Introduction to Modelling

Rafiqul Gani
(Plus material from Ian Cameron)

PSE for SPEED
Skyttemosen 6, DK-3450 Allerod, Denmark
rgani2018@gmail.com

www.pseforspeed.com

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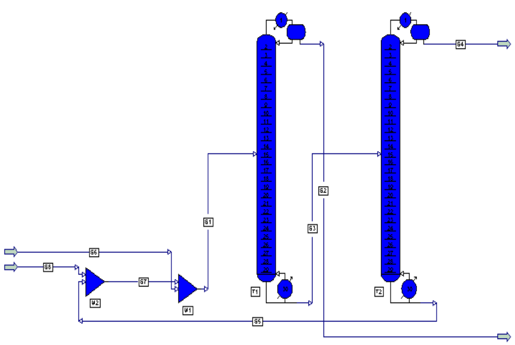
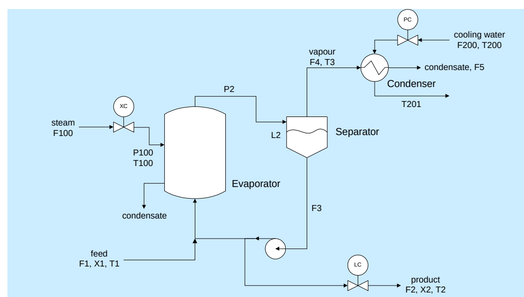
Examples of process modelling - 1

Process simulation (mass & energy balance)



Stream summary: Calculated variable values of process streams

Sugar drying and control



Sugar flowrate versus time under startup and airflow changes

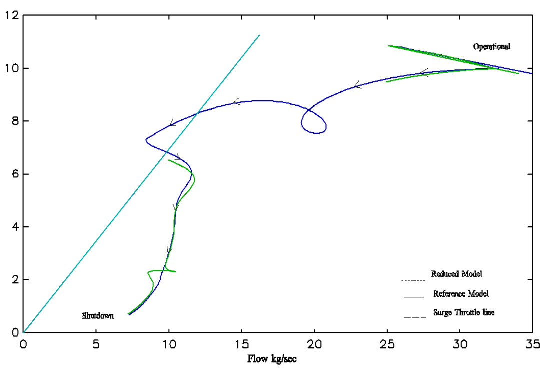
Simulation of waste water treatment facility

S1	S11	S2	S12
Mixed	Vapor	Vapor	Vapor
292,5756	590,0000	590,0000	590,0000
1,0000	1,0000	1,0000	1,0000
13,3936	82,6858	82,6584	82,6601
25,9916	26,9433	26,9639	26,9639
0,7010	1,0000	1,0000	1,0000

Stream summary: Calculated variable values of process streams

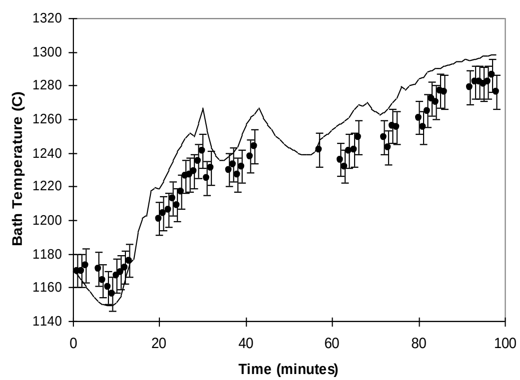
Examples of process modelling - 2

Surge Control Design for a Hydrogen Compressor



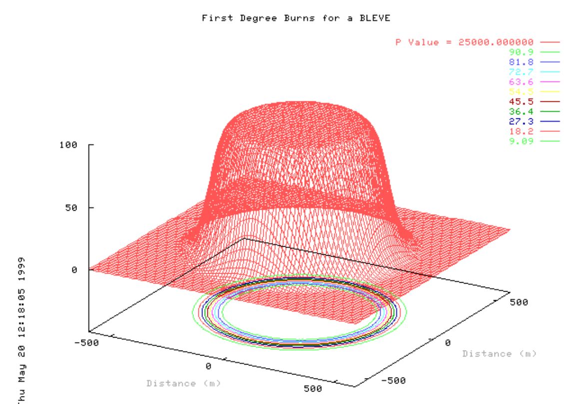
Head (bar) versus flowrate (kg/s) during controlled shutdown

Fed Batch Metallurgical Reactor



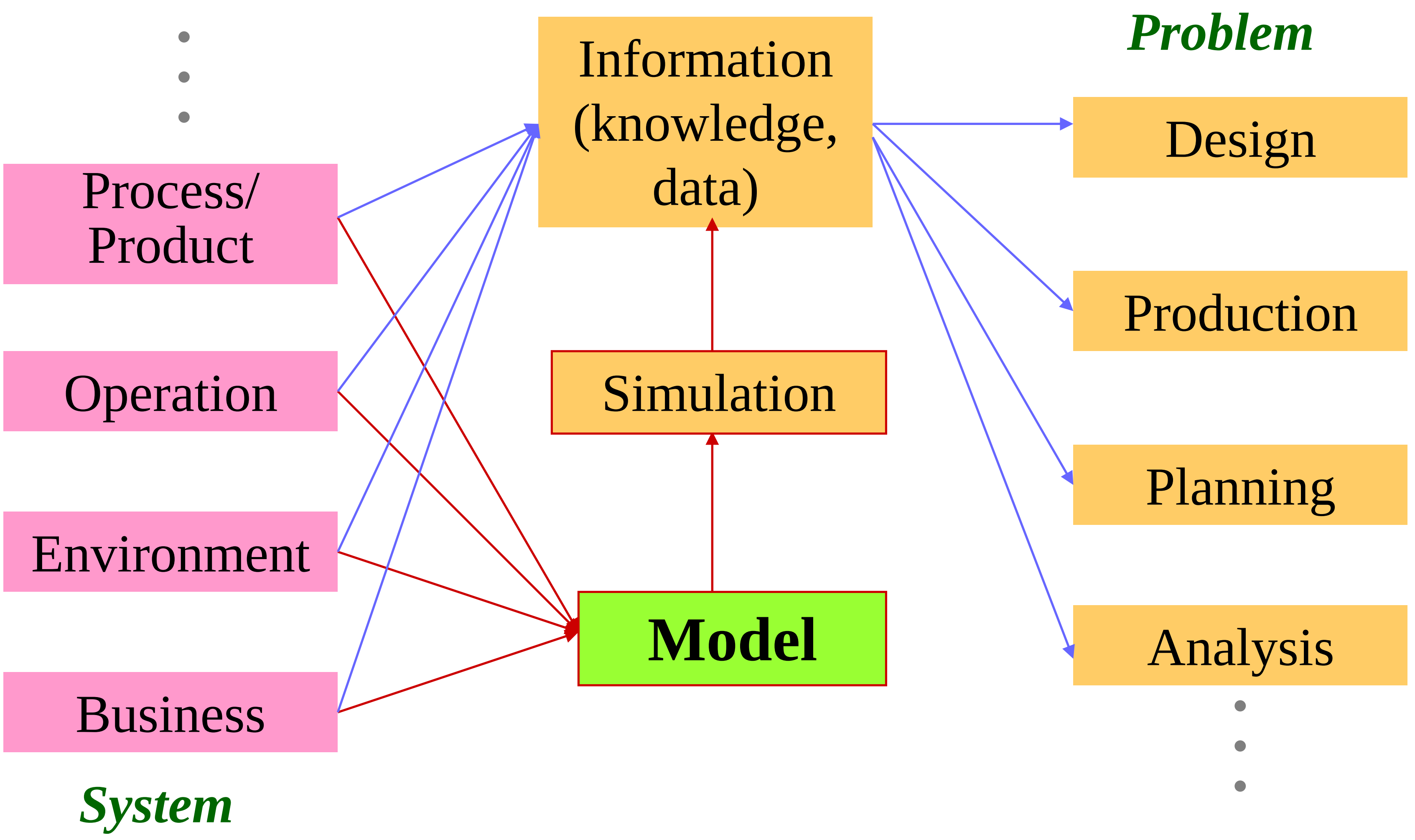
Temperature versus time during fed batch operation

Safety and Risk Assessment (BLEVE Radiation)



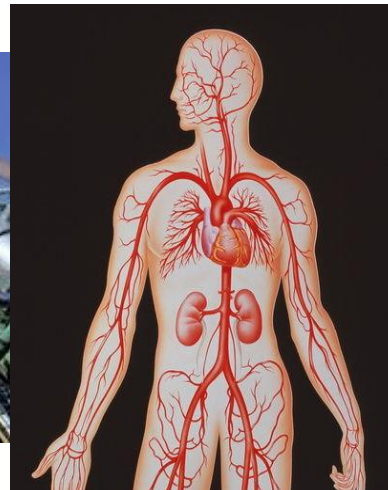
3D surface showing percent first degree burns for a BLEVE

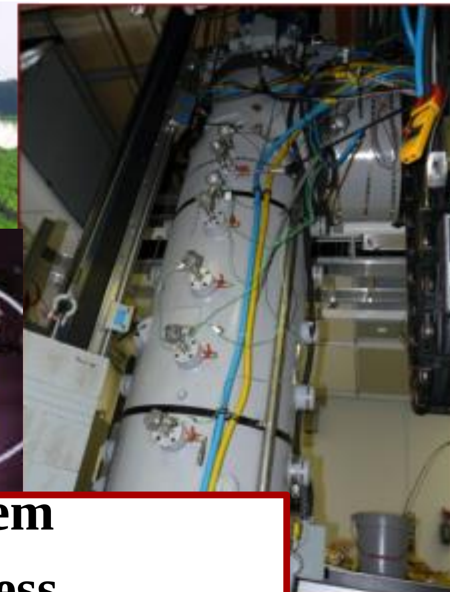
Why we need models?



The role of modeling

Modeling is an important enabler to face current and future challenges in product-process engineering

Improved understanding of the domain system

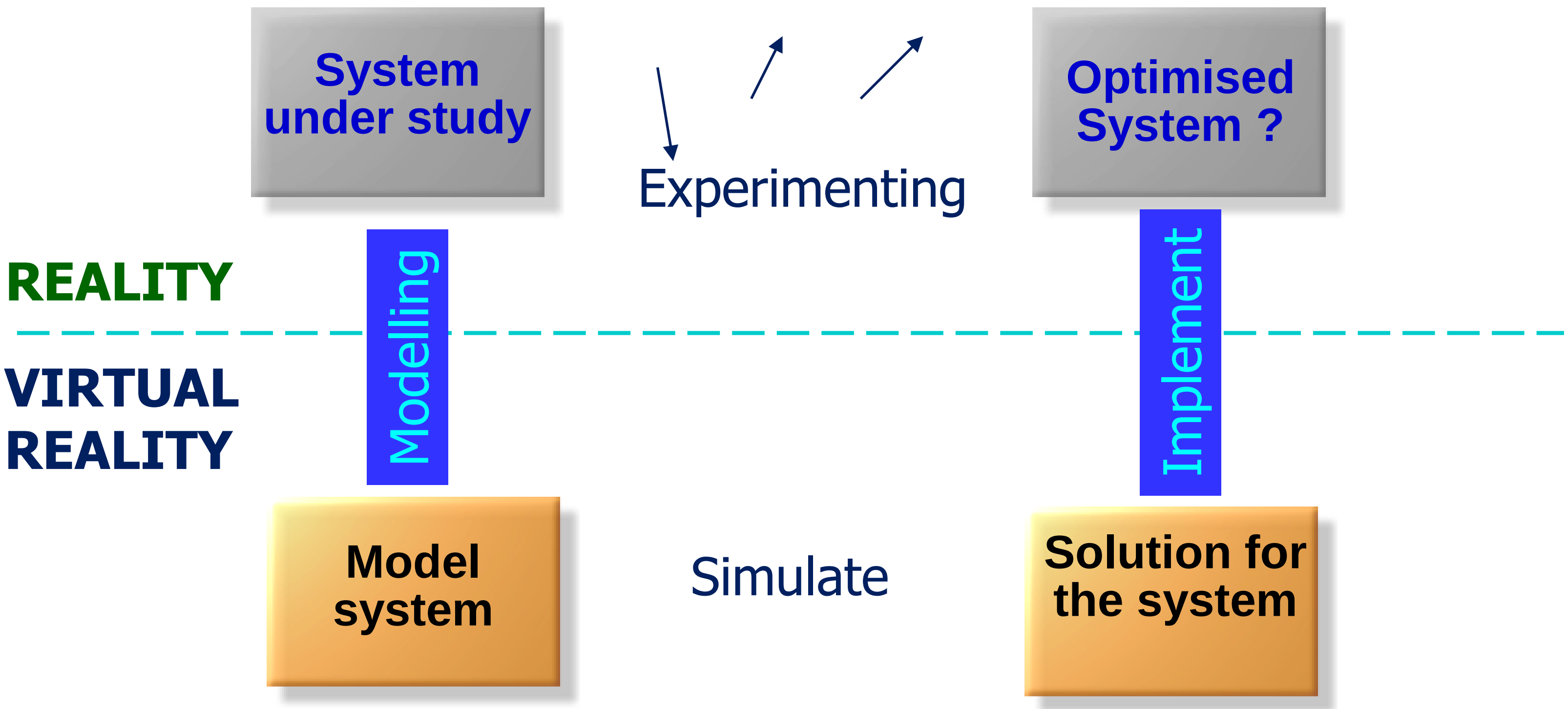
Prediction and optimization of product process behavior

Reduce number of resource-demanding experiments

Deliver truly innovative solutions

The role of modelling should not be to just replace experiments

The we need models?



What is a model?

"A model (M) for a system (S) and an experiment (E) is anything to which M can be applied in order to answer questions about S" (Minsky, 1965)

Modelling wisdom

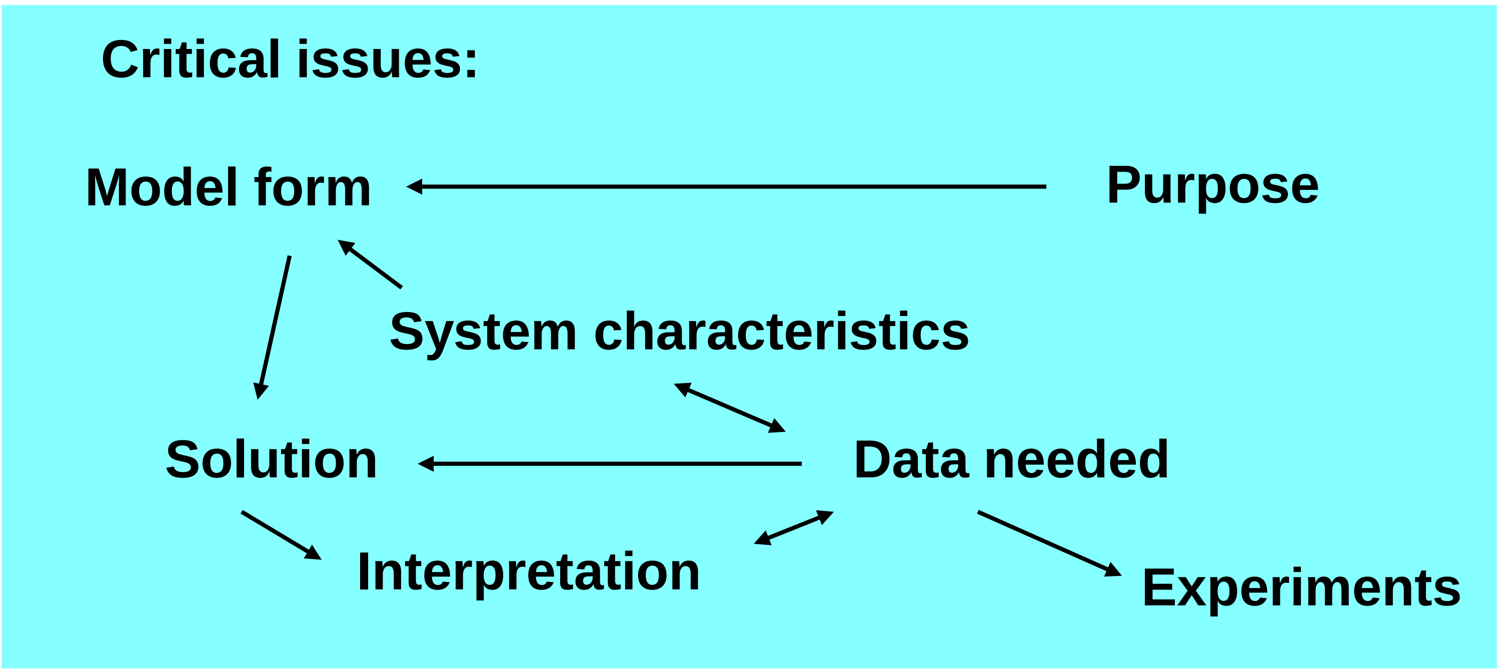
All models are wrong ….

…. some are useful !

… George Box

Concept of a model in PSE

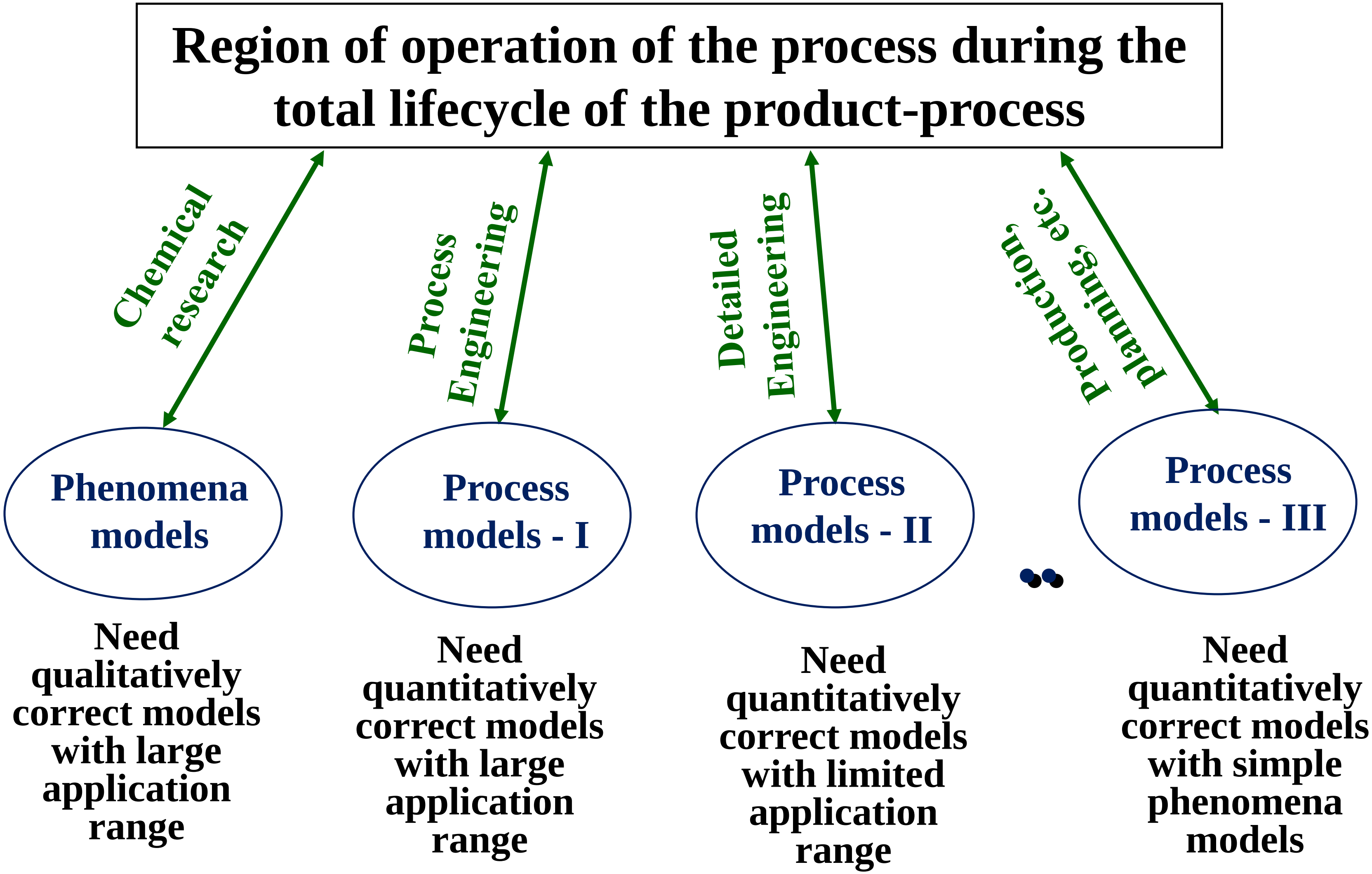
“A mathematical representation (M) of a physical system (S) for a specific purpose (P) and experiment (E)” - ***representing reality with virtual reality for a purpose!***



How the principal modeling steps support the requirements of a process modeling tool

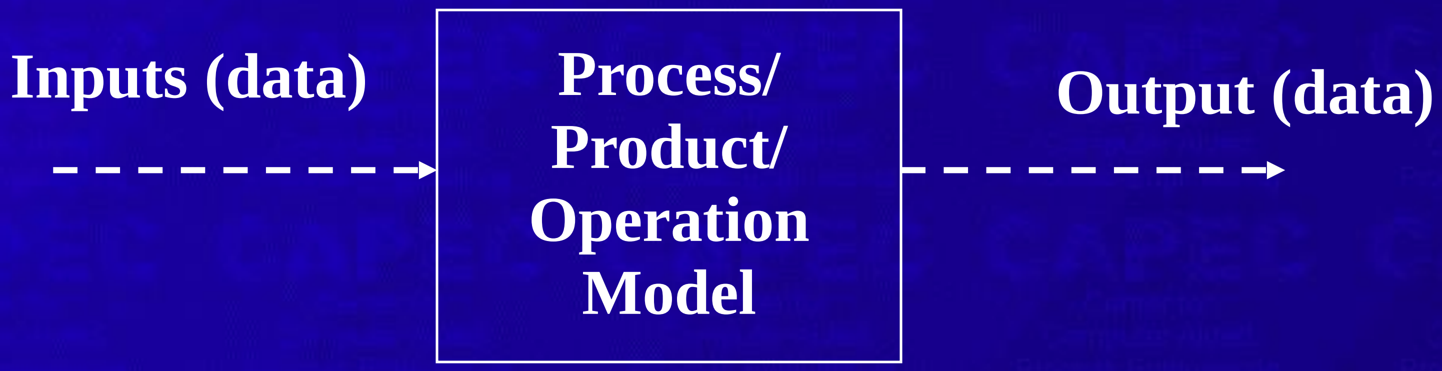
Requirements to a process modeling tool		How to support these requirements
Reuse of existing models	⇐	Aggregation of predefined building blocks
Generate various kinds of models	⇐	Aggregation of various different kinds of building blocks
Generate models with varying degree of details	⇐	Multi-level decomposition and aggre-gation of building blocks
Modification of existing models	⇐	Modify the content of an aggregated building block
	⇐	Add/delete building blocks to/from the aggregated set of building blocks
Continuous expansion of incorporated knowledge base	⇐	Adding new building blocks to the modeling tool
Expert help in setting up model equations	⇐	Assistance in the selection of which building blocks to use
	⇐	Assistance in setting up the model equation for new building blocks
	⇐	Data/action collection, i.e., collection of experience
Documentation and mainte-nance of the model equations	⇐	Data/action collection, i.e., collection of experience
	⇐	Building blocks with phenomena based information

Process modelling – process lifecycle



A systematic model building approach

General system schematic



General model schematic (modeling goals need to be established)

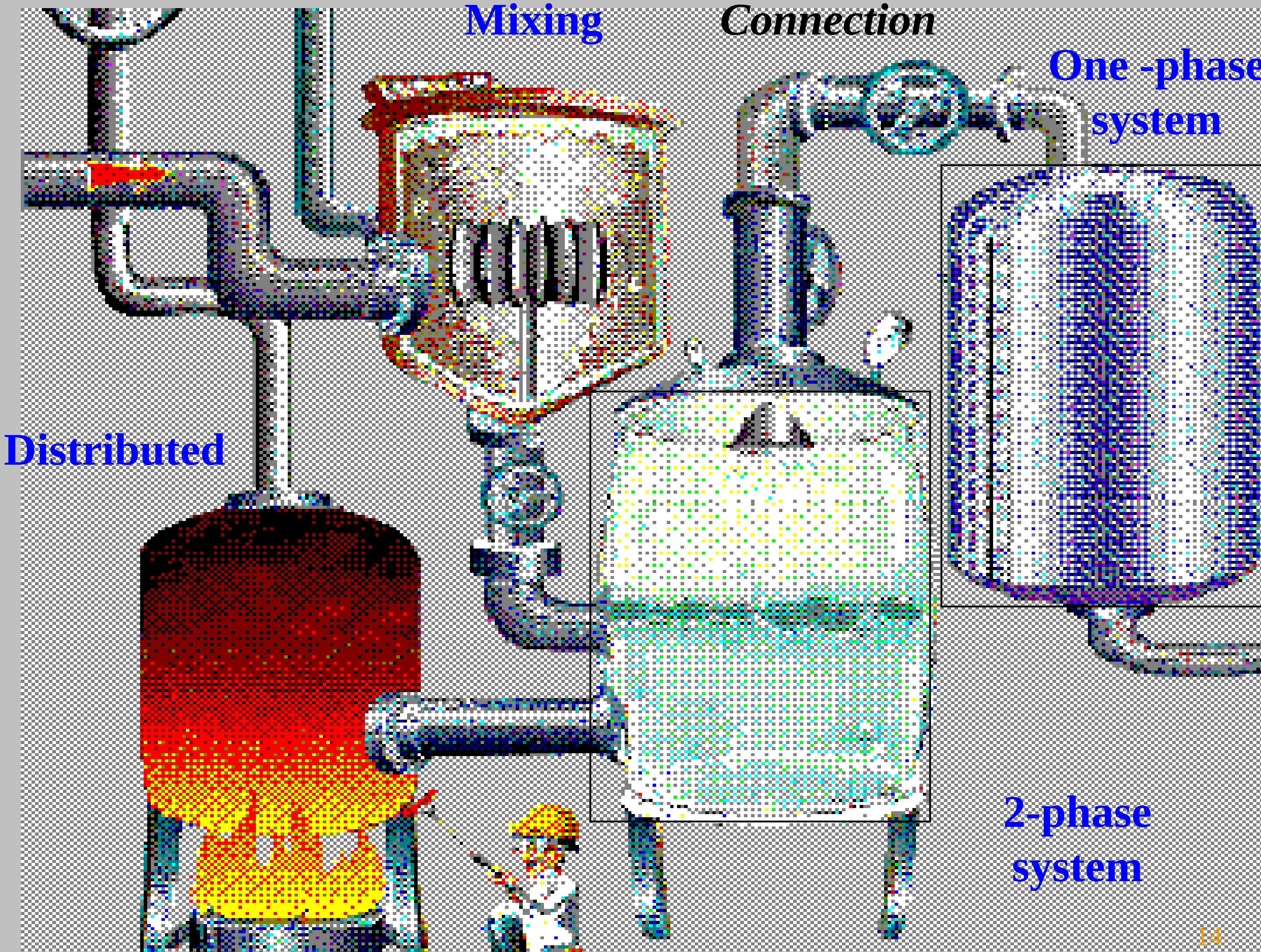
A systematic model building approach

Input(data) → **Process/ Product/ Operation Model** → Output (data)

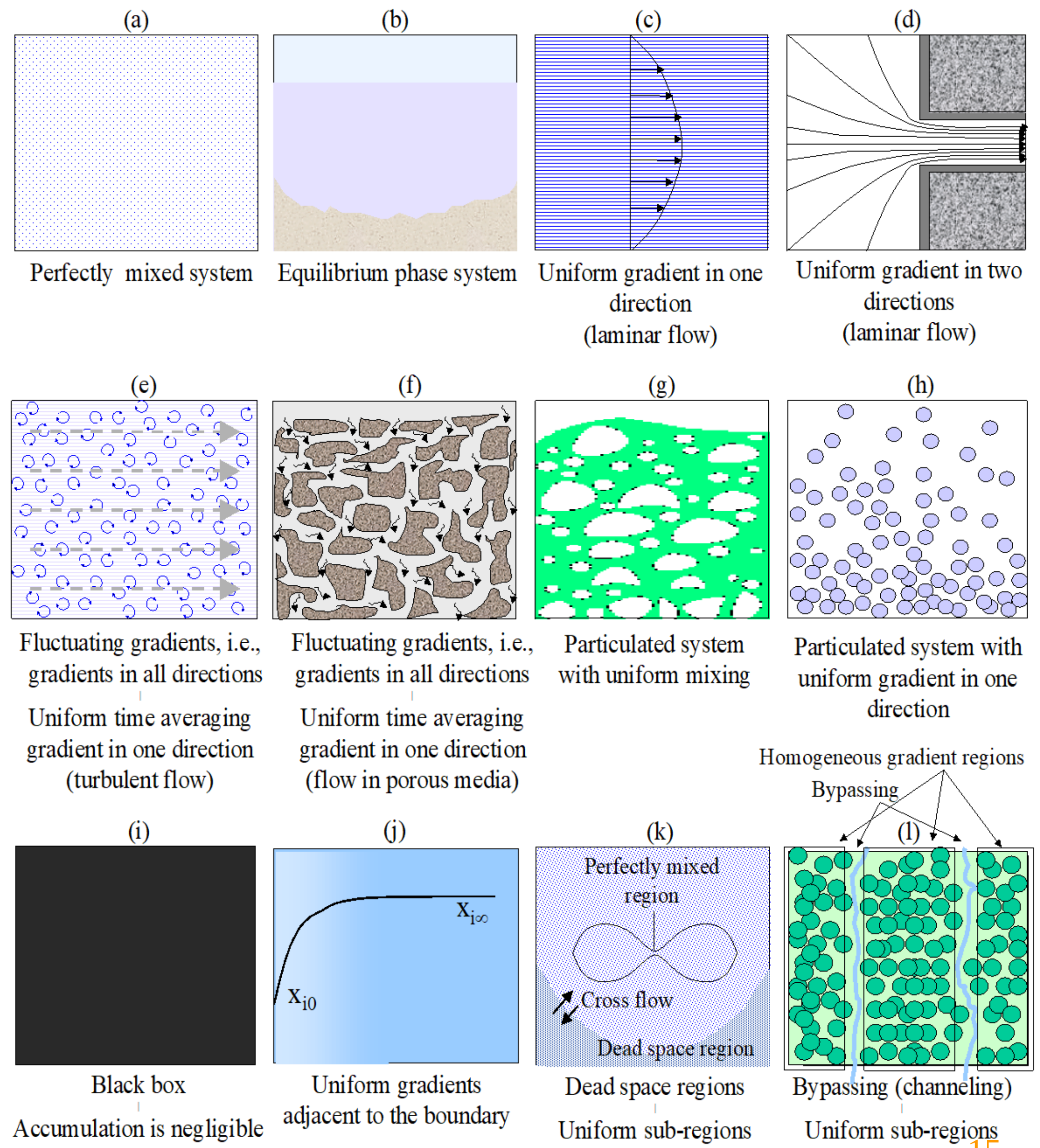
General model schematic (modeling goals need to be established)

Models

- **White-Box** → First principles model; no need of measured data; totally based on theory
- **Black-Box** → Not based on theory but on measured data; parameter estimation necessary
- **Grey-Box** → Combination of first principles, knowledge and measured data; realistic models


Mixing
Connection
One -phase
system
Distributed
2-phase
system

State of aggregation and phases within the system

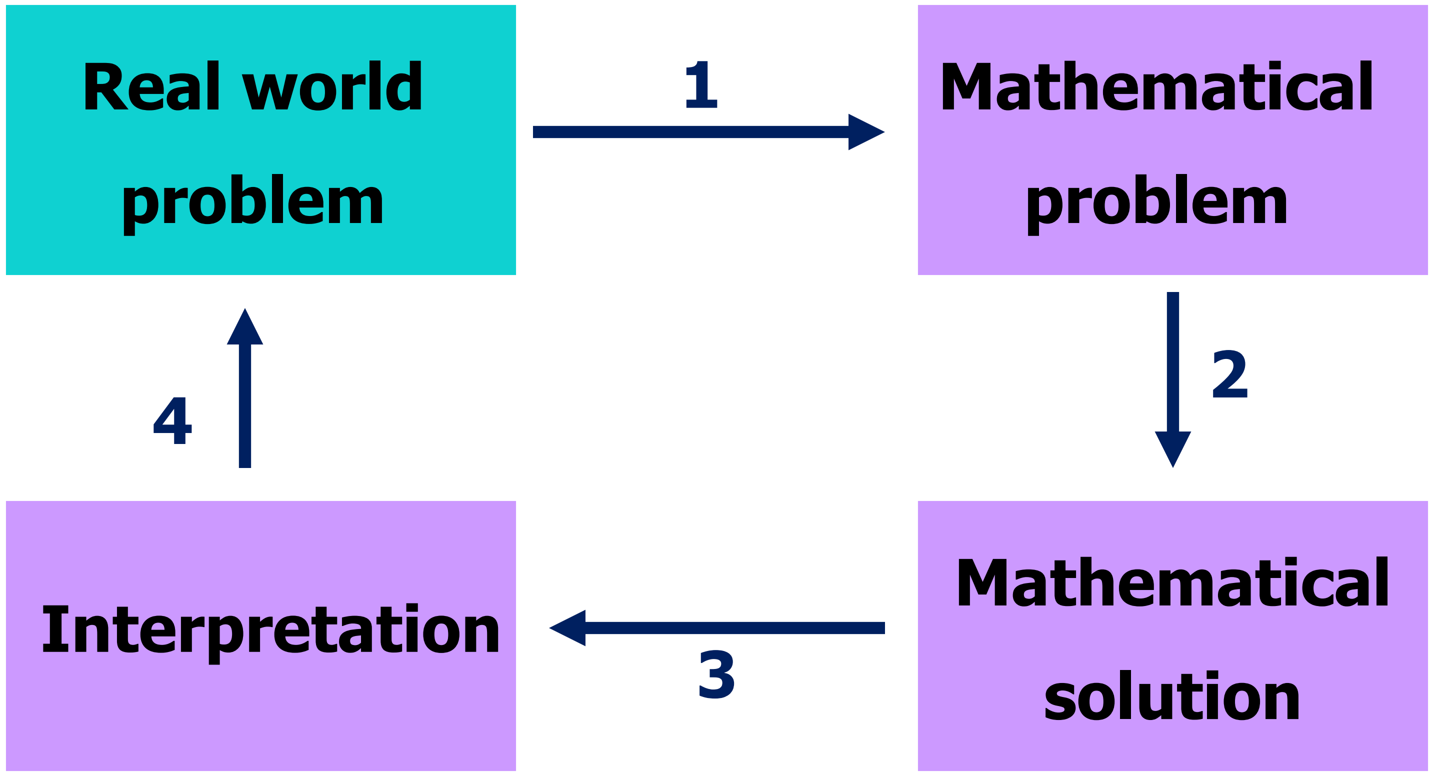


Conservation Principles

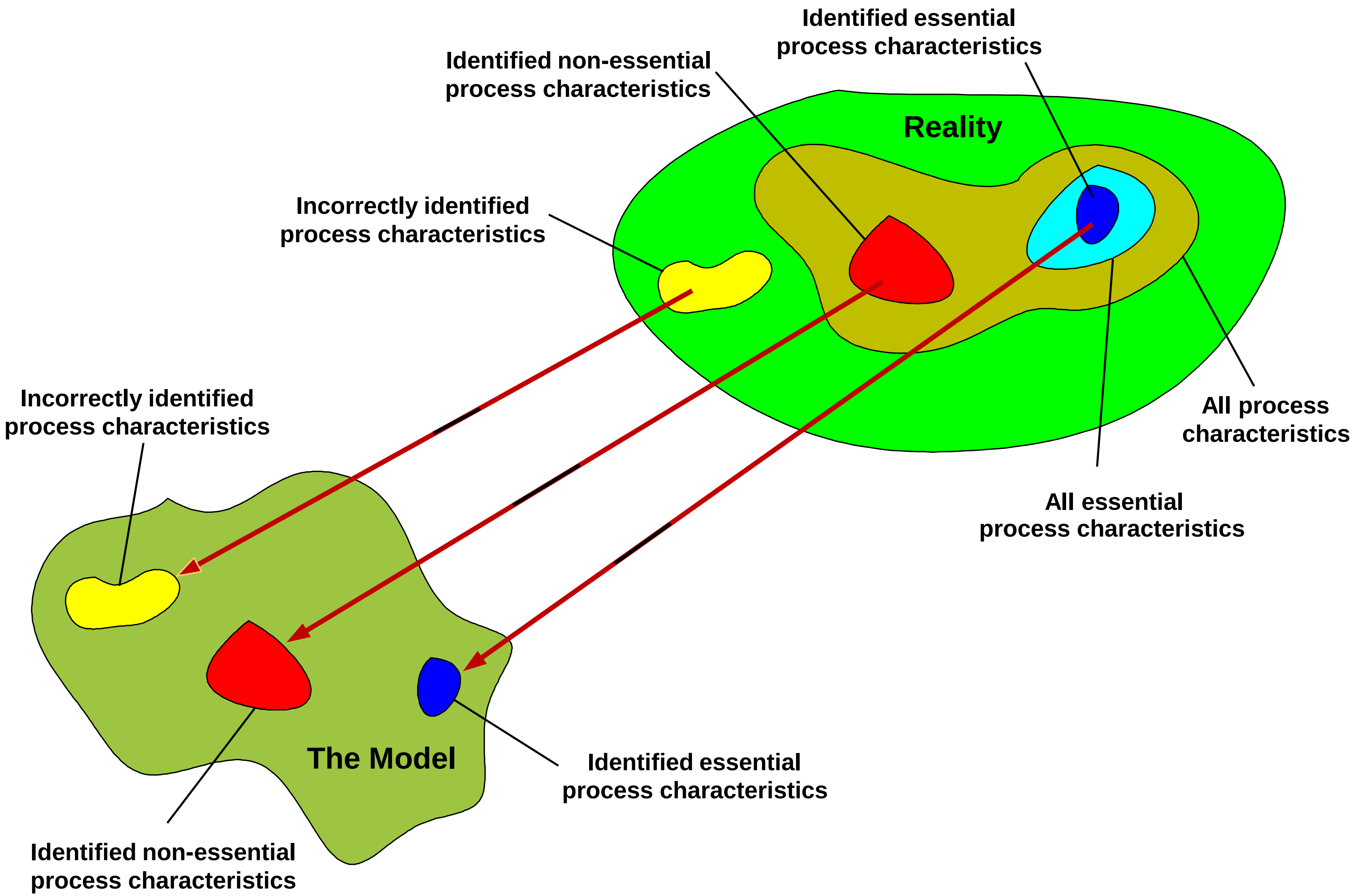
Thermodynamic Principles

- **Concept of space (region of interest; co-ordinate system in space)**
- **Scaler fields** *{P(x,y,z); P(v)}*
- **Vector fields** *{v(x,y,z,t); v(r,t)}*
- **State of aggregation and phases**
- **Extensive & intensive properties**
- **Phases & independent variables**

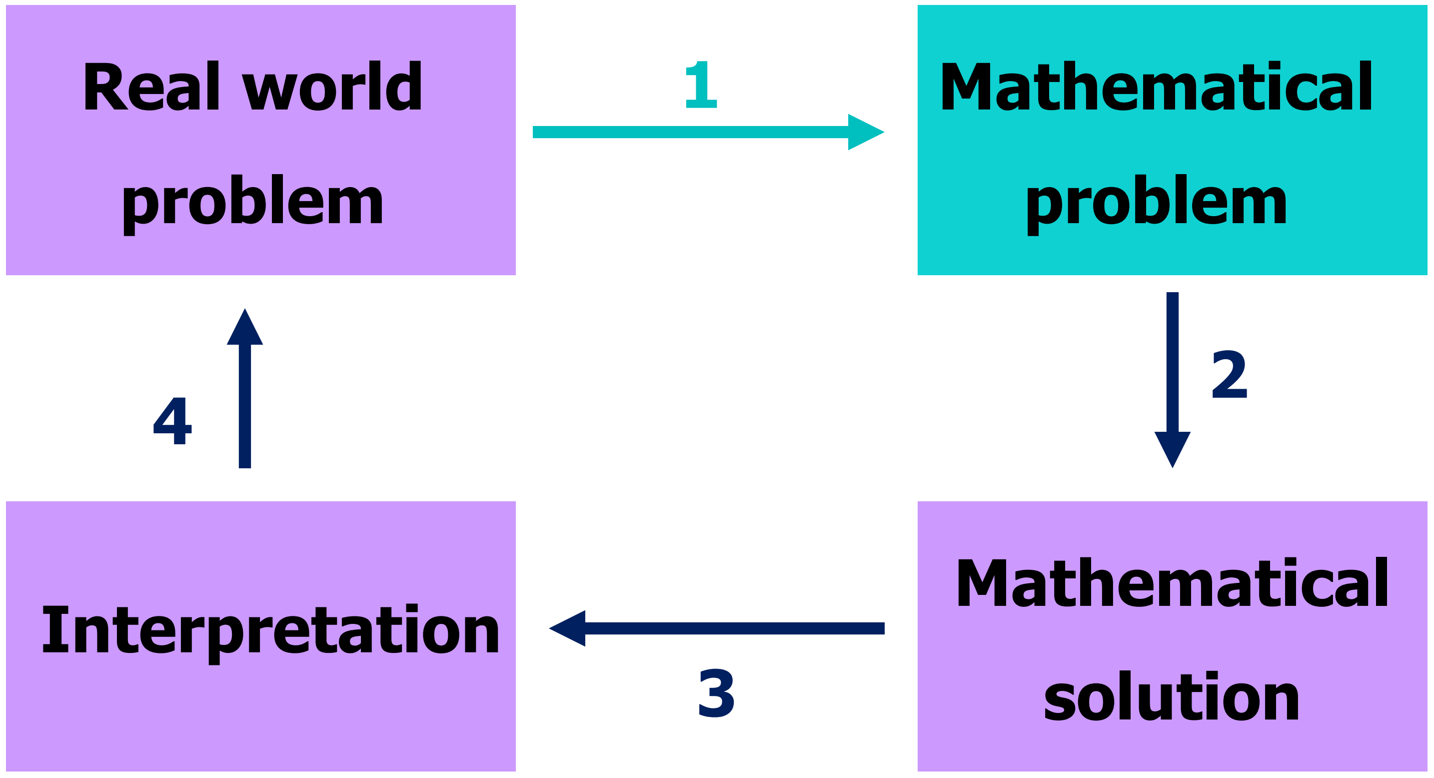
The Modelling Process



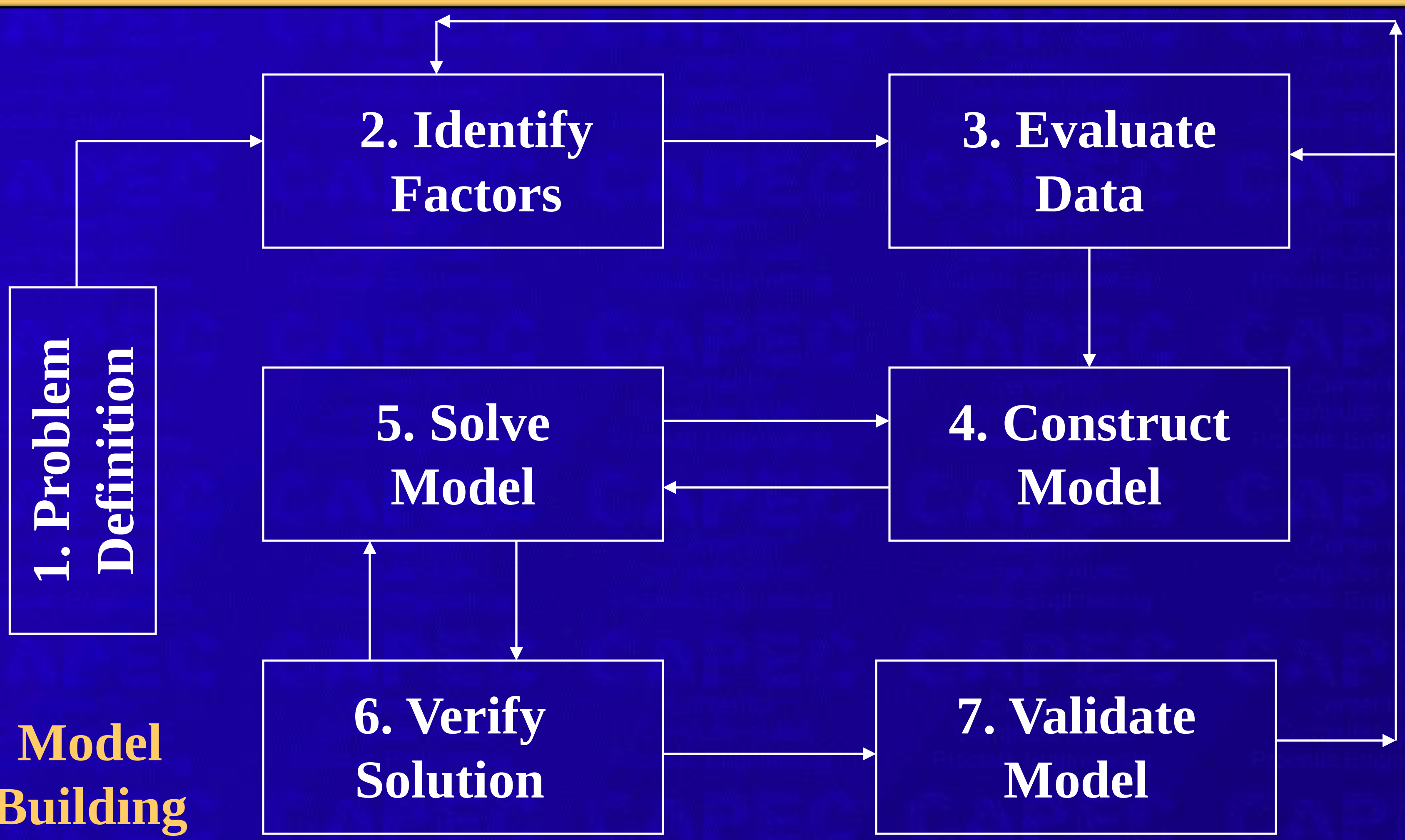
System versus model characteristics



The Modelling Process



A systematic model building approach



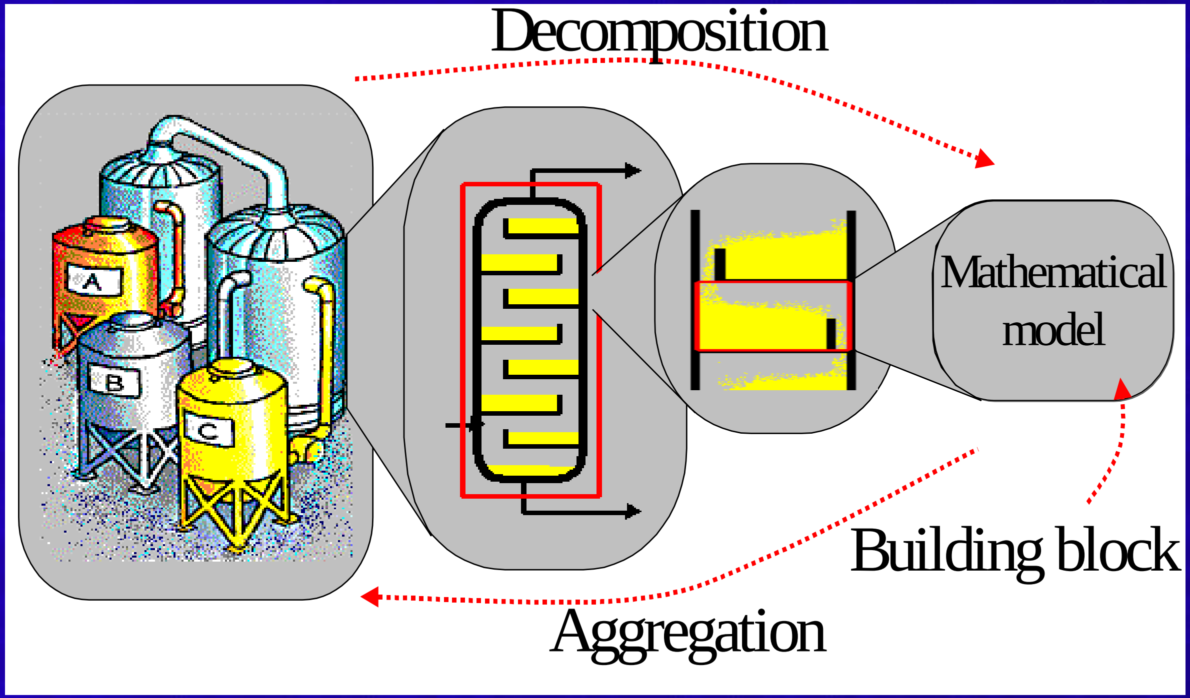
Model Building Steps

A systematic model building approach

Structural representation of models

1. **Assumptions**
2. **Equations & characteristic variables**
3. **Initial conditions (where applicable)**
4. **Boundary conditions (where applicable)**
5. **Parameters**

Model Construction



* Balance Equations

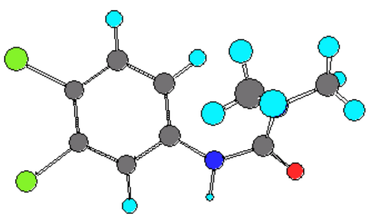
*Constraint Equations

*Constitutive Equations

Define Boundary **Describe System** **Develop Building Block**

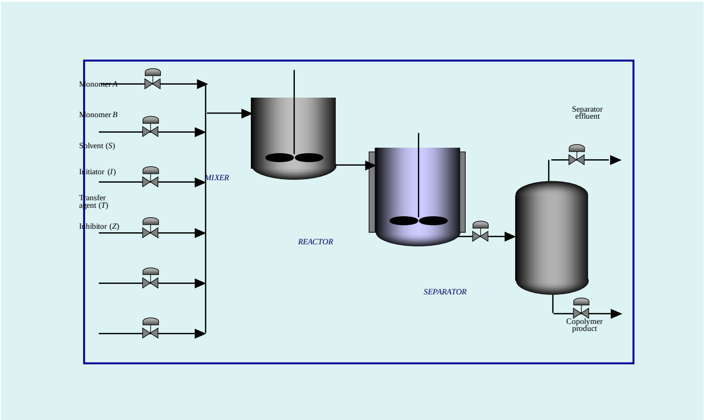
Chemical Process Modelling

The process of generating abstract or conceptual models, that is, representing reality with virtual reality for a purpose!



$$f(X) = \sum_i N_i C_i + w \sum_j M_j D_j + z \sum_k O_k E_k$$

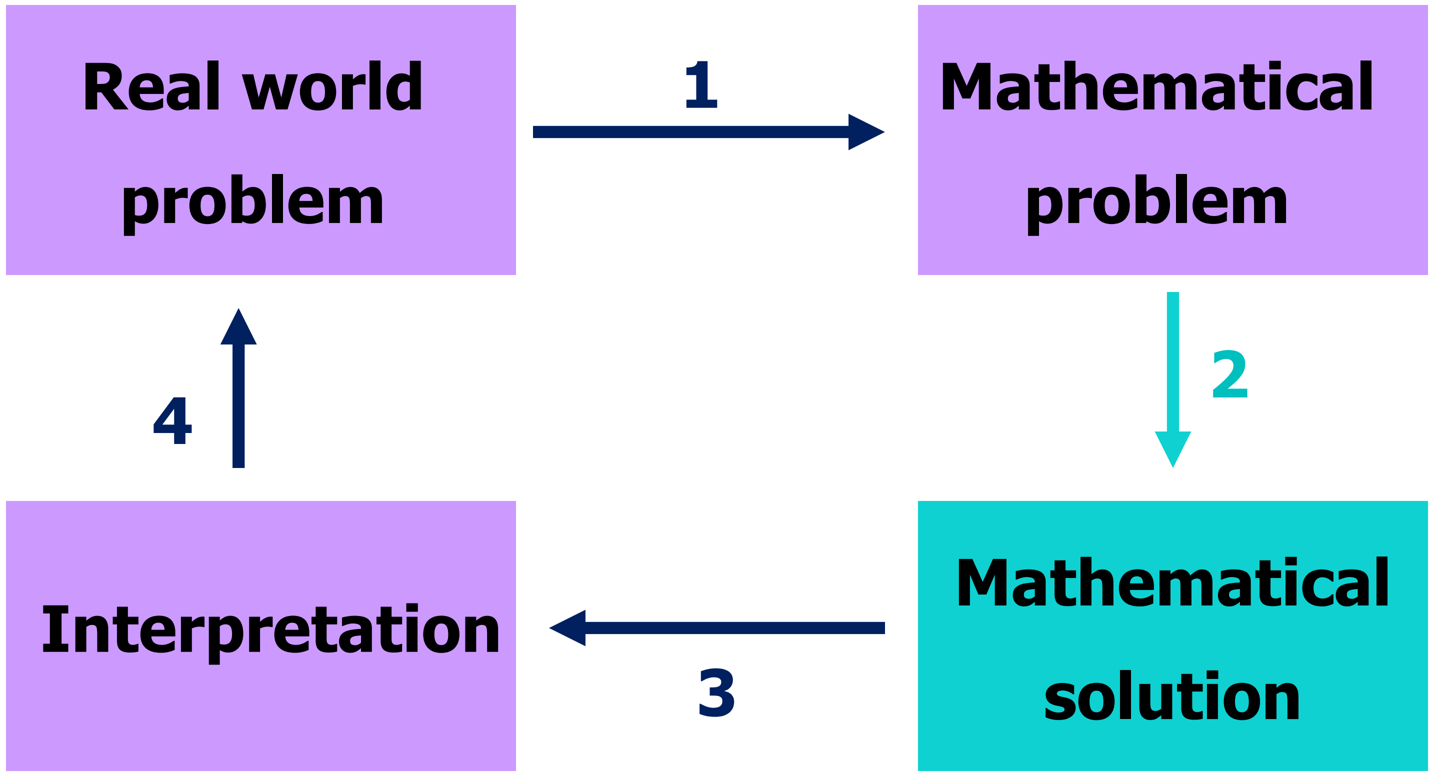
Predict behaviour*



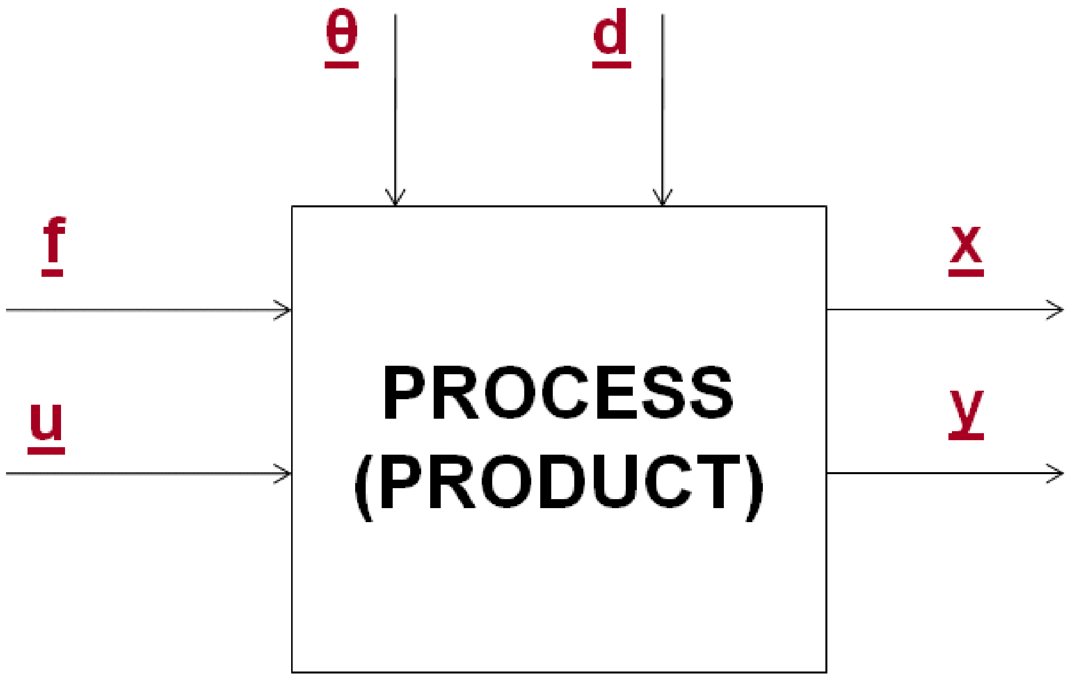
$$\frac{dm_A}{dt} = f_{A_i} - f_A - rV$$

$$\frac{dH}{dt} = f\hat{H}_i - f\hat{H}$$

The Modelling Process



Solution of mathematical models - 1



Models:

Process/property

$d\underline{x}/dt = f(\underline{f}, \underline{u}, \underline{d}, \underline{\theta}, \underline{x})$

$\underline{y} = g(\underline{x})$

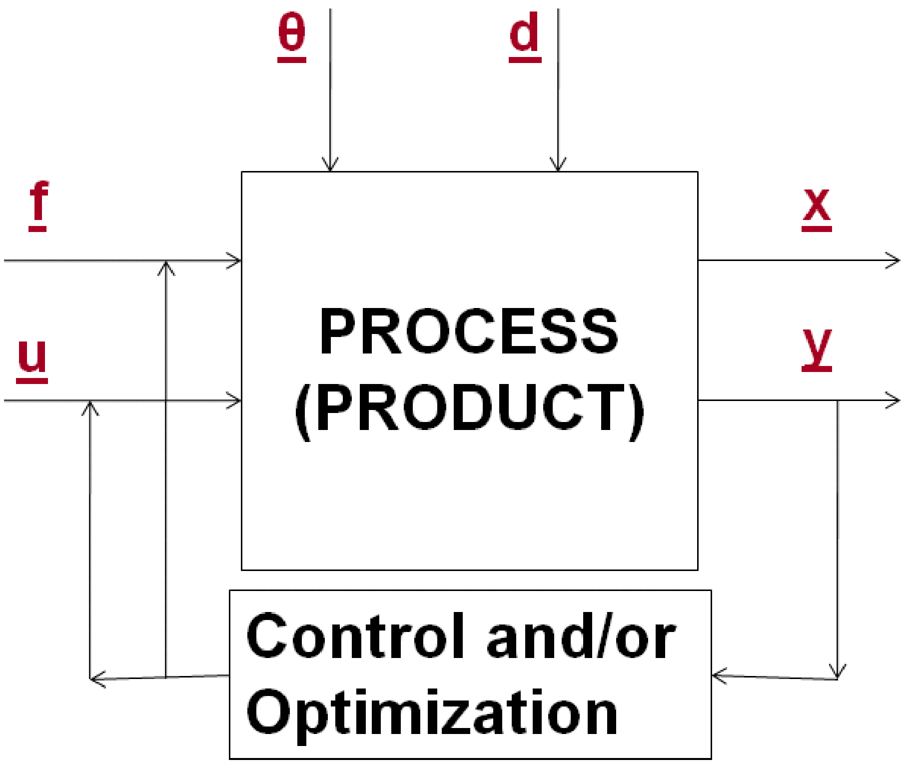
$\underline{\beta} = \beta\,(\underline{C}, \underline{f}, \underline{x})$

Analytical or numerical solution?

Given: $\underline{\theta}$, $\underline{d}$, $\underline{f}$, $\underline{u}$; calculate $\underline{x}$, $\underline{y}$ (simulation)

Process simulation; design; analysis (troubleshooting, safety, environmetal impact assessment, ...)

Model-based solution approaches



Models: $Fobj = f(\underline{x}, \underline{y})$

Process/property

$d\underline{x}/dt = f(\underline{f}, \underline{u}, \underline{d}, \underline{\theta}, \underline{x})$

$\underline{y} = g(\underline{x})$; $\underline{u} = g_c(\underline{y})$; $\underline{f} = g_o(\underline{y})$

$\underline{\beta} = \beta\ (\underline{C}, \underline{f}, \underline{x})$

Sustainability Metrics

$\underline{S}_e = S_e\ (\underline{f}, \underline{u}, \underline{x}, \underline{y}, \underline{d}, \underline{\theta})$

$\underline{S}_i = S_i\ (\underline{C}, \underline{f}, \underline{y})$

$\underline{S}_s = S_s$ (size, profit, ?)

Safety & Hazards

$\underline{H}_c = Hc\ (\underline{C}, \underline{f}, \underline{y}, \underline{d})$

$\underline{Hp} = H_p\ (\underline{u}, \underline{f}, \underline{x}, \underline{d}, \underline{\theta})$

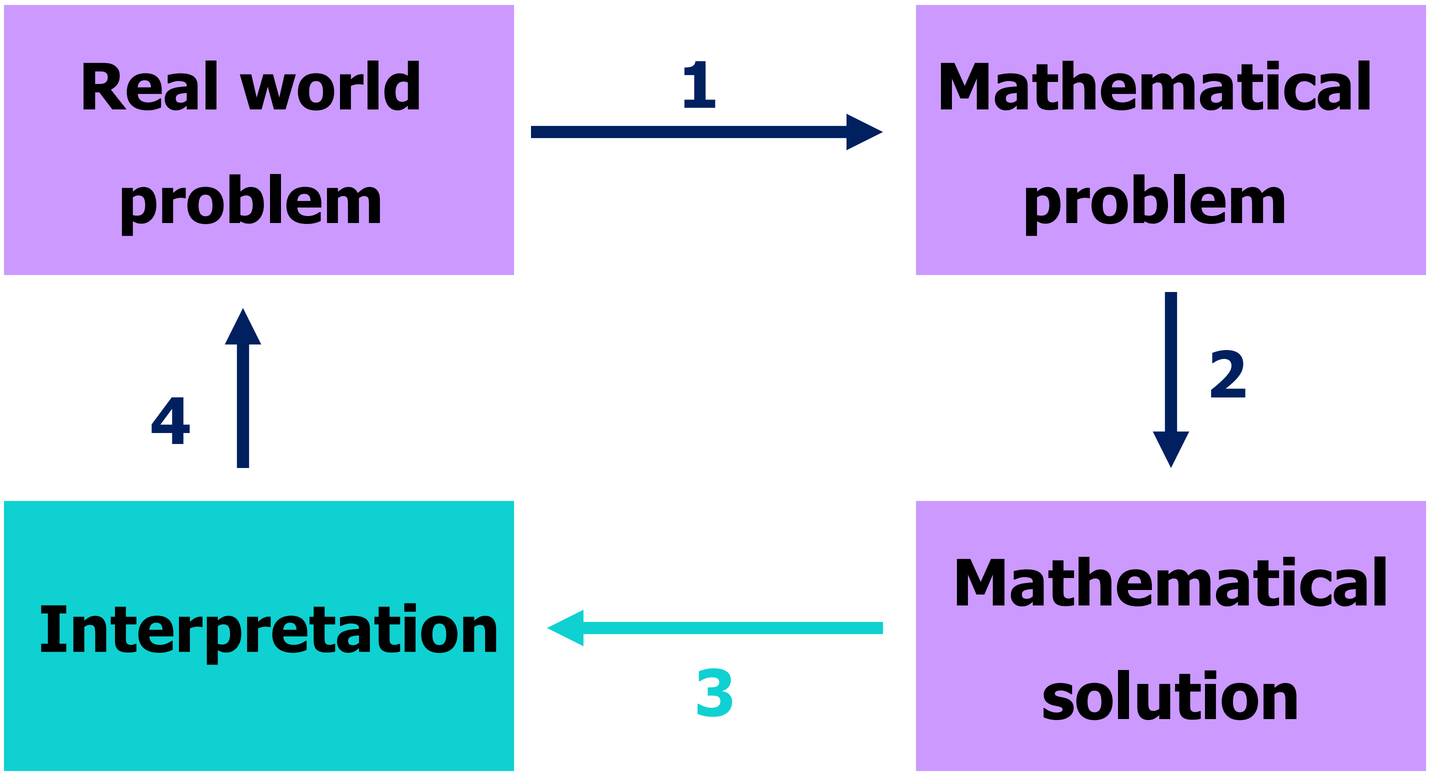
constraints

Given: $\underline{\theta}$, $\underline{d}$, $\underline{f}$, $\underline{u}$; calculate $\underline{x}$, $\underline{y}$ (simulation)

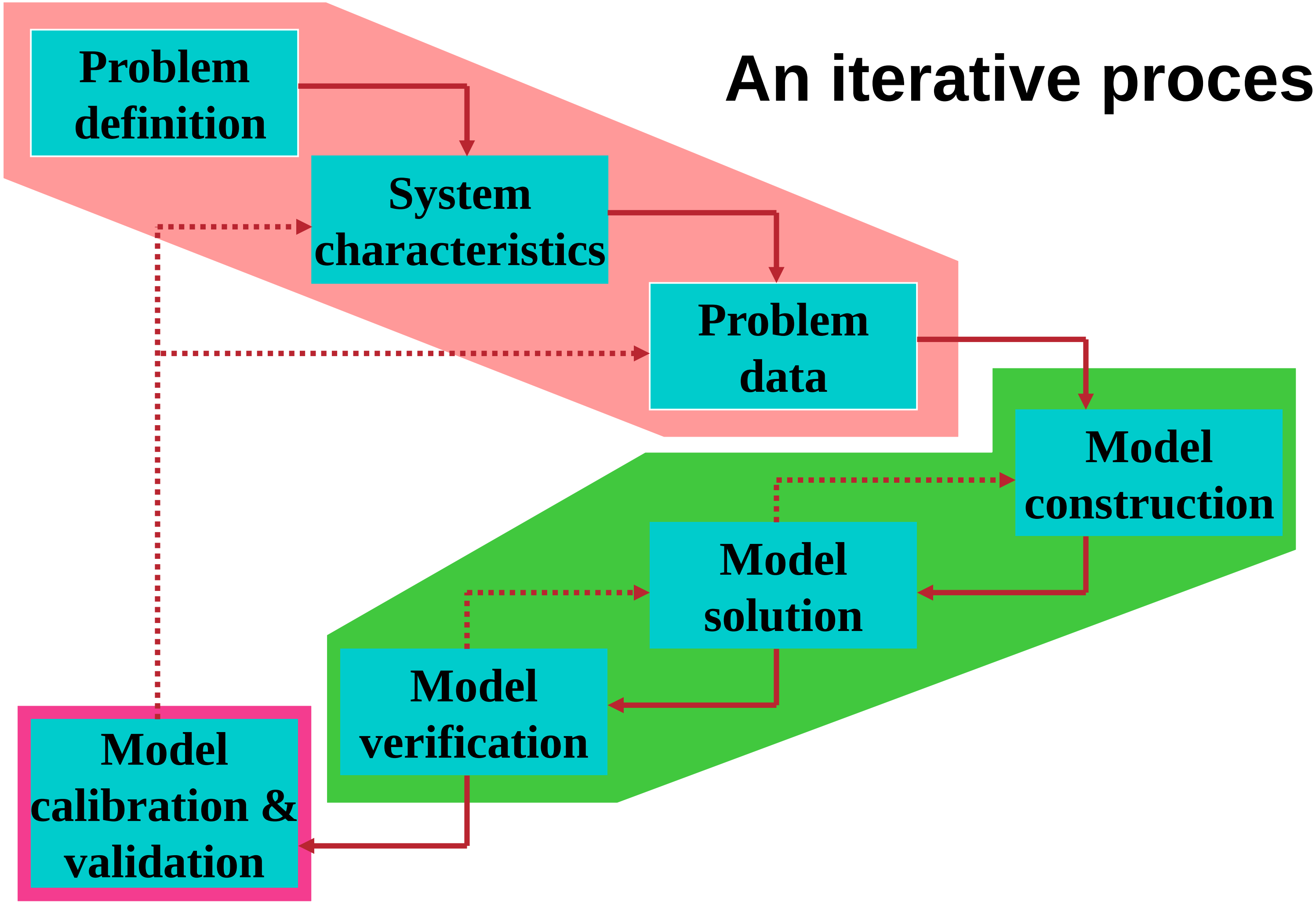
Given: $\underline{\theta}$, $\underline{f}$; minimize Fobj ($\underline{x}$, $\underline{y}$); subject to constraints (models, product quality, ...)

Process simulation; design; control, diagnosis, operator training, safety, analysis (environmetal impact assessment, ..)

The Modelling Process



The Modelling Process



An iterative process

Model classification & forms

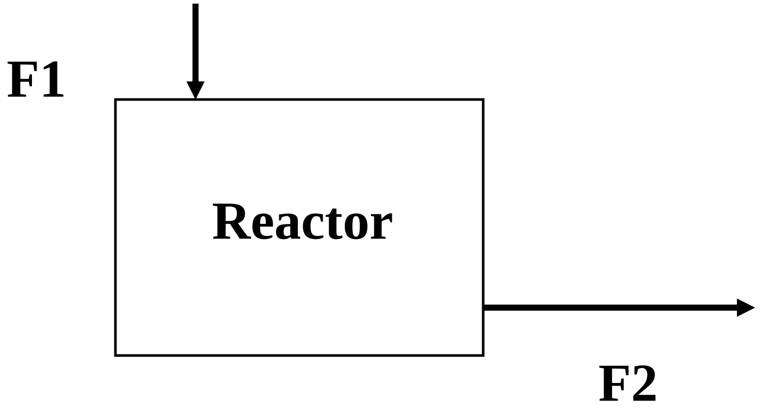
- Mechanistic vs. Empirical
- Stochastic vs. Deterministic
- Lumped vs. Distributed
- Linear vs. Nonlinear
- Continuous vs. Discrete
- Dynamic vs. Steady state

- Deterministic: NLAE/ODE/PDAEs
- Stochastic: NLAE/DE/Integral PDAEs
- Lumped: NLAE/ODE
- Distributed: Elliptic/Parabolic PDE
- Linear: AE/ODE
- Continuous: NLAE/ODE
- Discrete: -/DE

Summary of model characteristics

- Models can be developed in hierarchies
- Models exist in relative precision
- Models cause us to think about our system
- Models are developed at a cost in terms of time & money
- Models require parameter estimation and constants
- Models should be identifiable in terms of their parameters
- Models may need simplification to become useful
- Models may be difficult or impossible to validate
- Models can become intractable w.r.t their numerical solution

Use of mathematical models - 1



Reaction : A → B

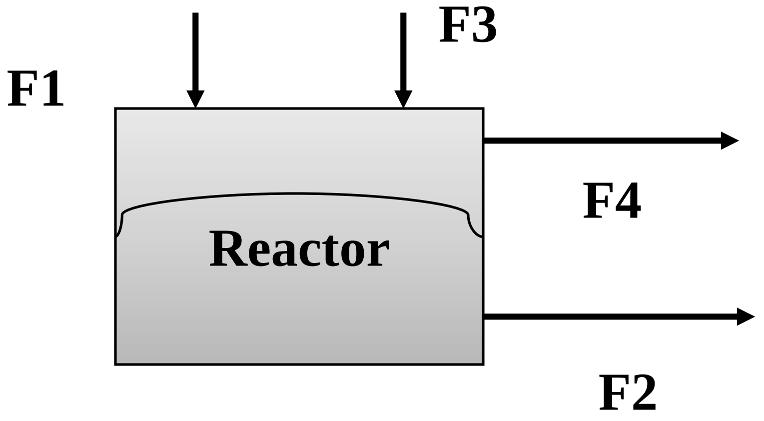
High conversion at temperature = 340 K

Embed reactor model into operation model

Batch Operation Model

1. **Charge Feed (open F1 & close F2)**
2. **Close F1**
3. **Heat until temperature = 340 K**
4. **Control temperature at 340 K**
5. **Discharge when X_B is ≥ 0.9**
6. **…….**

Use of mathematical models - 2



Reaction : A → B

Maximum conversion of 50% A at T = 340 K

Extract B from reactor with solvent!

Solvent ID and effects need to be modeled

Embed reactor model into operation model

Batch Operation/Design Model

1. **Charge Feed (open F1 & close F2)**
2. **Close F1**
3. **Heat until temperature = 340 K**
4. **Control temperature at 340 K**
5. **Charge solvent by opening F3**
6. **Extract B by opening F4**
7. **…….**

Model based calculations

Calculator or solver

Robust & efficient solution strategy

Modelling tools: construction; model reuse; model analysis; model aggregation; model decomposition; model identification; ….

Model object

Model library

Customized simulator

CAPE-OPEN standards; plug & play

Own reading

- What common models do we associate with heat transfer ?
  - Conduction…? Fourier's model (1822)
  - Convection …? Newton's model (1701)
  - Radiation …? Stefan-Boltzmann (1879)
- What are some of the key characteristics of these models ?
- What classification do you give them ?
- What are some of the impediments to effective model building ?