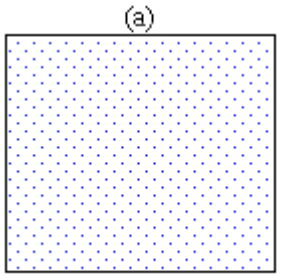


Accuracy (verification)

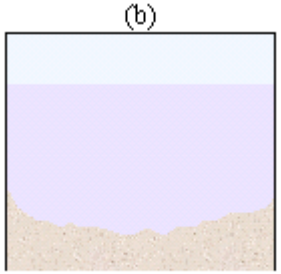
Predictive power (design)



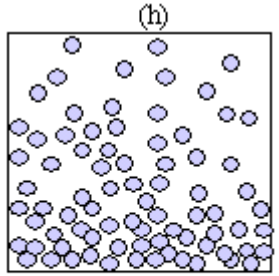
Black box



Perfectly mixed system



Equilibrium phase system



Particulated system with uniform gradient in one direction

Generate & use models at various scales

Property Models

Correlations — Pi = Ai + [Bi/(Ci + T)]

Molecular — Zc = (Pc*Vc)/(83.14*Tc)

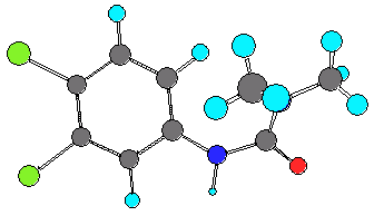
CH3-; -CH2-; -OH; …..

Groups — Tb = 222.543*log(Sum.Groups.I + Sum.Groups.II + Sum.Groups.III)

C, H, O, N, S, ….

Atoms — P=∑niPi + b(vχ0) + 2c(vχ1)

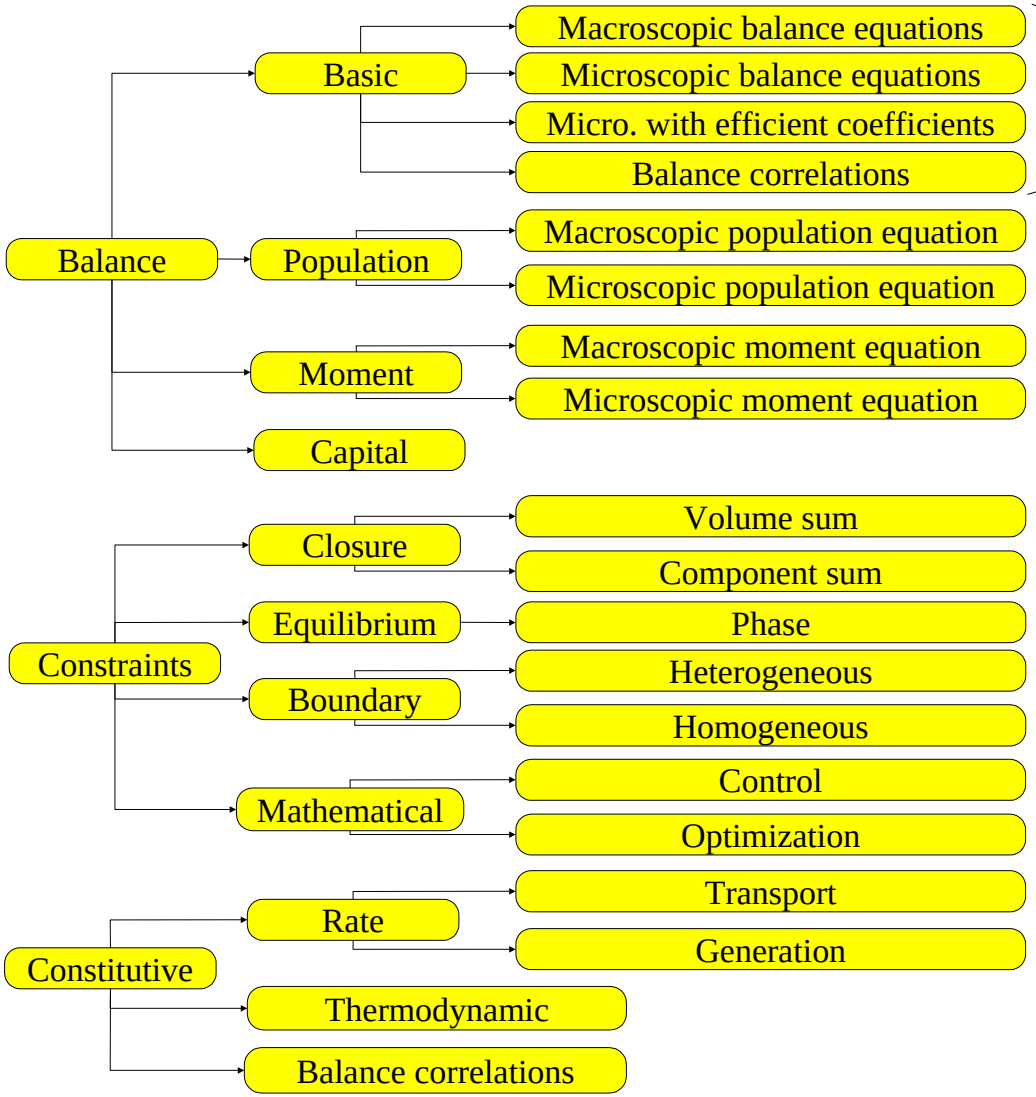
Micro



Accuracy (verification)

Predictive power (design)

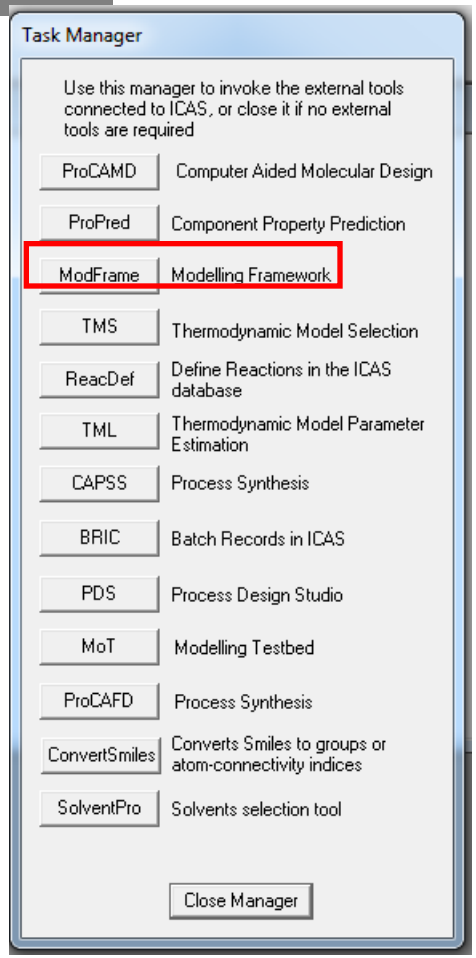
Examples of model construction & solution

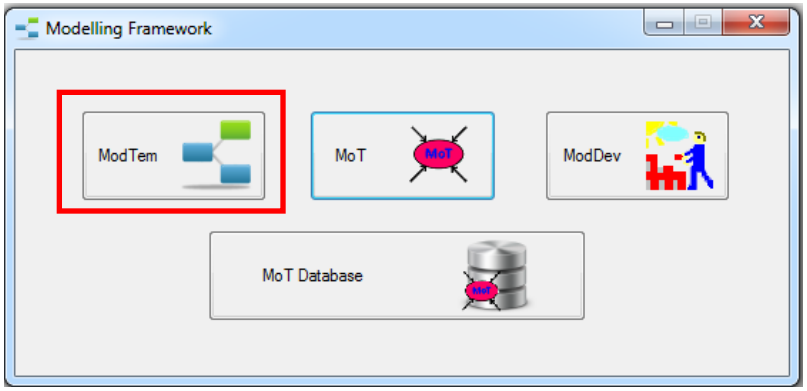


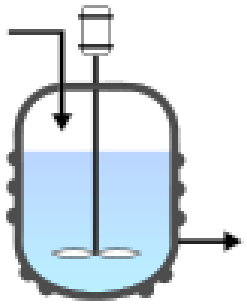
Can be transferred into balance equations for other extensive quantities by symbolic manipulation

Describe modelling needs through a model derivation taxonomy – start from the left for each class of model equation and identify the end-point on the right. Retrieve the equations from a library for each end-point

Model-based tools – Product design

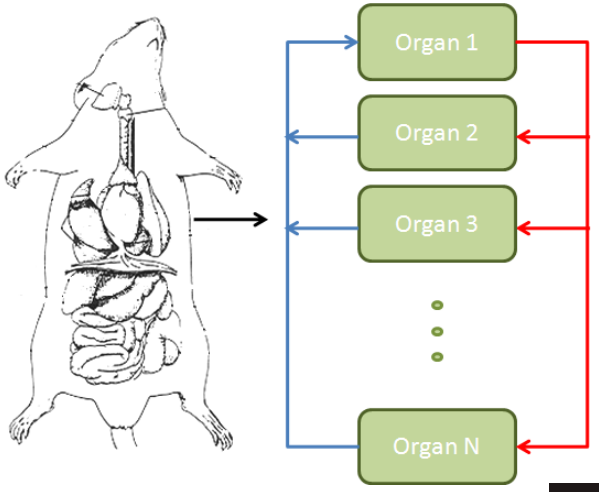


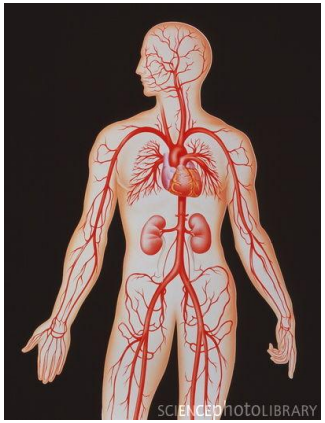




Computer-Aided Modelling: Pharmacokinetics

Pharmacokinetic modeling of drug distribution in rats





1. Retrieval and analysis of different candidate models

   Phase I: Modelling objective and system information

   Phase II.B: Multi-scale model construction

2. Discrimination between model candidates, estimation of identifiable model parameters

   Phase III: Model identification/discrimination

   Phase IV: Model evaluation/validation

3. Strategy for scale-up (to human)

-> Highlight modelling methodology (different work-flows) and software tool.

A Mosat, E Lueshen, M. Heitzig, C. Hall, A A Linninger, G. Sin, R. Gani, 2013, "First principles pharmacokinetic modeling – A quantitative study on Cycloporin", Computers & Chemical Engineering, 54, 97-110; see also another paper in CACE 2014

Current & future challenges

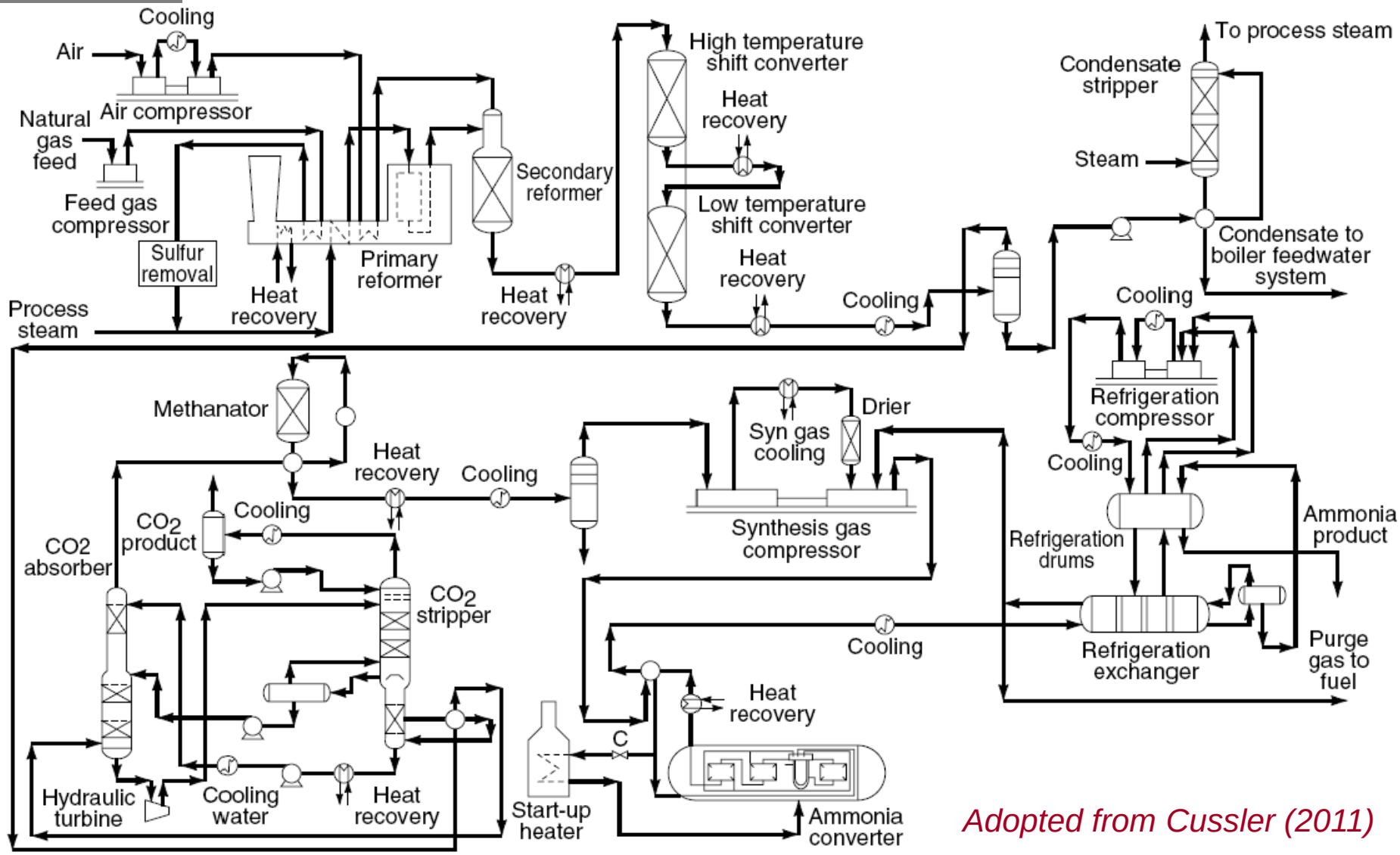
The key chemical products

	Commodities	Molecules	Microstructures
Key	Cost	Speed	Function
Basis	Unit Ops	Chemistry	Microstructure
Risk	Feedstock	Discovery	Science

Skills Required?

Adopted from Cussler (2011)

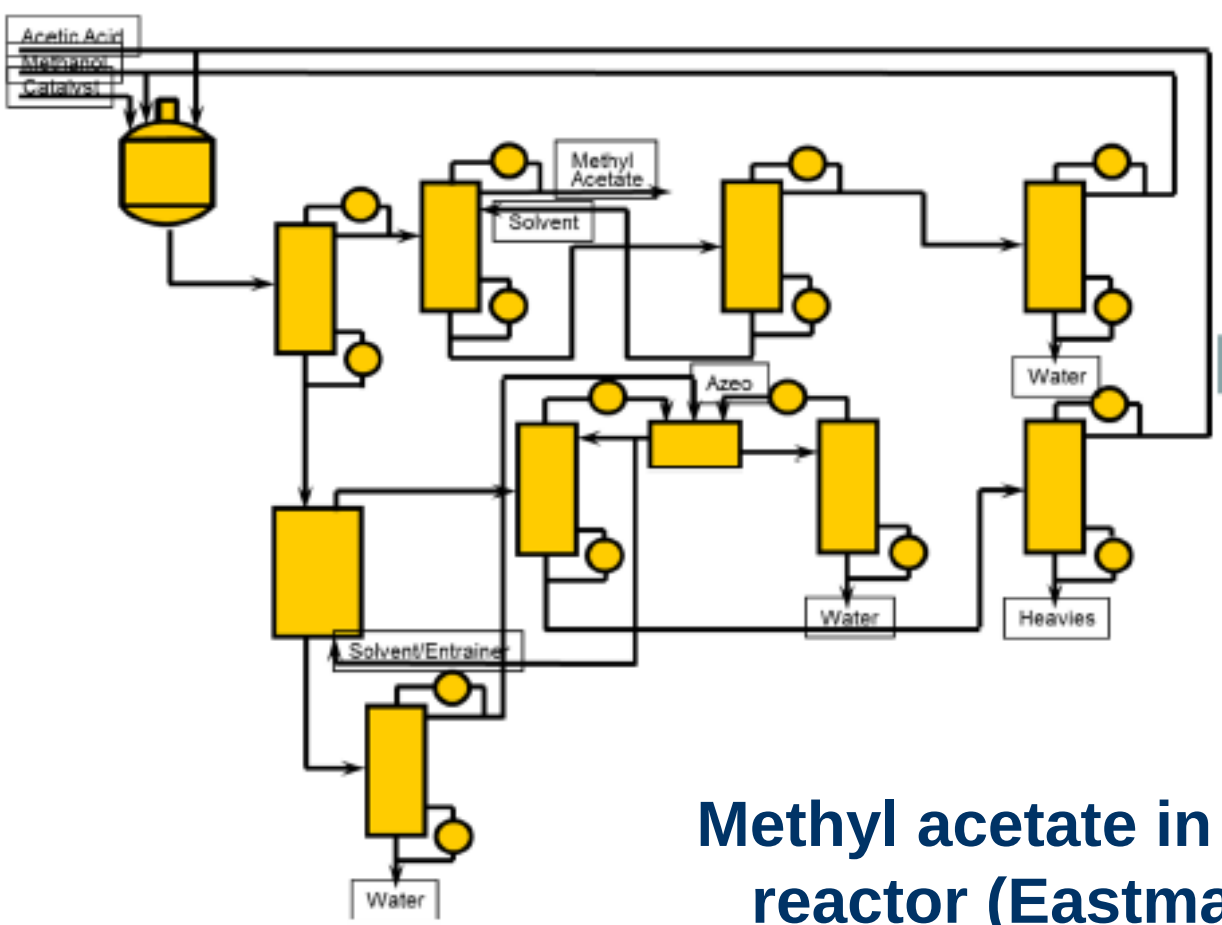
Problems we can solve very well!

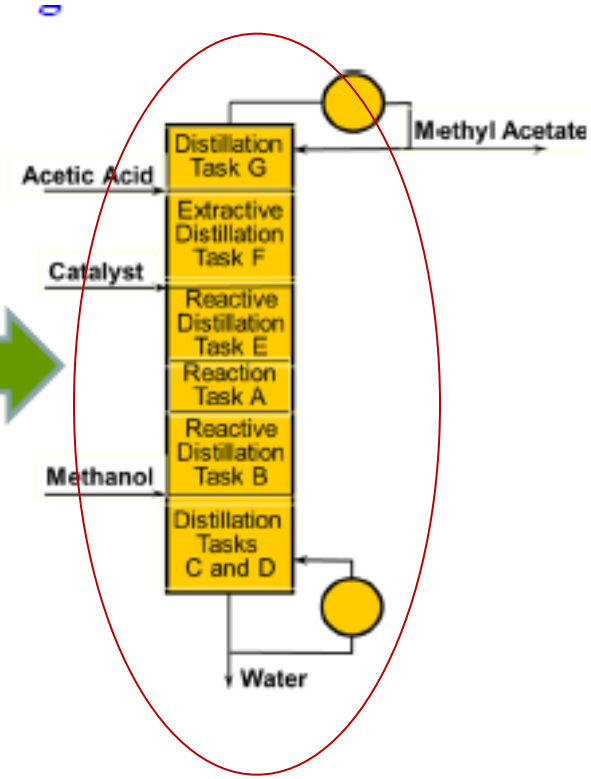


Adopted from Cussler (2011)

Current & future challenges: Processes

How to find innovative solutions?





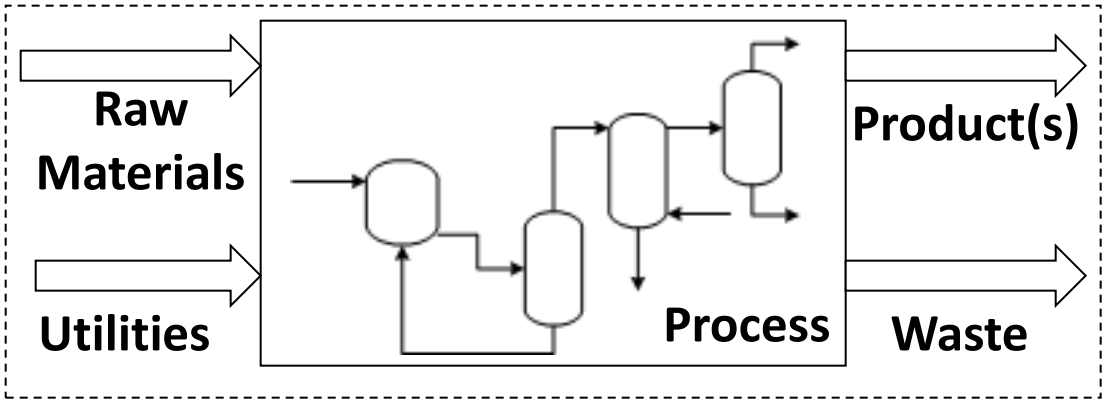
Methyl acetate in multifunctional reactor (Eastman Chemicals)

How to tackle the enlarged problem size?

Chemical and bio-based industry faces enormous challenges to achieve and/or respond to:

Establish sustainable production

Adopt to changing markets



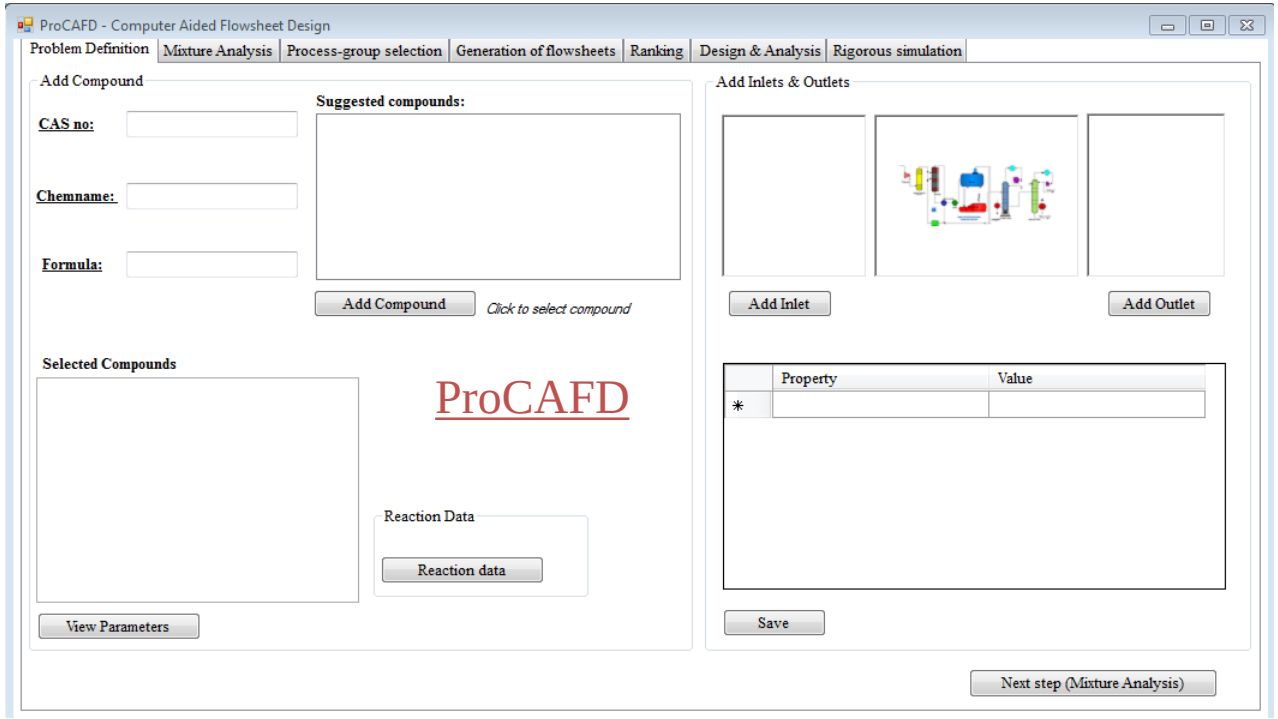
Survive global competition

Demands for innovative products

Processes need to be:

Sustainable (Economically feasible; Reduced waste; Utility efficient; Environmentally acceptable); Safe; Operable; .....

Framework & Tool for Computer Aided Flowsheet Generation

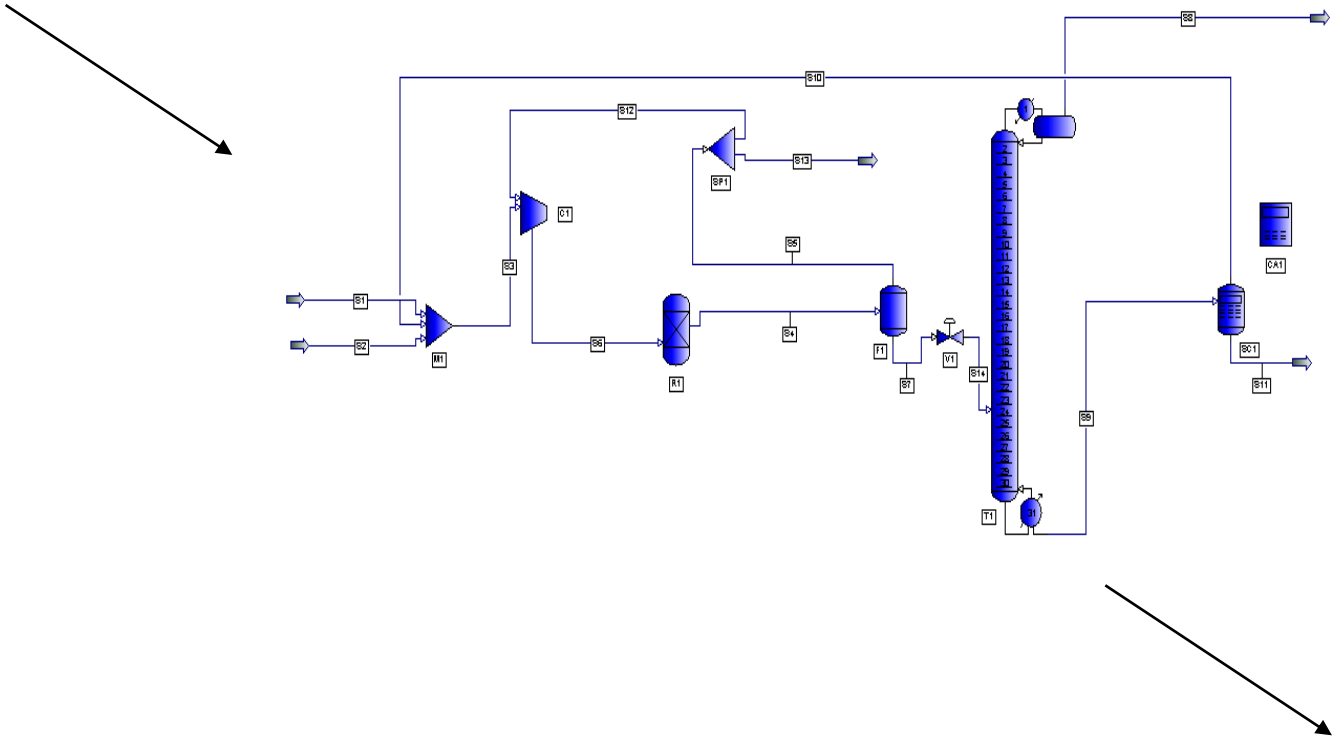


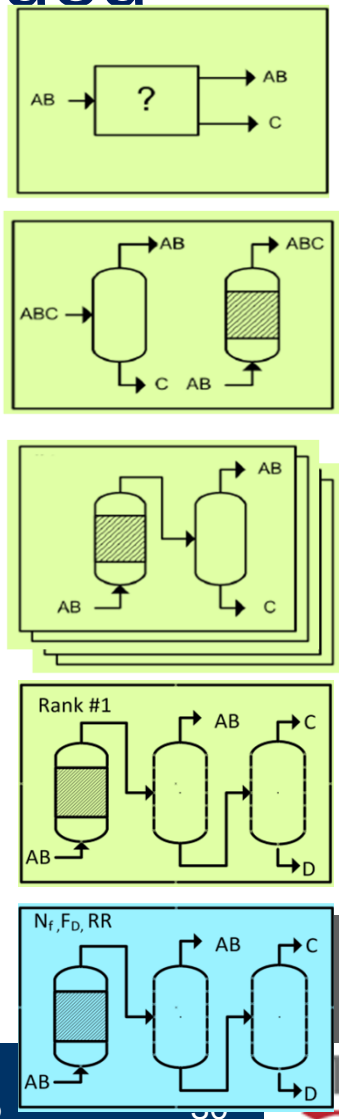
A Computer-Aided Tool to:

- ❖Generate all feasible process flow-sheets (To generate novel/innovative solutions).
- ❖Quick & efficient evaluation of alternatives.
- ❖Design & Analysis of Alternatives
- ❖That requires minimal computation resources and expert knowledge.

Framework & Tool for Computer Aided Flowsheet Generation

(iA)(rAB/pABCD)<1<2[<(iB)](gmemABC/D)[(oD)](A/BC)1(B/C)2(oC)





Molecular Products

The key chemical products

	Commodities	Molecules	Microstructures
Key	Cost	Speed	Function
Basis	Unit Ops	Chemistry	Microstructure
Risk	Feedstock	Discovery	Science

Skills Required?

Adopted from Cussler (2011)

Products with Special Microstructures

The key chemical products

	Commodities	Molecules	Microstructures
Key	Cost	Speed	Function
Basis	Unit Ops	Chemistry	Microstructure
Risk	Feedstock	Discovery	Science

Skills Required?

Adopted from Cussler (2011)

Examples of chemical products

Positive contribution to the modern society

Survival of the modern society depends on the products from ChE

Formulate & solve these problems?

Jet-fuel blend

Liquid formulations & emulsions

Gasoline blend

Scientifically specified needs

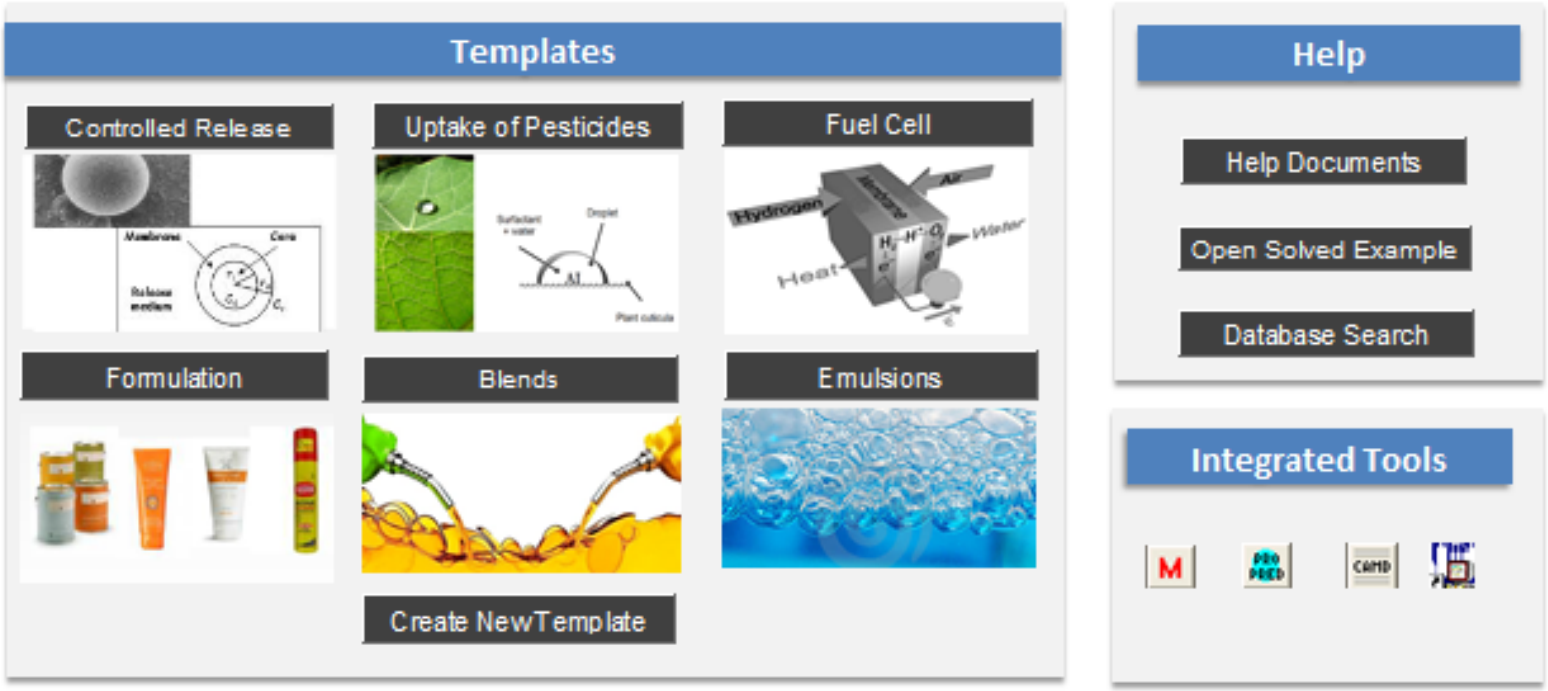
Needs defined by consumer reactions

Model-based tools – Product design

Is there a need for a product simulator?

VPPD - Lab
Virtual Product-Process Design Lab

The chemical product simulator



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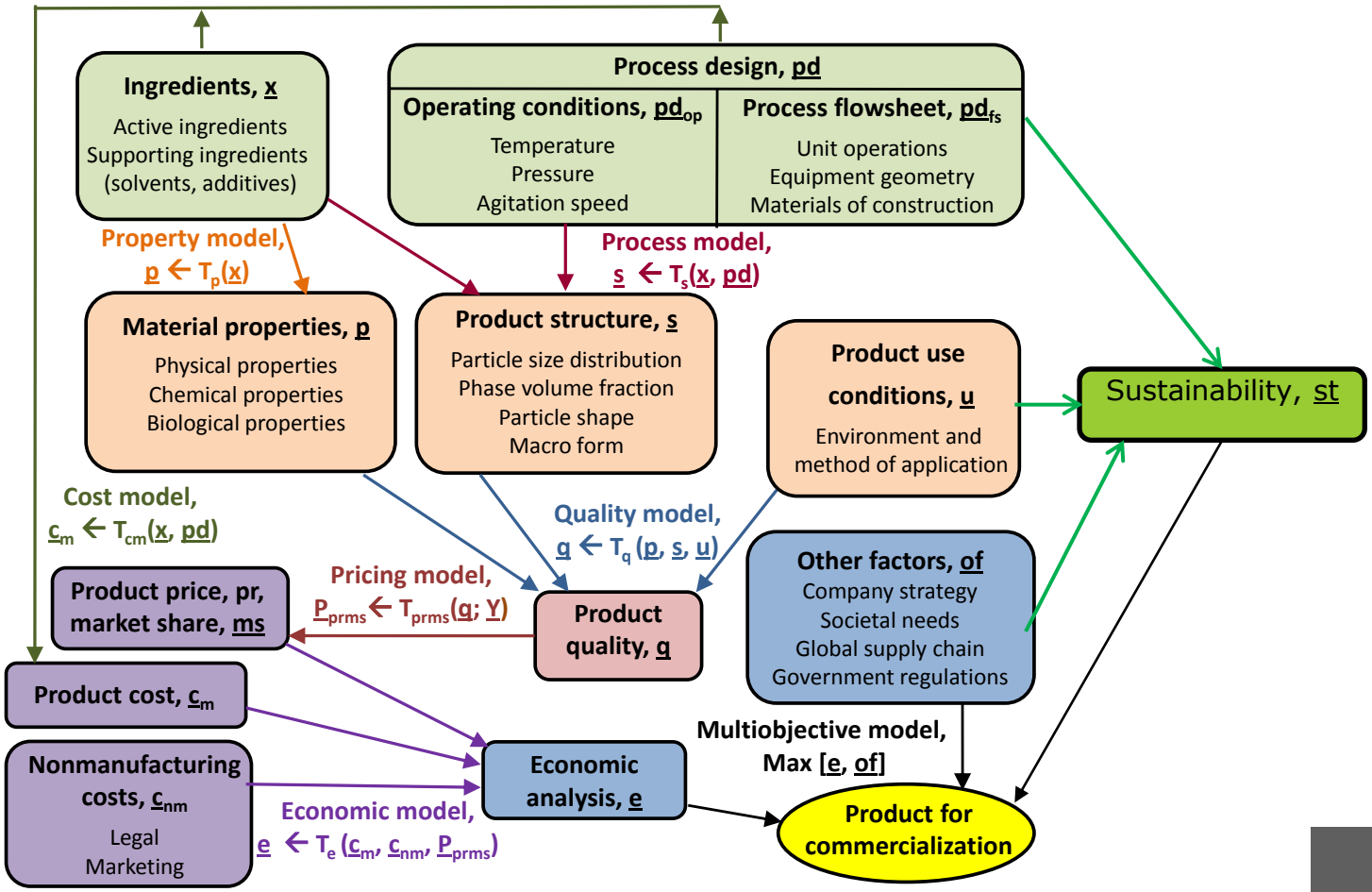
Model-based tools – Product design

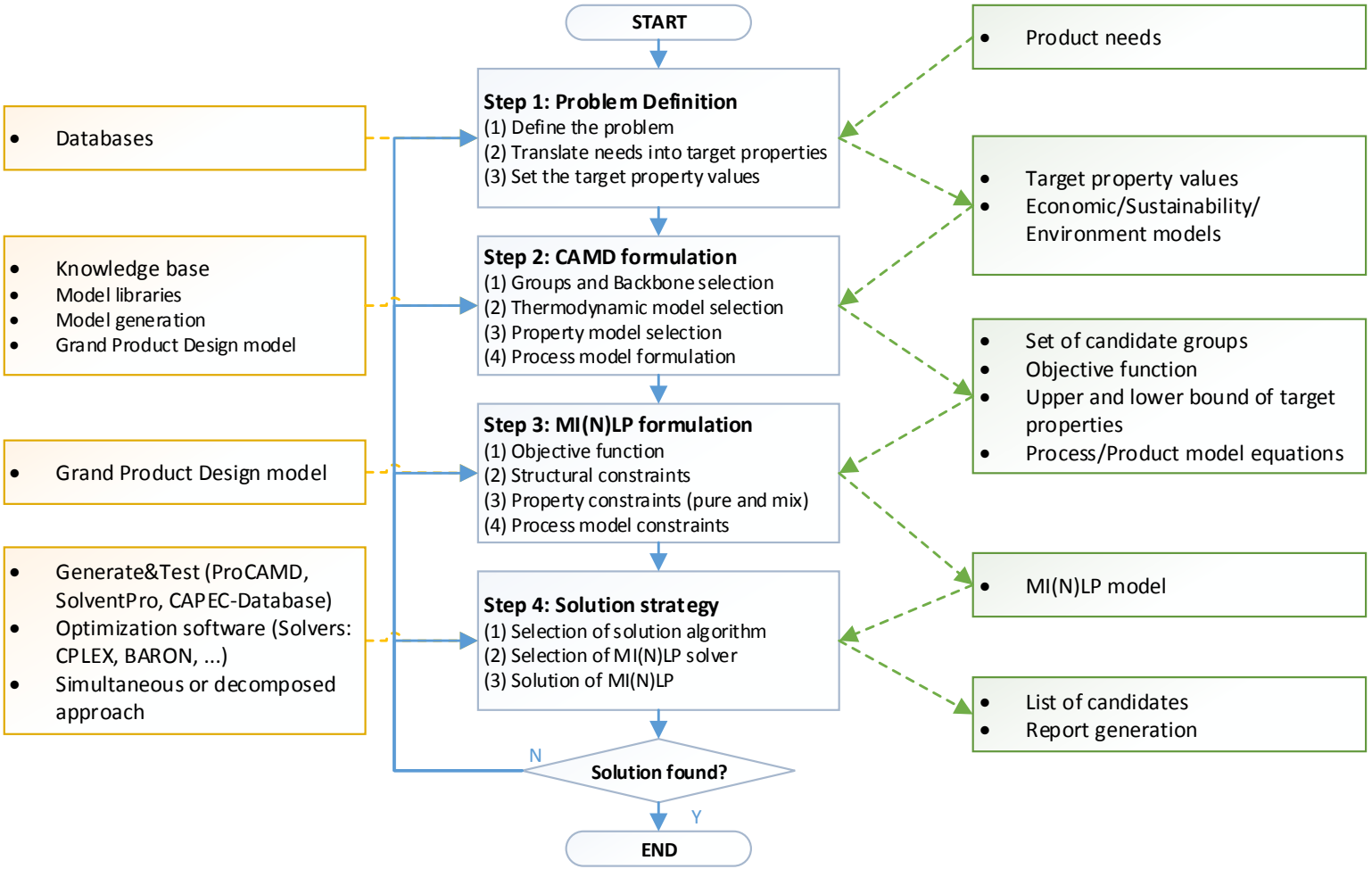
The Grand Product Design Model?



Model-based tools – Product design

The Mathematical Problem & Solution?

Methods and Tools | Work Flow | Information Flow



Issues & questions for the future

- **Should we look for solutions that are not so simulator specific?**
  - **Are simulators able to solve the problems we are interested in?**
- **Should we develop new model-based methods & tools?**
  - **Should we let the vendor companies develop the tools?**
- **How to find the innovative solutions we need?**
  - **Can this be done with the current tools?**
- **We (PSE-academia) need to take back the leadership role**

Conclusions & issues

Need to address the grand challenges – energy, water, food & environment

Need to look and develop beyond the current methods and tools

Need efficient management of the complexity is the key

Need to develop model based systems that provide truly innovative & new solutions

……

Future Research Challenges in PSE

How do we go from here . . .

Azapagic 2013

Future Research Challenges in PSE

……. Somewhere here?

Azapagic 2013