Optimisation in a Process Engineering Context

Eva Sorensen

Chemical Engineering

Product and Process Systems Engineering

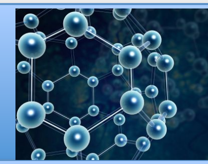
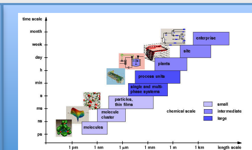
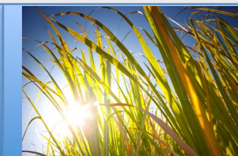
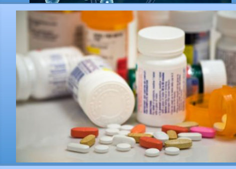
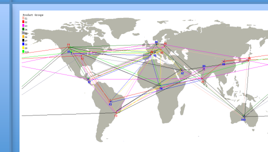
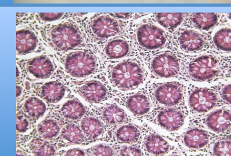
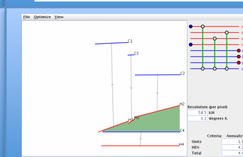
David Bogle, Vivek Dua, Eric Fraga, Lazaros Papageorgiou,

Eva Sorensen and Michail Stamatakis

Application Domains

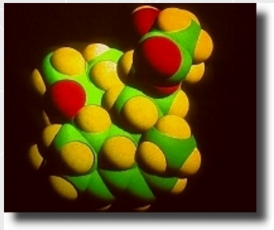
Our key areas of research:

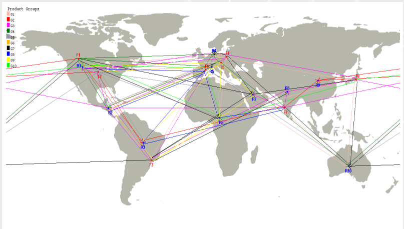
Competence Areas

Competence Areas	Chemical Manufacturing Systems	Biological Systems Engineering	Supply Chains of the Future	Energy Systems Engineering
Product and Process Design				
Operations and Control				
Modelling and Model Solution Tools				

Process Engineering

- ***Process Systems Engineering*** *is concerned with the improvement of decision making processes for the creation and operation of the chemical supply chain.*



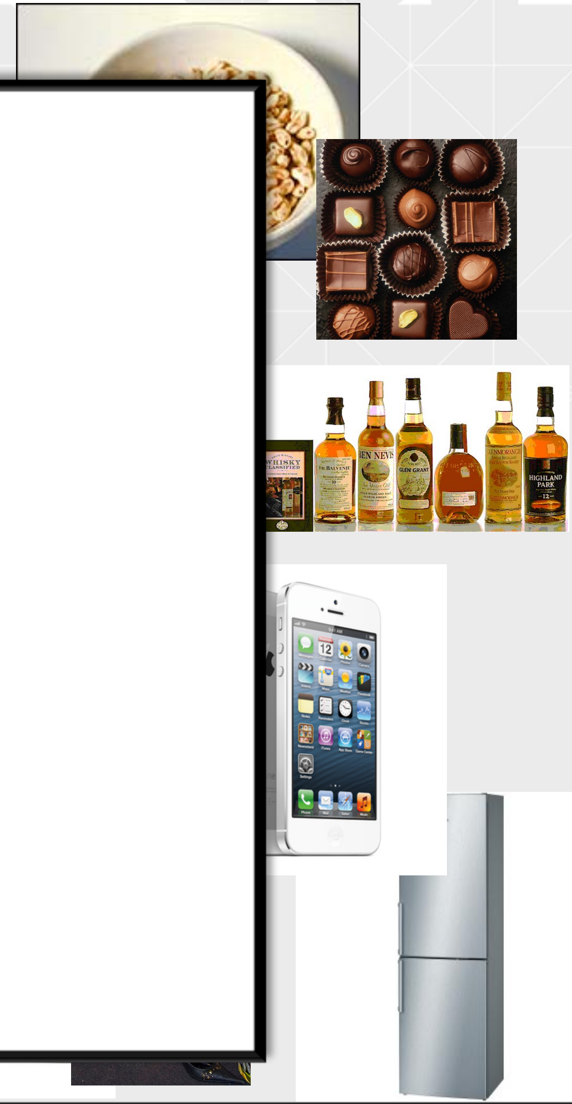



- *It deals with the discovery, design, manufacture and distribution of chemical products in the context of many conflicting goals.*

Grossmann and Westerberg, Carnegie Mellon University

“Chemical products”

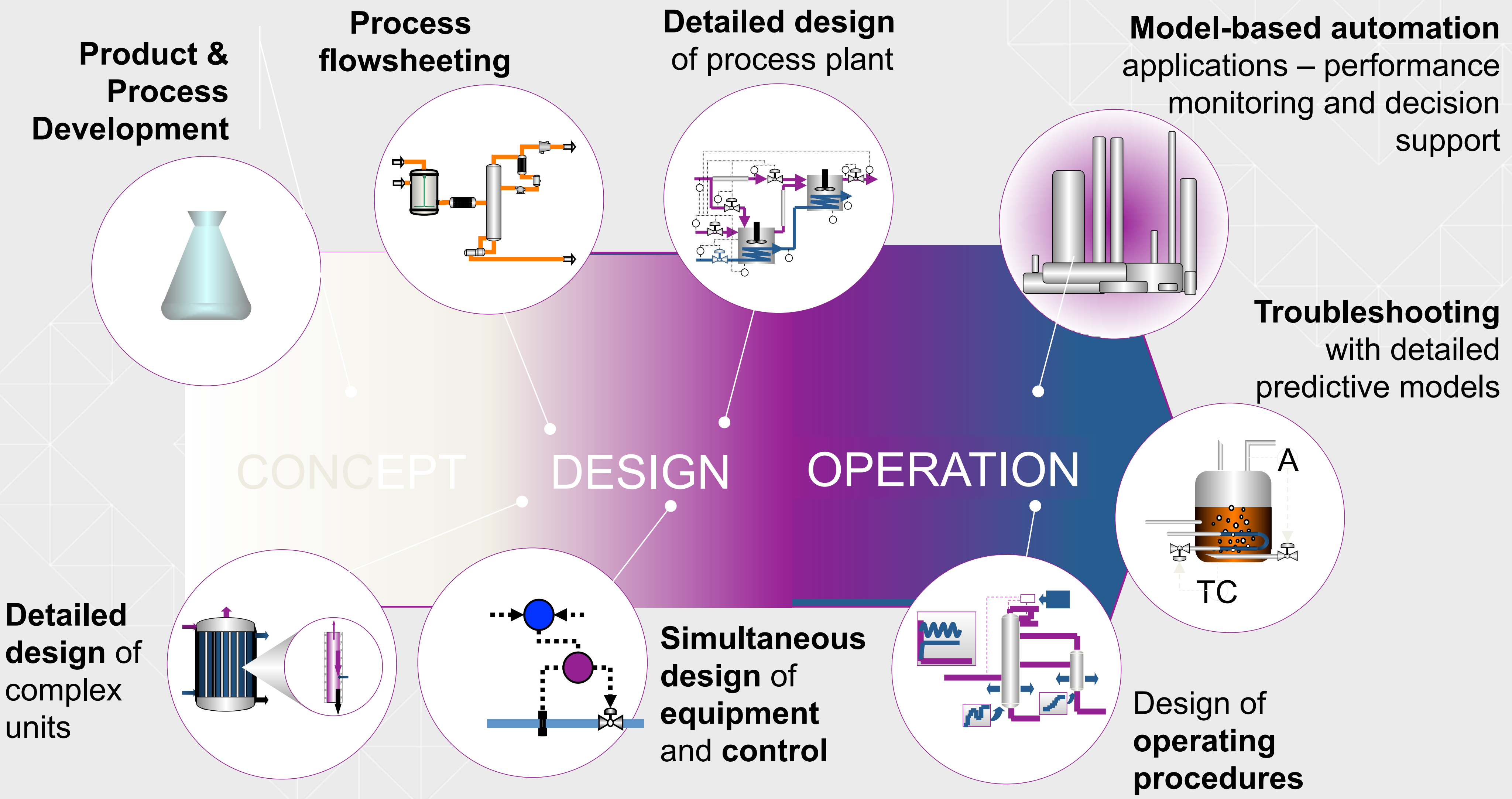
“Chemical products”



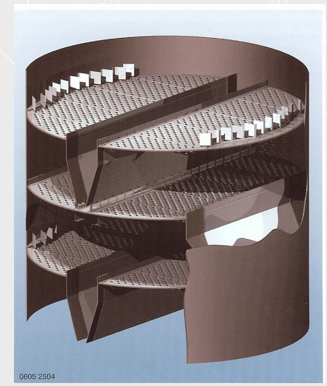
Application Domains:

- Chemical Manufacturing Systems
- *Molecular Systems Engineering*
- Biological Systems Engineering
- Supply Chains of the Future
- Energy Systems Engineering

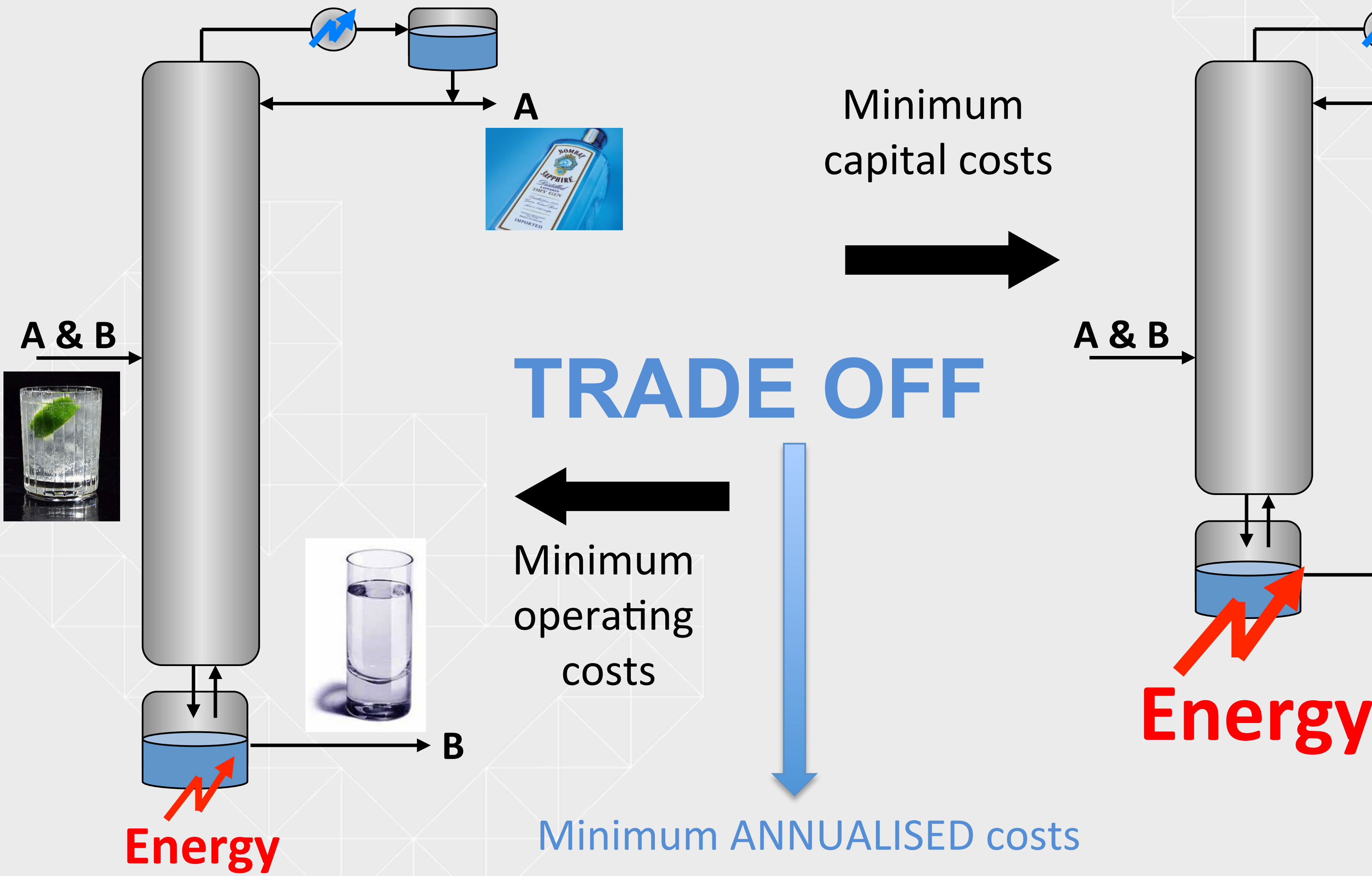
Process Engineering pipeline



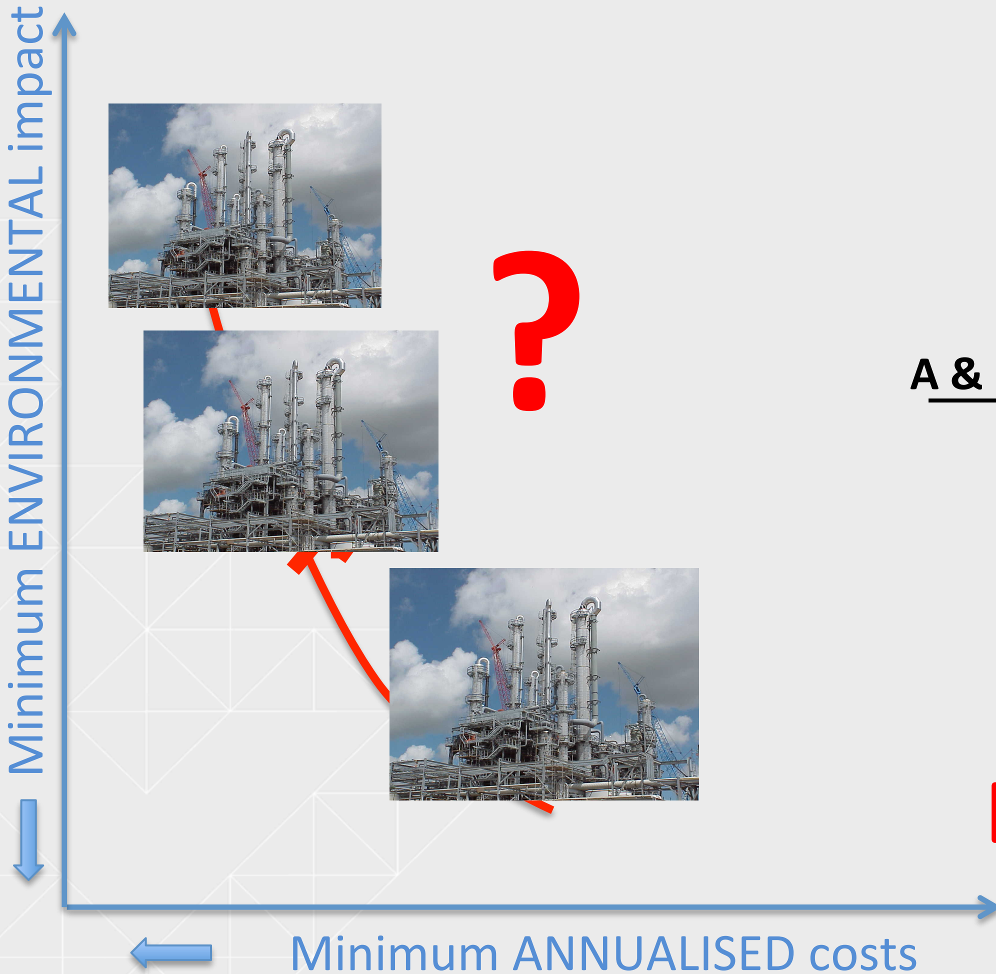
Distillation column design

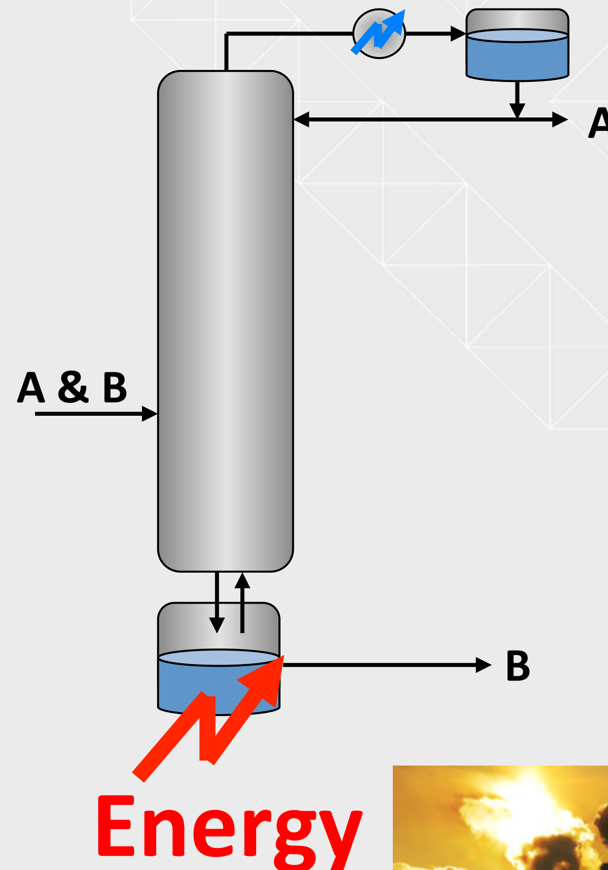


Distillation column design *contd.*

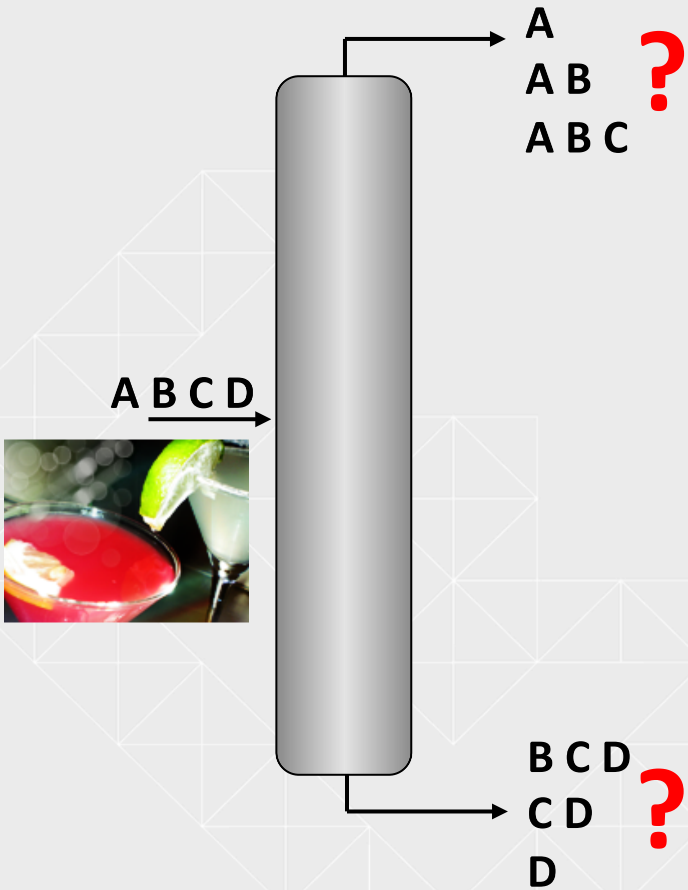


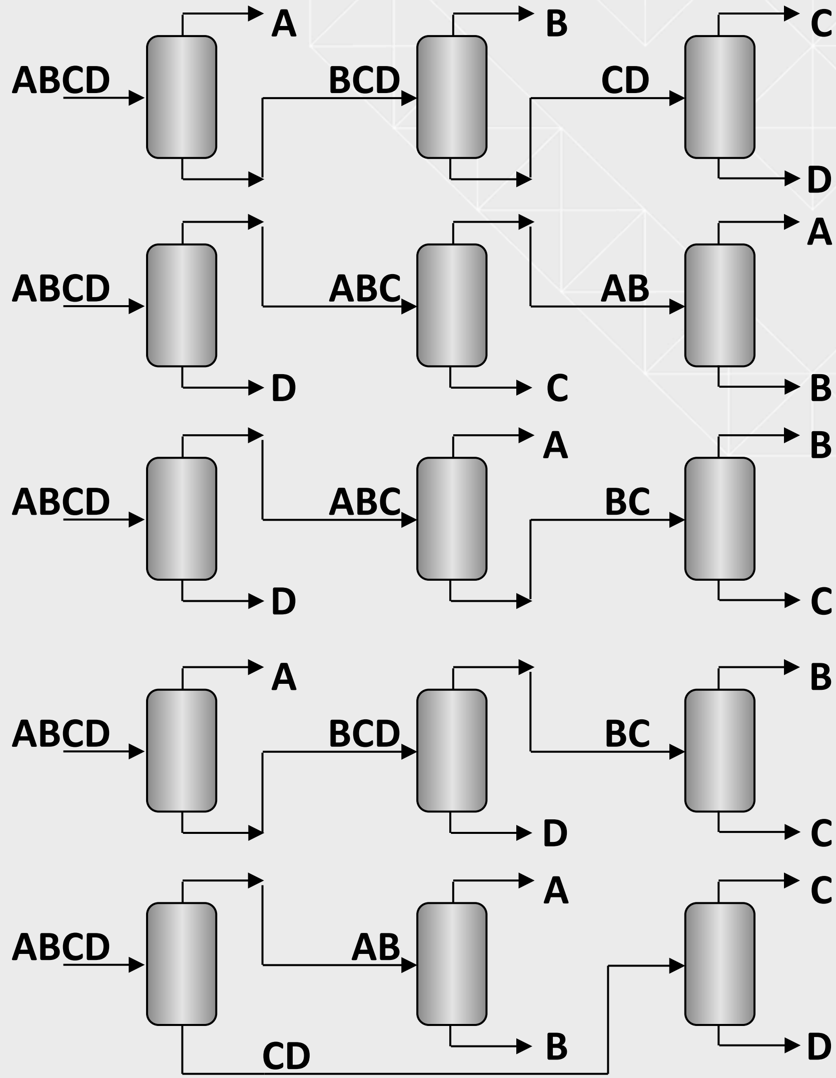
Distillation column design *contd.*





Column scheduling





Model?

The use of validated predictive models for…

Quantified uncertainty in the model predictions

Quantitative prediction of the effects of design & operating decisions on KPIs, within the accuracy necessary to achieve the business objectives

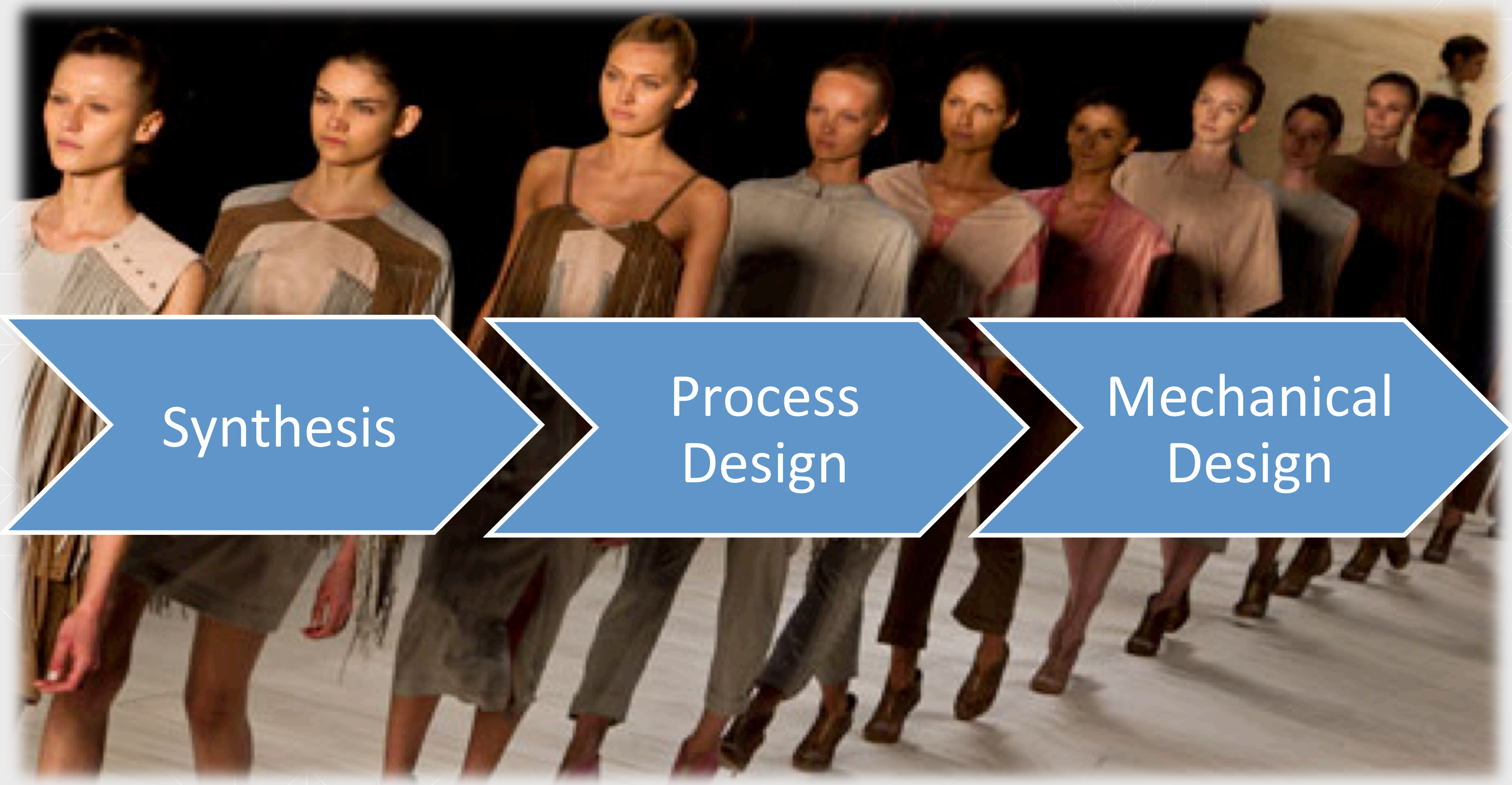
Quantification of technological risk involved in model-based decisions

Optimisation of process design & operation by comprehensive exploration of alternatives

Effective targeting of experimental R&D towards minimisation of this risk

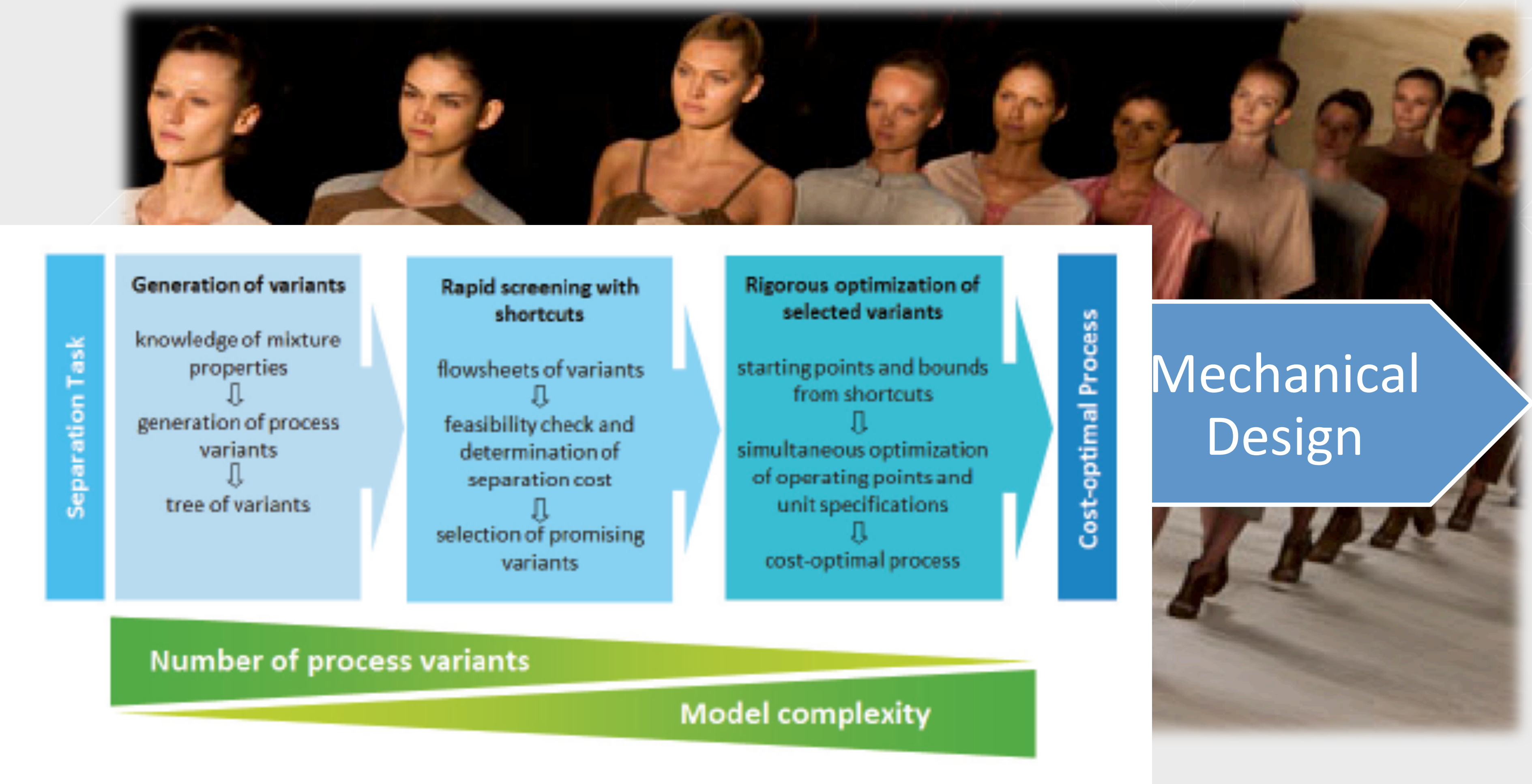
Model?

Catwalk!



Model?

Catwalk!

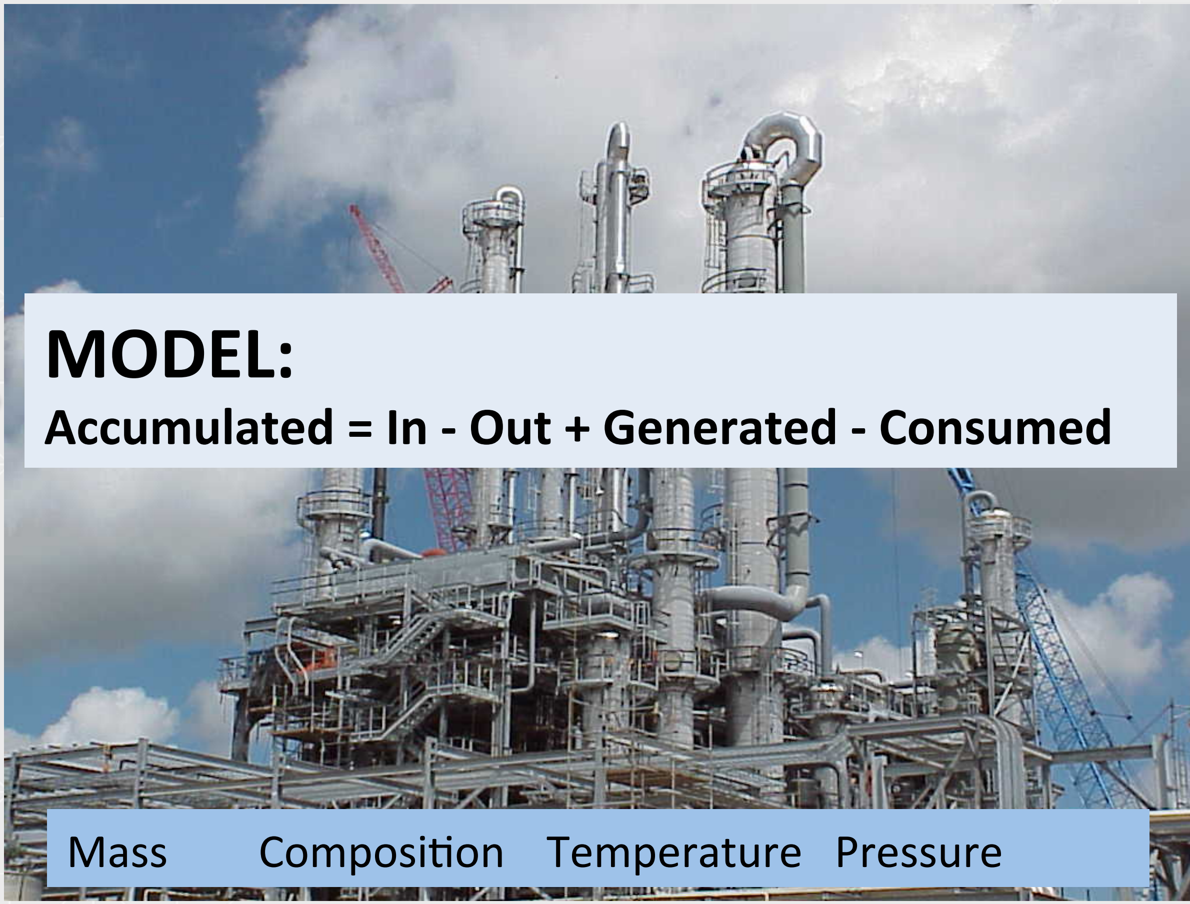


Mechanical Design

Model?

Mathematical mass and energy balances

Mass
Composition
Temperature
Pressure



MODEL:

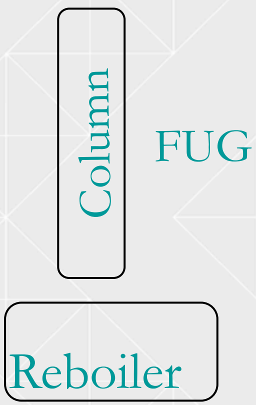
Accumulated = In - Out + Generated - Consumed

Mass Composition Temperature Pressure

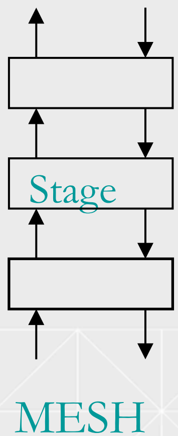
Mass
Composition
Temperature
Pressure

Model details - distillation

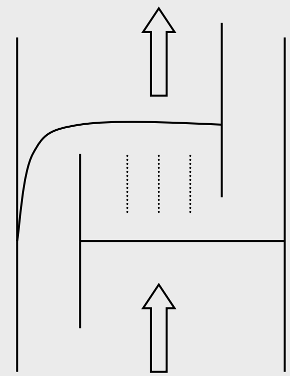
Simplified Models



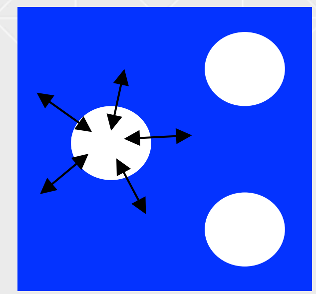
Rigorous Models



Detailed Models



Rate-based Models



Tray model

$$\frac{dM_{i,j}}{dt} = L_{j-1}x_{i,j-1} + V_{j+1}y_{i,j+1} - L_j x_{i,j} - V_j y_{i,j} \quad , \quad i = 1,\ldots,NC$$

$$\frac{dU_j}{dt} = L_{j-1}h^L_{j-1} + V_{j+1}h^V_{j+1} - L_j h^L_j - V_j h^V_j$$

$$M_{i,j} = M^L_j x_{i,j} + M^V_j y_{i,j} \quad , \quad i = 1,\ldots,NC$$

$$U_j = M^L_j h^L_j + M^V_j h^V_j - P_j \upsilon_j$$

$$\frac{M^L_j}{\rho^L_j} + \frac{M^V_j}{\rho^V_j} = \upsilon_j$$

$$\sum_{i=1}^{NC} x_{i,j} = \sum_{i=1}^{NC} y_{i,j} = 1$$

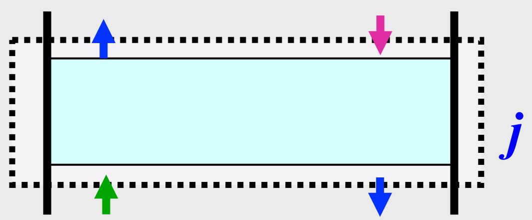
$$y_{i,j} = K_{i,j}x_{i,j} \quad , \quad i = 1,\ldots,NC$$

$$h^L_j = h^L\left(T_j, P_j, \underline{x}_j\right) \; ; \; h^V_j = h^V\left(T_j, P_j, \underline{y}_j\right)$$

$$\rho^L_j = \rho^L\left(T_j, P_j, \underline{x}_j\right) \; ; \; \rho^V_j = \rho^V\left(T_j, P_j, \underline{y}_j\right)$$

$$K_{i,j} = K_i\left(T_j, P_j, \underline{x}_j, \underline{y}_j\right) \quad , \quad i = 1,\ldots, NC$$

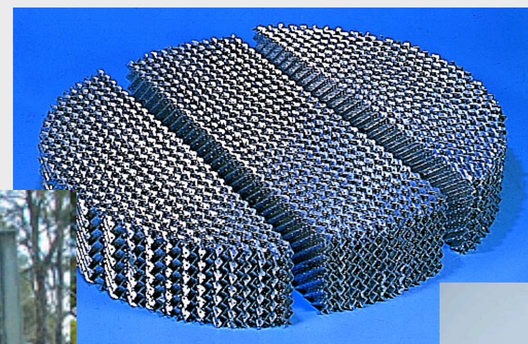
Single tray only!!!!

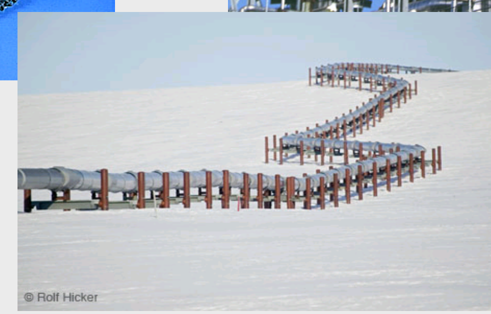


Model details – spatial variations

Properties vary with respect to one or more spatial dimensions as well as with time:

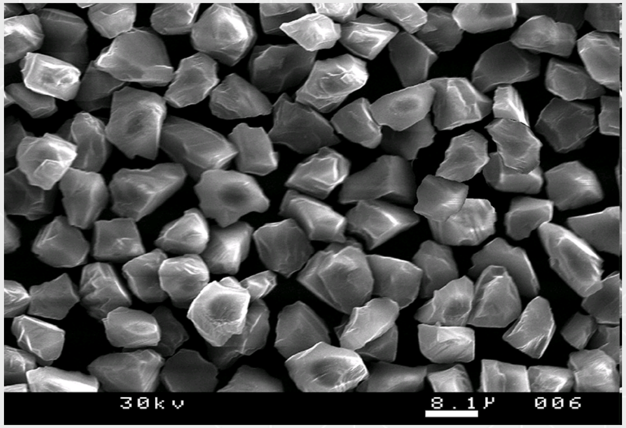
- Tubular reactors
- Packed bed columns (adsorption/absorption/distillati chromatography)
- Pipelines
- *etc*

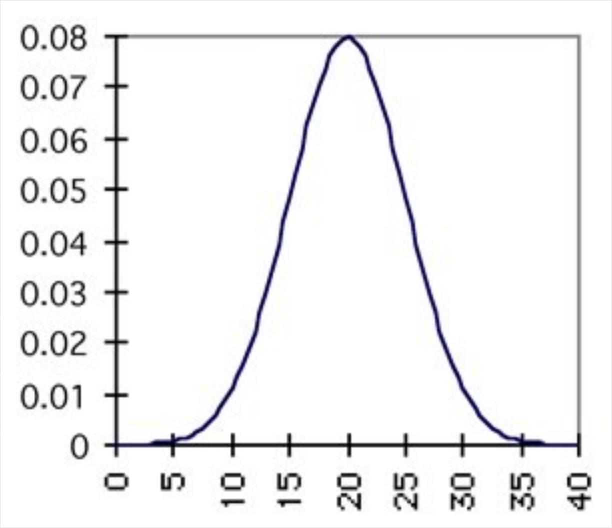


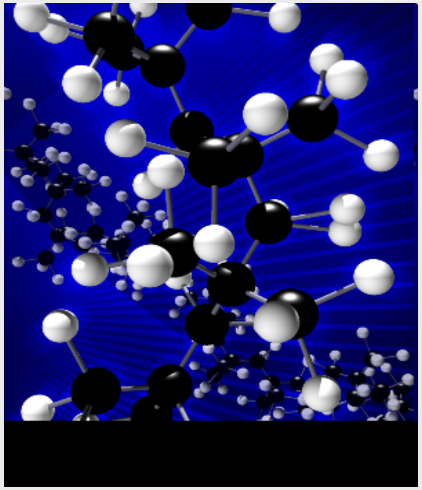


Model details – Probability density

- Probability density functions instead of single scalar values:
  - Crystallisation units (size of crystals)
  - Polymerisation reactors (length of polymer chains)
- For such processes, the properties may *also* vary with both time and spatial position.







Optimisation Problem Formulation

Minimise & ***Minimise*** & .....

Objective function 1 & *Objective function 2*

Subject to:

Model equations — *DAE/PDAE, nonlinear*

Design variable bounds — *discrete and continuous*

Operational variable bounds — *continuous*

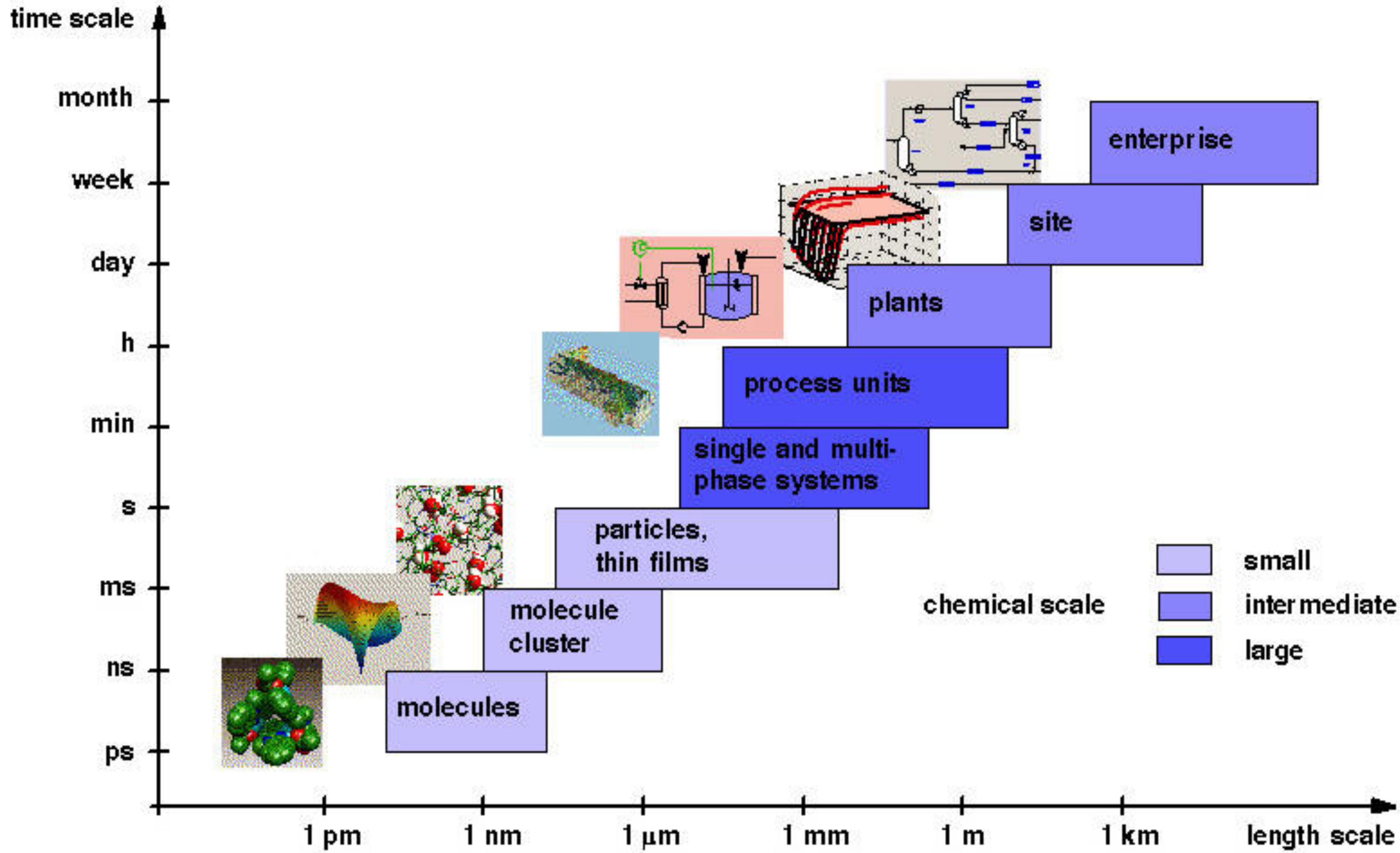
To determine:

Design variables (constant)

Operation variables (time dependent)

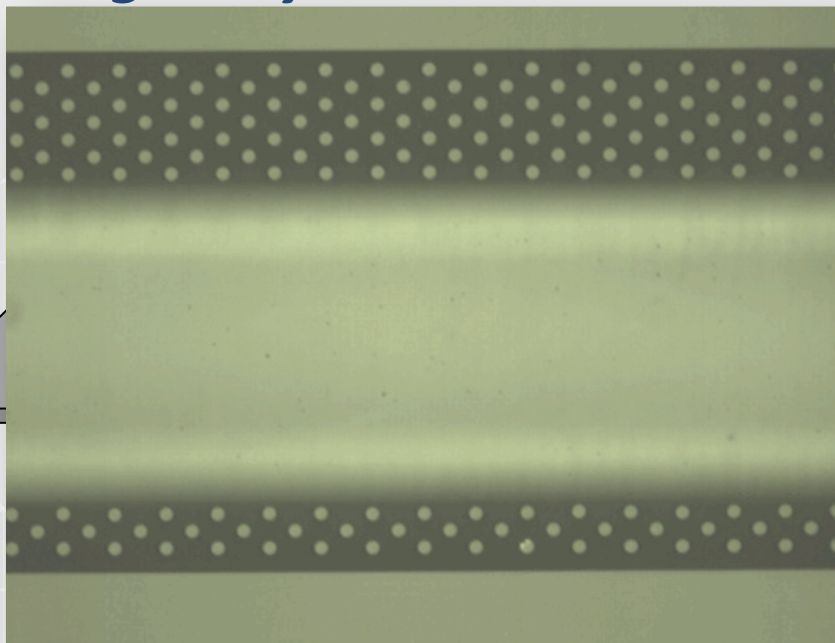
EXAMPLES

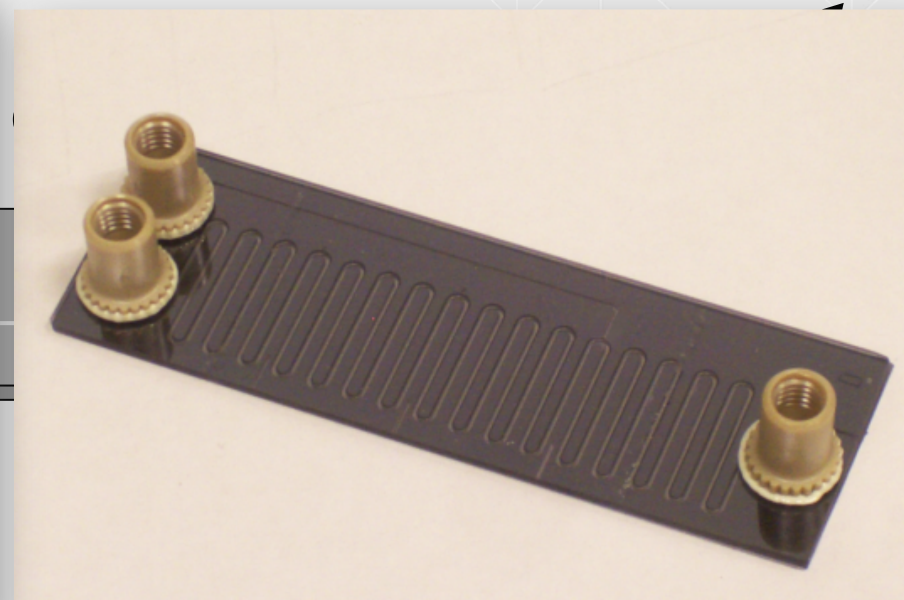
Multi-scale considerations



Micro distillation

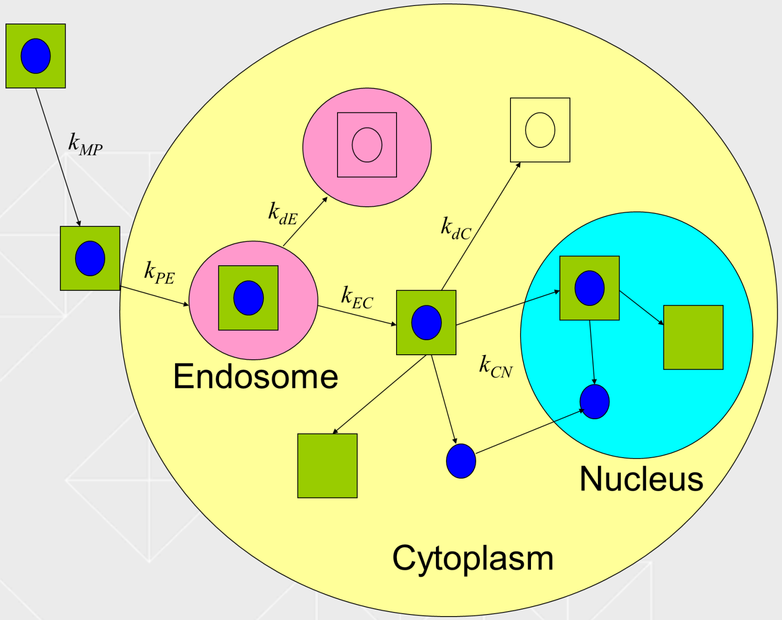
- To fabricate micro-distillation chips based on ***zero-gravity distillation***





- To demonstrate fluid separation and assess separation performance

Optimal control of Gene Delivery



$$\frac{dM}{dt} = -k_{MP}M + u$$

$$\frac{dP}{dt} = k_{MP}M - (k_{PE} + k_{PC} + k_{dP})P$$

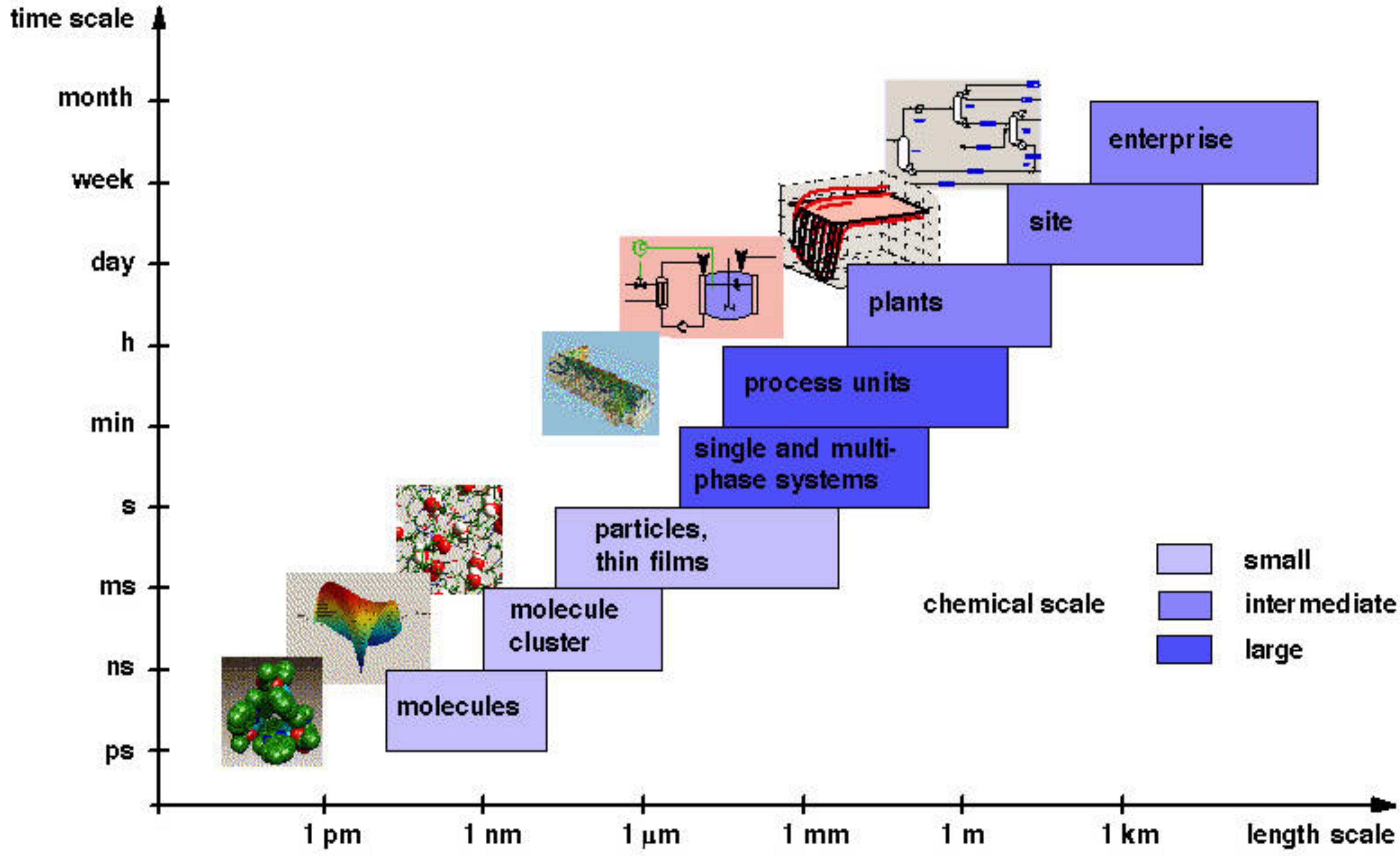
$$\frac{dE}{dt} = k_{PE}P - (k_{EC} + k_{dE})E$$

$$\frac{dC}{dt} = k_{EC}E - (k_{CN} + k_{dC})C$$

$$\frac{dN}{dt} = k_{CN}N$$

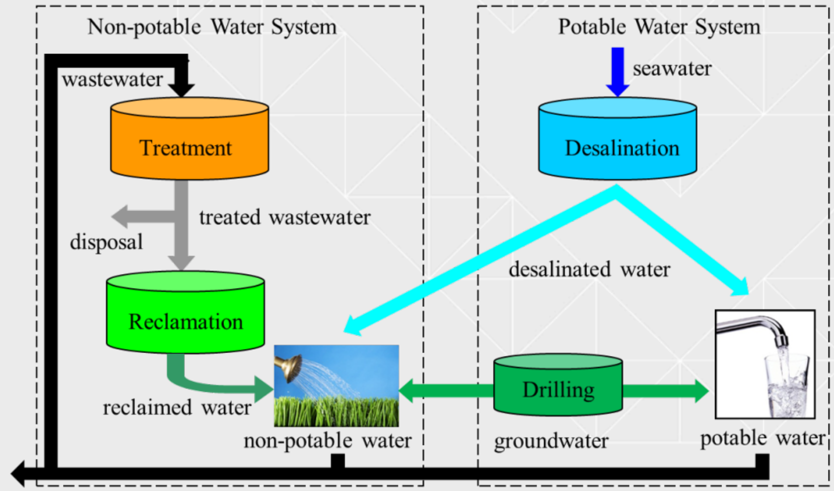
Compute optimal gene delivery profile to maximise efficacy and minimise toxicity subject to model equations and constraints.

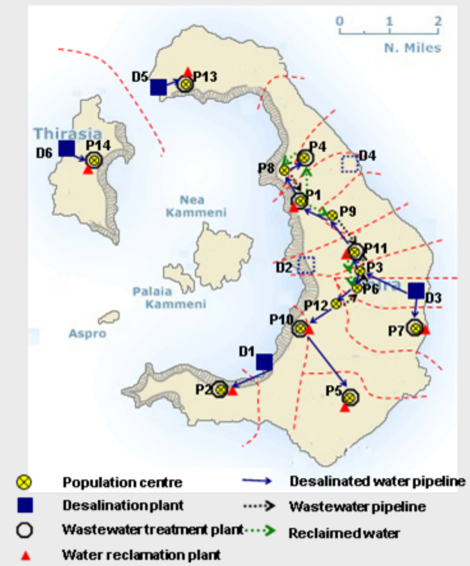
Recall: Multi-scale considerations



Water Resource Management

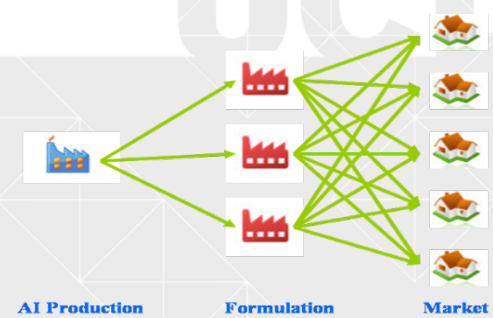
- Non-conventional water resources are crucial to water deficient areas
  - Desalinated water
  - Treated wastewater
  - Reclaimed water
- MIP approaches proposed for integrated water resources management
- Decisions:
  - Plants locations, capacities and productions
  - Pipeline networks and flows
  - Pumping stations
  - Storage tanks
- Objective: annualised total cost
  - Capital costs (plant/pipeline/pumping station/storage tank)
  - Operating costs (production/pumping)



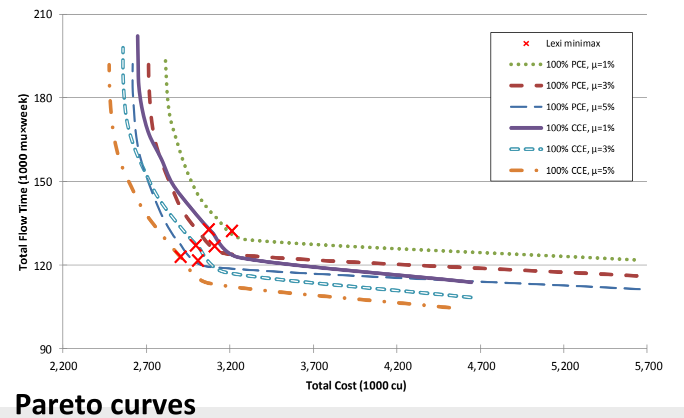


Global Supply Chain Planning

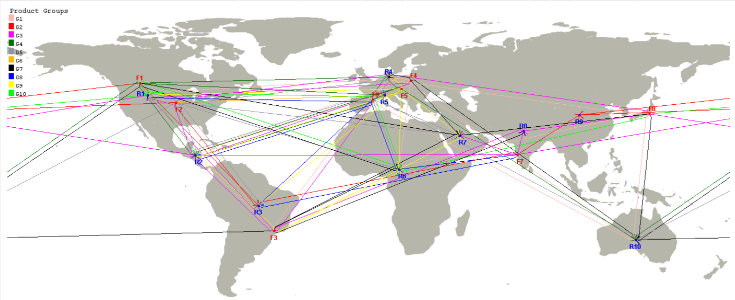
- Three key supply chain performance metrics are considered:
  - Cost
  - Responsiveness (flow time)
  - Customer service level (lost sales)
- Two solution approaches for multiobjective MILP model:
  - ε-constraint method → Pareto solutions
  - Lexicographic minimax method → Fair solution



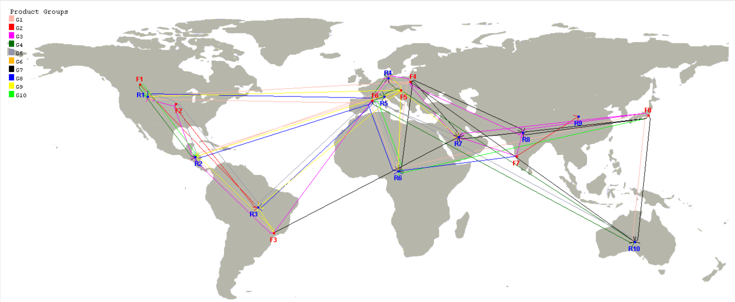
Global supply chain network



Pareto curves

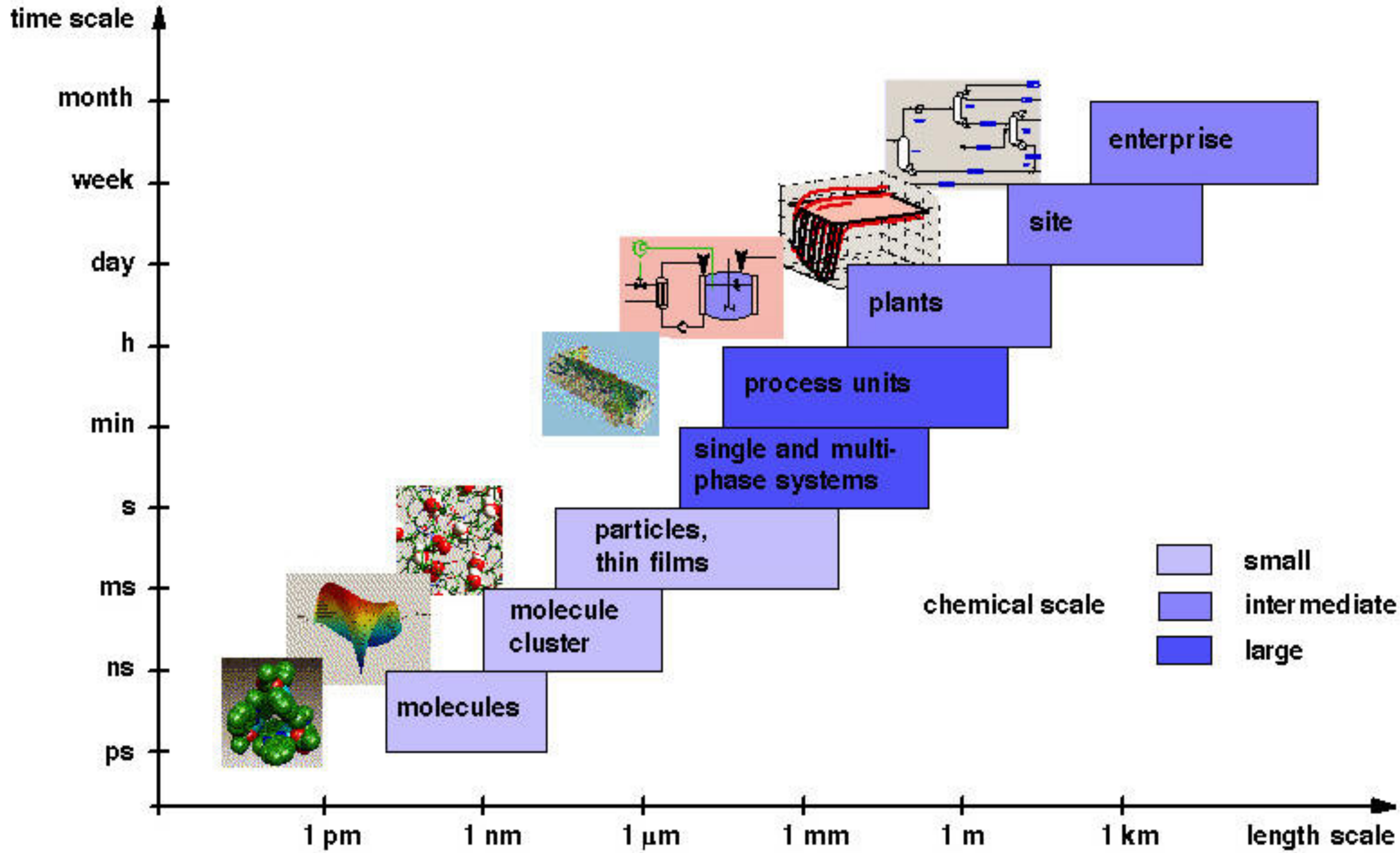


Minimum cost



Minimum flow

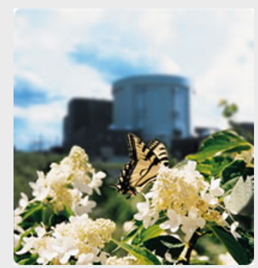
Recall: Multi-scale considerations



Main constraints

PHYSICS/CHEMISTRY

SAFETY



SUSTAINABILITY

Optimisation problem

Integer:
columns
plants
etc

Continuous:
Energy
Flowrates
etc

Integer:
columns
plants
etc

Continuous:
Energy = f(t)
Flowrates = f(t)
etc

MINLP

MIDO

UCL ENGINEERING

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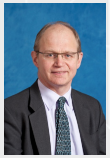
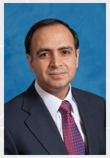

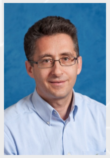

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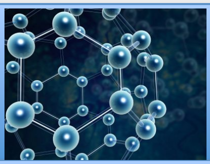
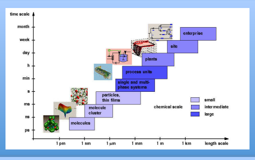
Chemical Manufacturing Systems | Biological Systems Engineering | Supply Chains of the Future | Energy Systems Engineering

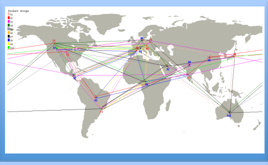
Competence Areas

Product and Process Design


Operations and Control






Modelling and Model Solution Tools