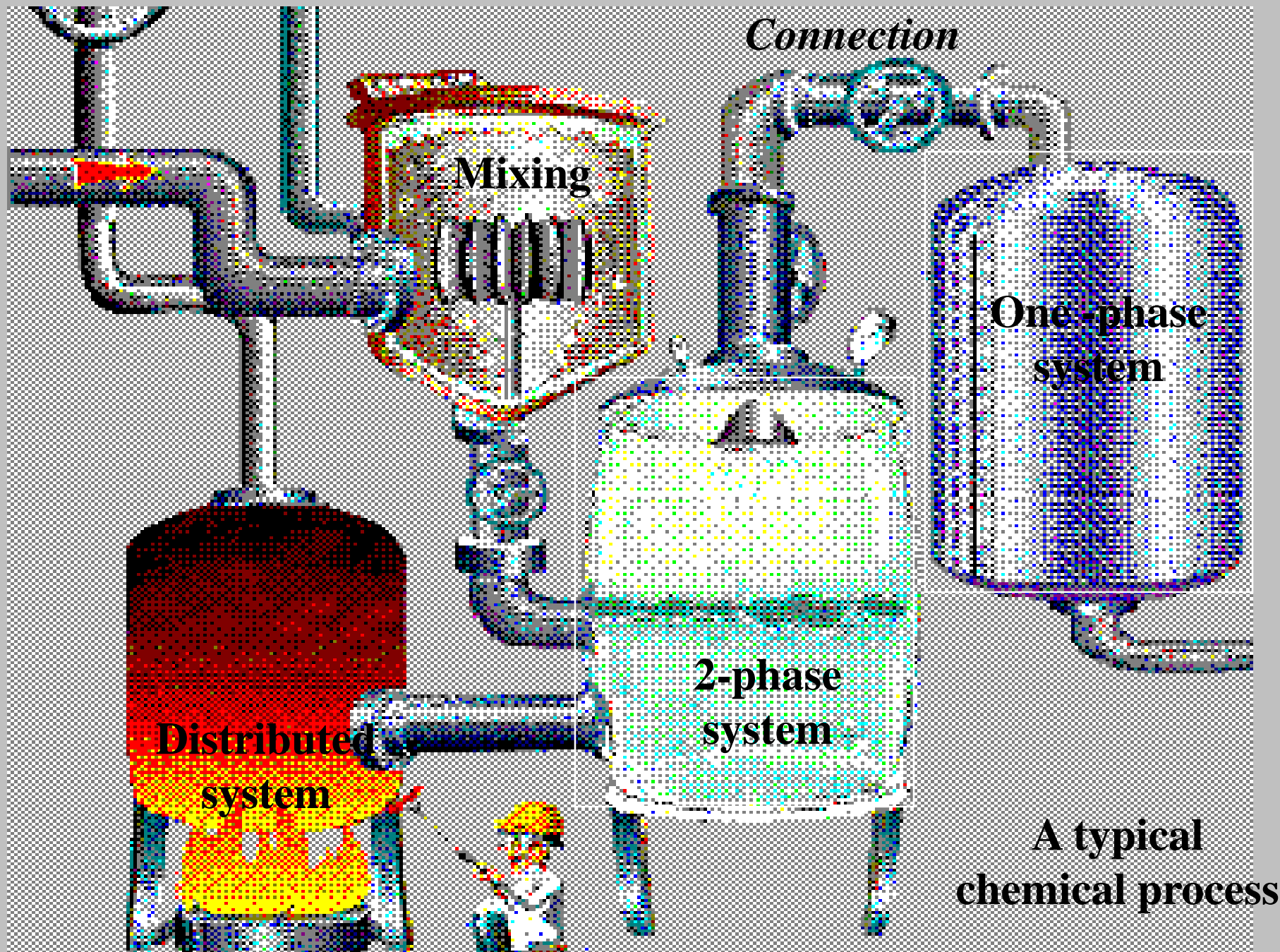


# **Lecture 4a: Systematic (computer) aided model generation**

**ICAS - ModDev**

**Rafiqul Gani**

**CAPEC, Department of Chemical and Biochemical  
Engineering, Technical University of Denmark,  
Lyngby**



*Connection*

**Mixing**

**Distributed  
system**

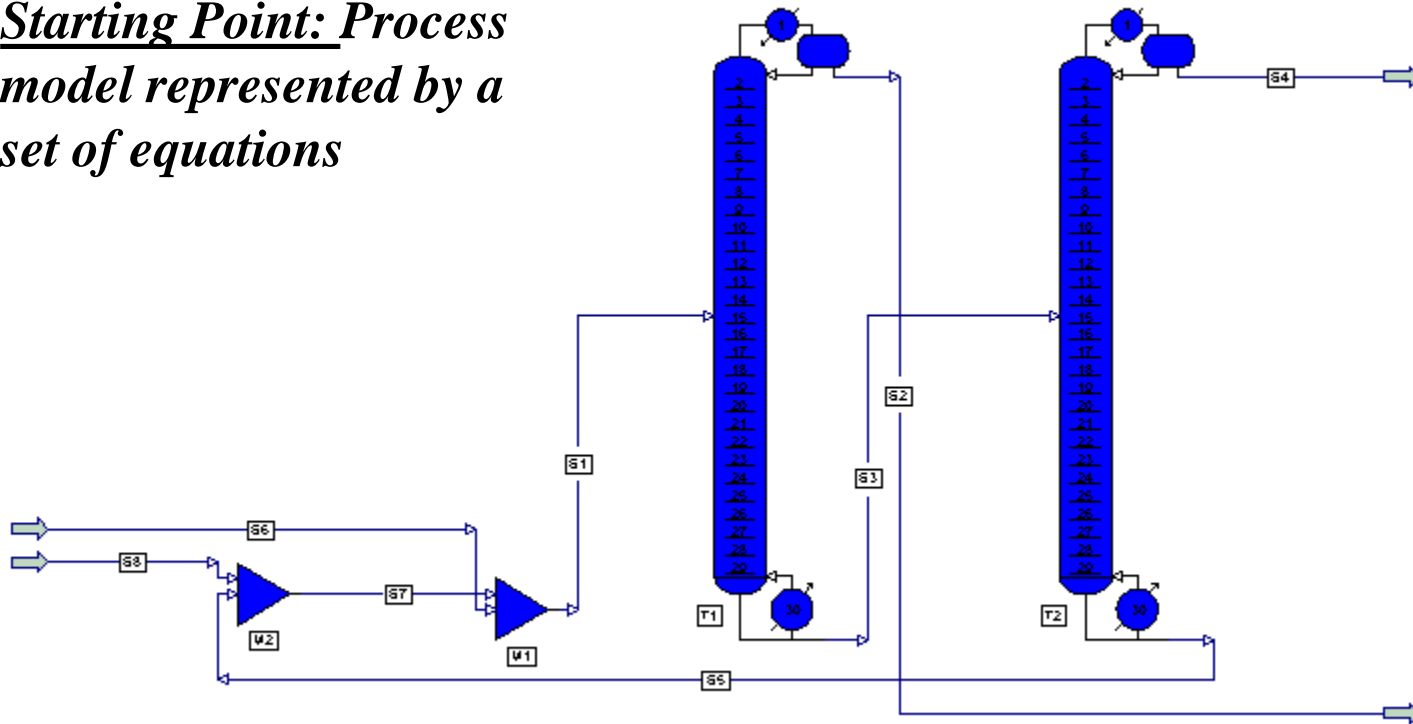
**2-phase  
system**

**One-phase  
system**

**A typical  
chemical process**

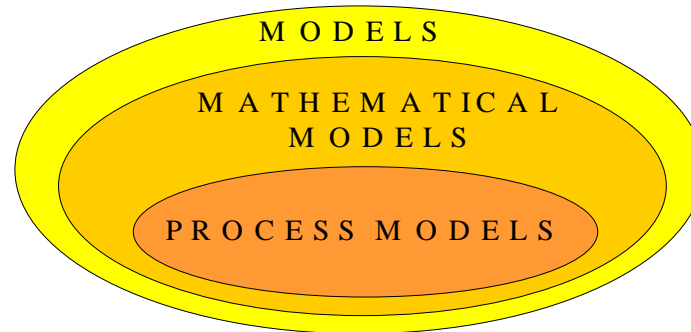
# Model Construction: Separation System

*Starting Point: Process model represented by a set of equations*



*In addition to the mathematical models (and their solution), construct also models for operation, the environment and business*

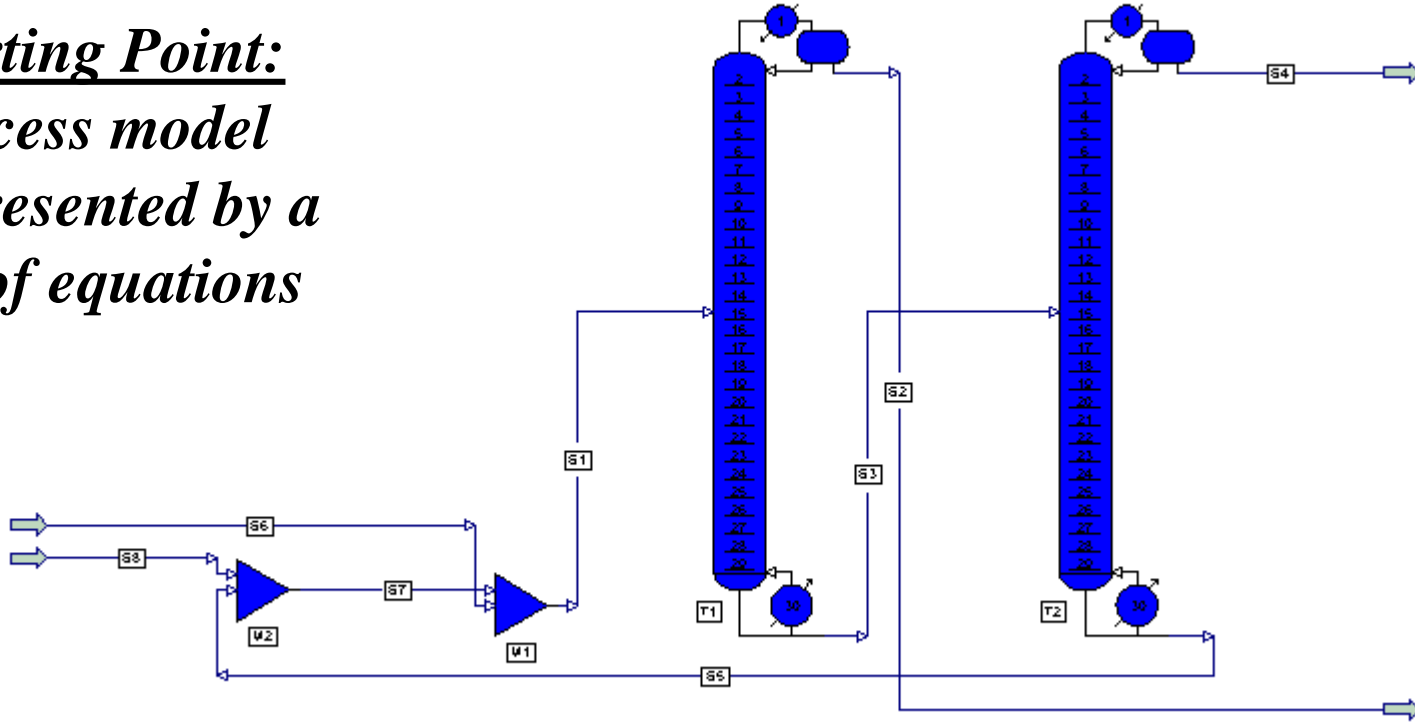
# Model Construction Steps



- **Derive the model equations**
  - **Analyze model equations**
- **Translate the model equations to a solvable form; create library for use with a simulator or for on-line solution**

# Model Generation Approaches

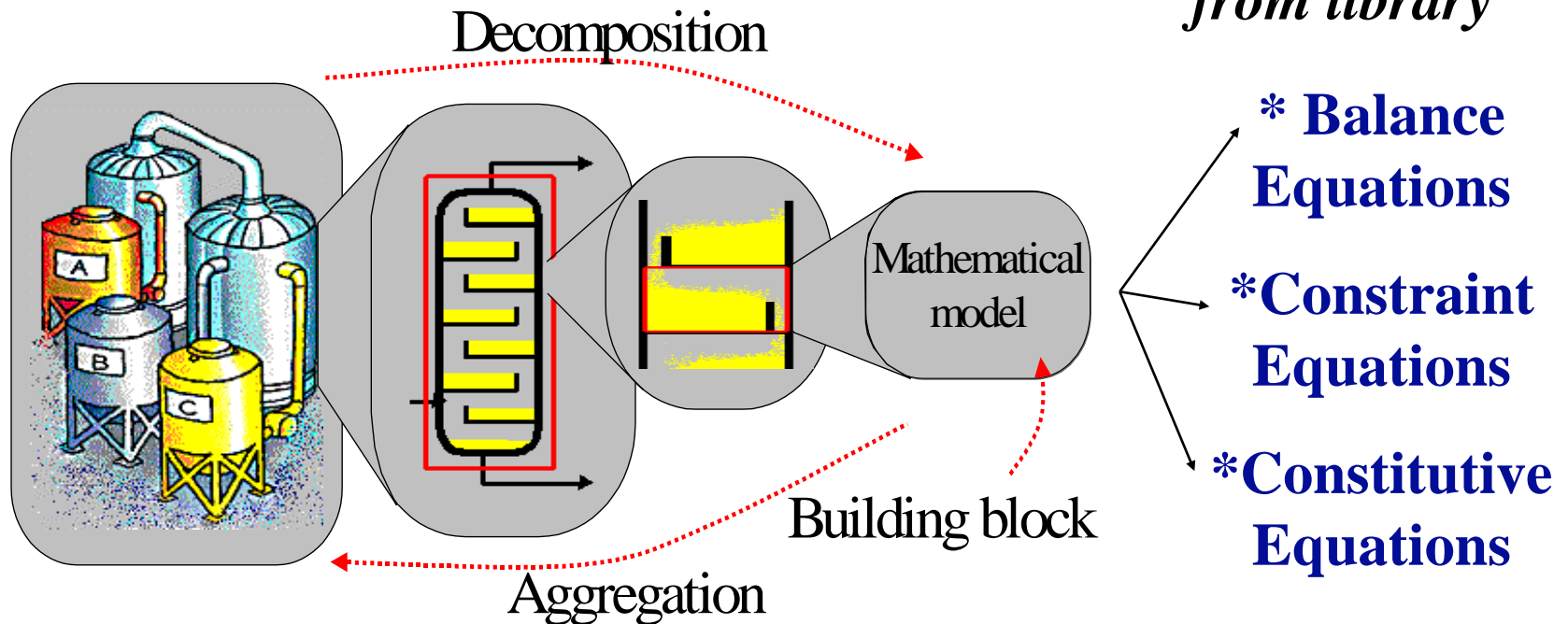
Starting Point:  
*Process model  
represented by a  
set of equations*



*Generate process models of different form defined by  
operation/design objectives (from simulators with model  
libraries)*

# Model Generation: Another Approach

4. *Extract equations from library*

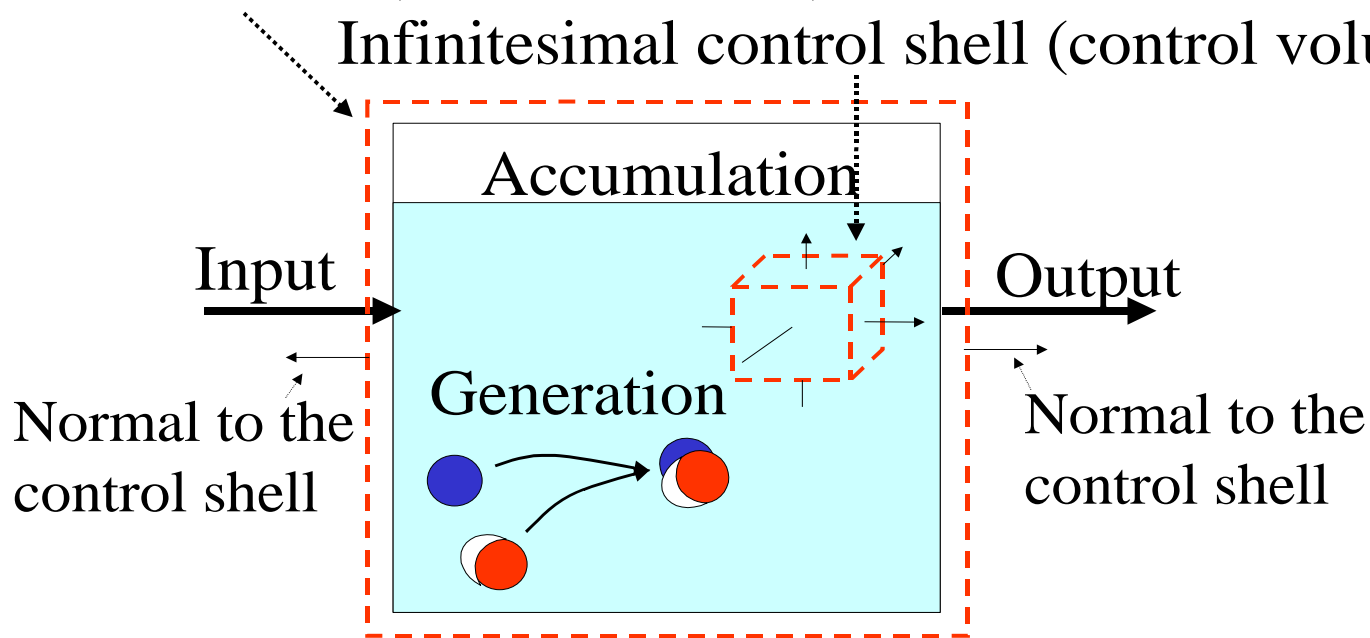


**1. Define Boundary    2. Describe System    3. Identify Building Blocks**

# Example: Derivation of the generic form of the balance equation using an arbitrary control shell (control volume)

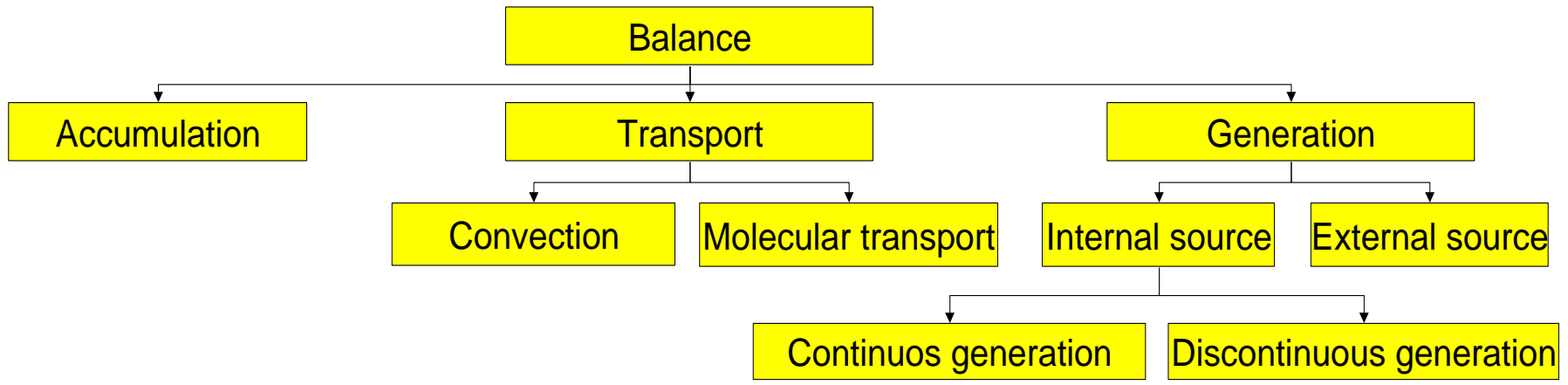
Control shell (control volume)

Infinitesimal control shell (control volume)



$$Accumulation = Input - Output + Generation$$

# Balance Equation Generation



**Plus**

**Constitutive Relations**

**Conditional Relations**



# Model (equation) Generation

**Each control shell & connection is associated to a set of model (fundamental) building blocks**

**Each model building block is either represented by a *Reference Model* or a generic (*Created Model*)**

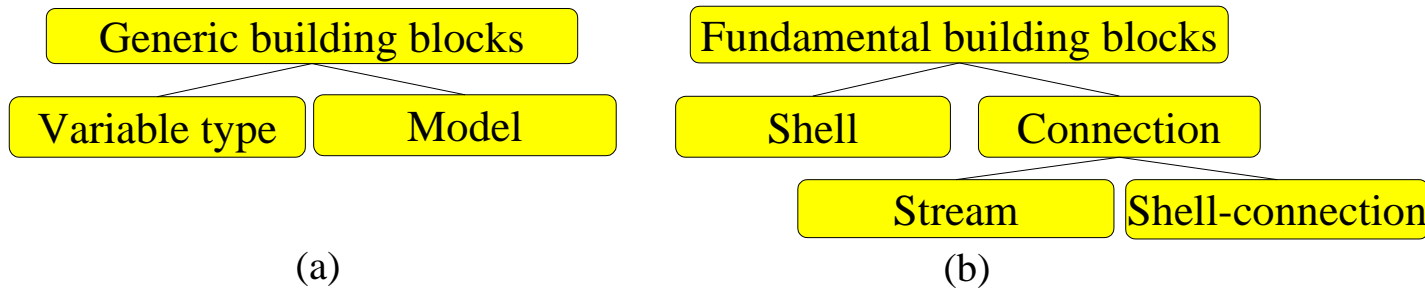
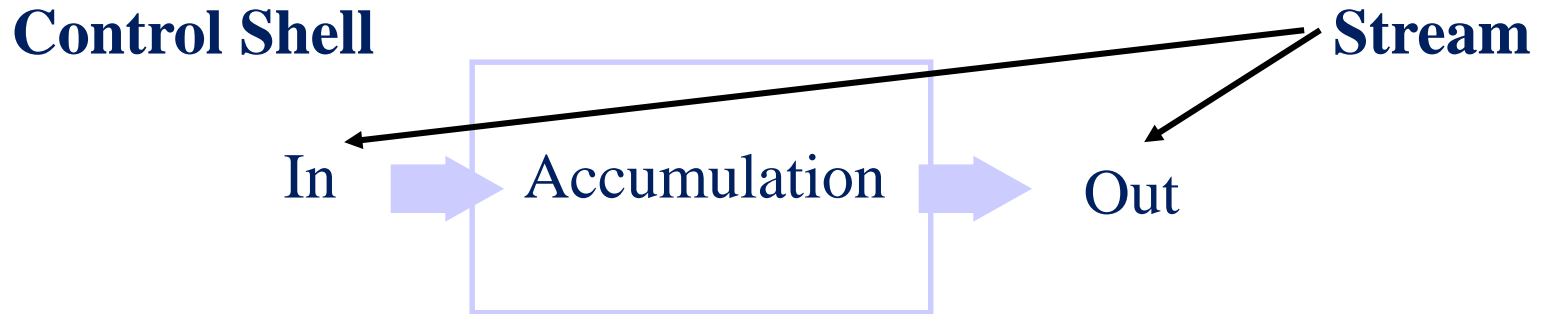
**building block (model)**

**Model equations  
available in the  
knowledge base**

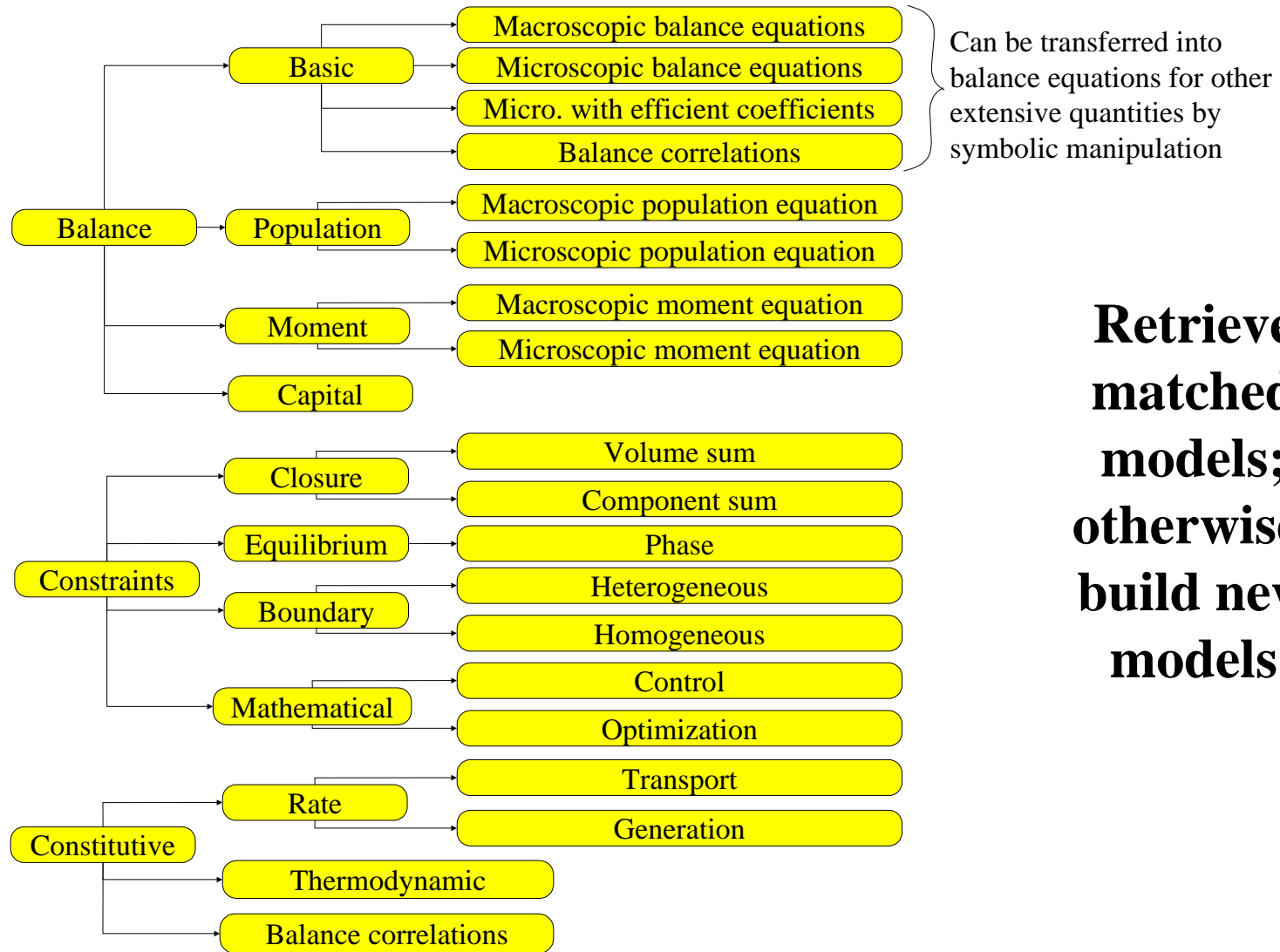
**Model equations  
not available in the  
knowledge base**

# Process ↔ Model Equations

Relationship between process and model equation is established through descriptions of control shells (system boundaries) and connections



# Generation of model equations for control shells

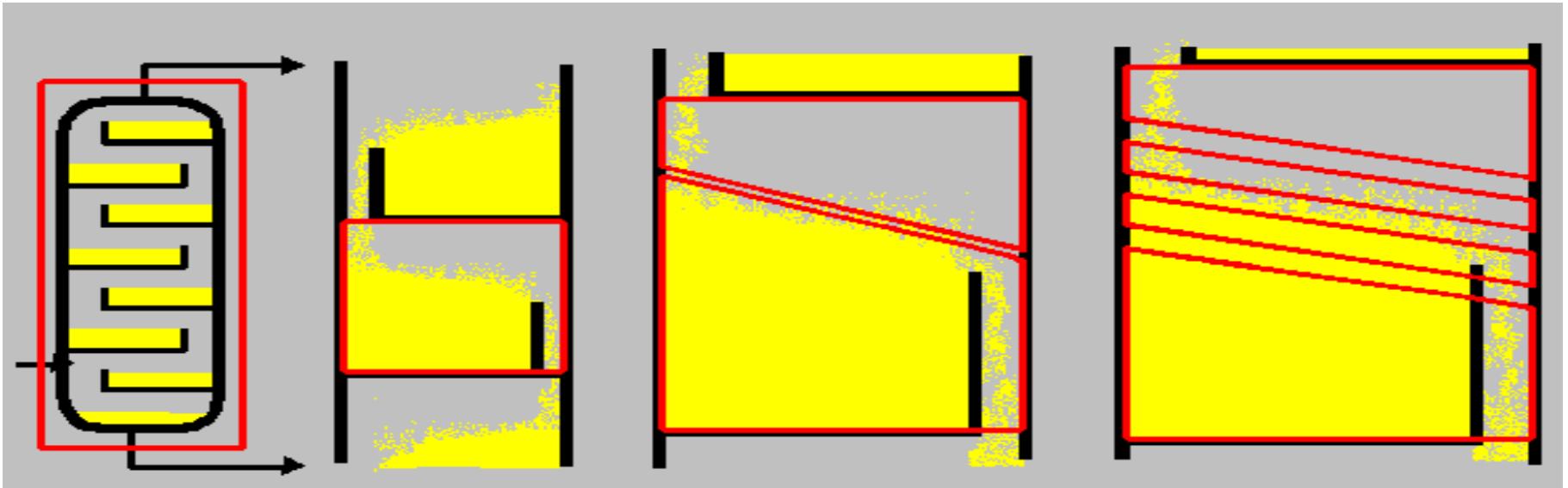


**Retrieve  
matched  
models;  
otherwise,  
build new  
models**

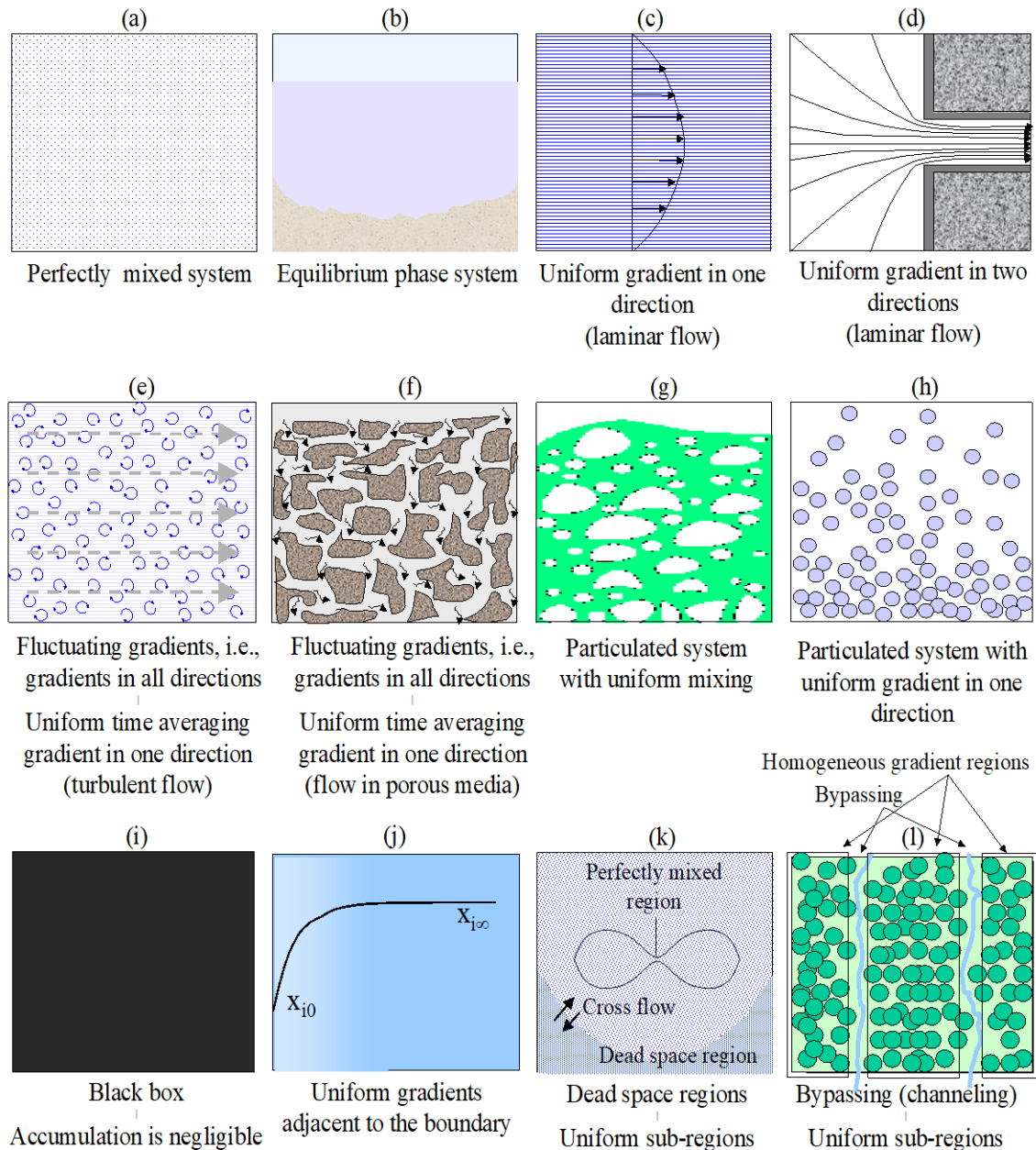
# Describe control shells & connections

To model the various type of processes, the control shell must be defined such that the partial gradients (with respect to  $T$ ,  $P$  and  $f_I$ ) within the boundaries are either:

- Negligible
- Incorporated in an interface or overall flux model
- Dependent on some product specification (design)



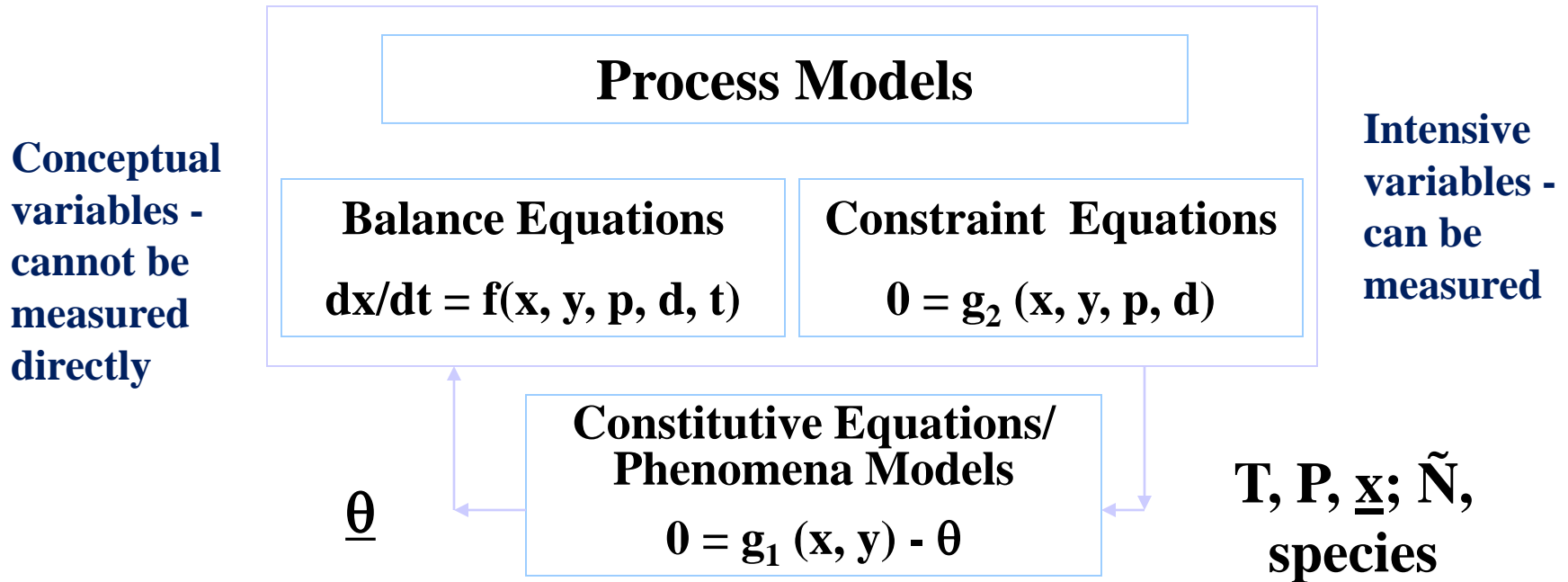
# Description of the control shell: Define the state of aggregation and phases within the system



# Relationship between control volumes & balance equations

	Perfectly mixed	Homogeneous gradients	Homogeneous time averaging gradients
One region	Figure 2.4a – Figure 2.4b Macroscopic balances	Figure 2.4c – Figure 2.4d Microscopic balances	Figure 2.4e – Figure 2.4f Microscopic balances with efficient coefficients
Several regions	Figure 2.4i Black-box: The accumulation is assumed negligible and the physical description of what is happening inside the control shell is not considered (input-output model)	Figure 2.4k - Figure 2.4l Combined models: Each sub-region is modeled with either of the five surrounding balance combination	Figure 2.4j Boundary gradient system: Systems where the film gradients can be included in interphase flux models
Particulated systems	Figure 2.4g Macroscopic balances + Macroscopic population balance OR Macroscopic balances + Macro-moment balance		Figure 2.4h Microscopic balances with efficient coefficients + Microscopic population balance OR Microscopic balances with efficient coefficients + Macro-moment balance

# Classification of Model Equations

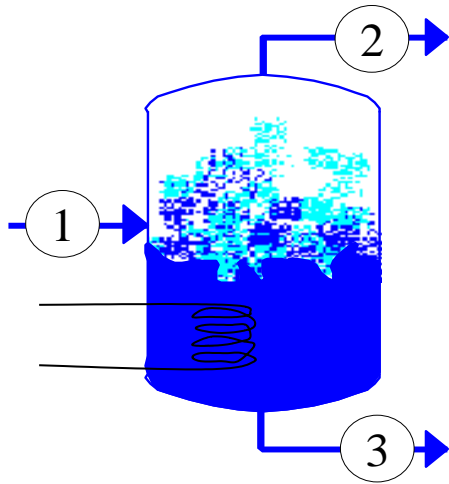


*Constitutive equations (not rigorous) relate conceptual variables to measurable variables & species parameters.  $\theta_i = f_i(T, P, \underline{x}; \underline{m})$*

*Mimic behaviour of the process (system)*

*Different types of models can be obtained through different choices of the different model sub-classes*

# Describe Problem: Steady state PT-Flash



## STREAM CONNECTION OBJECT

Name: 3

Models for quantities:

Energy (enthalpy):  $H_3 = @FUNC\_E(2, f_{3[]}, T_3, P_3)$

Models for the “from”-connection: (*equilibrium*)

Energy connection:  $T_3 = T_{flash}$

Momentum connection:  $P_3 = P_{flash}$

## SHELL OBJECT

Name: *flash*

Assumed phase condition: *Calculate (VL)*

Equilibrium model:  $0 = f_{2i}/ft_2 - K_{flash} * f_{3i}/ft_{3i}$  @KEQ( $T_{flash}$ ,  $P_{flash}$ ,  $f_{2[]}$ ,  $f_{3[]}$ , # $K_{flash}$ )

## SHELL CONNECTION OBJECT

Name: *heater*

Connection models:

Energy connection:  $Q_{heater} = Q_{flash}$

Lecture 4a: Advanced Computer Aided Modelling



# Model generation through ICAS-ModDev

Describe the shell and connections of the processes to be modelled through ModDev, which will then generate the necessary model equations.

Note that for constitutive models, if the appropriate model is not present in the library, a user-supplied model would be necessary. Also, the conditional equations may need to be supplied by the user. The model for a shell may be re-used as many times as necessary

# Tools & options in ModDev (ModGen)

Fundamental shell connection object

Fundamental shell object

Fundamental stream object

Draw modeling objects

Analyze and manipulate the model equations

Select external solver

Interphase with solver

ModDef

The screenshot shows the ModGen software interface with the following components:

- Diagram:** A process flow diagram for a stage  $p$ . It features a yellow rectangular block labeled "stage(p)".
  - Input streams:  $l(p+1)$  (top),  $v(p)$  (right), and  $-feed(p)$  (left).
  - Output streams:  $l(p)$  (bottom) and  $v(p+1)$  (right).
- Equation List:** A list of 12 equations defining the stage's behavior:
  - $6: P_v(p)=P\_stage(p)$
  - $7: ft\_v(p)=sum\_j(f\_v(p))$
  - $8: H_v(p)=@FUNC\_E(2,f\_v(p),T\_v(p),P\_v(p))$
  - $9: @KEQ(T\_stage(p),P\_stage(p),f\_v(p),f\_l(p),K_{eq\_stage}(p))$
  - $10: 0=f\_v(p)/ft\_v(p)-K_{eq\_stage}(p)_i f\_l(p)/ft\_l(p)$
  - $11: 0=+f\_l(p+1)-f\_l(p)+f\_v(p+1)-f\_v(p)+f\_feed(p)_i$
  - $12: 0=+ft\_l(p+1)*H\_l(p+1)-ft\_l(p)*H\_l(p)+ft\_v(p+1)*H\_v(p+1)-ft\_v(p)*H\_v(p)+ft\_feed(p)*H\_v(p)$
- Toolbar:** Contains various icons for file operations, drawing, and solver selection. Specific solvers like ASCII, ICAS, and GPRON are highlighted.
- Menu Bar:** Includes File, Edit, View, Draw, Format, Model, Window, and Help.
- Status Bar:** Shows "Ready" and the date/time "21:06:56 02/25/98".

# Tools & options in ModDev (ModGen) - define shell

The screenshot displays the ModDev software interface. On the left, a diagram shows a rectangular shell labeled 'Shell1' with two input streams (1 and 2) on the left side and one output stream (3) on the right side. On the right, the 'Shell description' dialog box is open, showing the following configuration options:

- Name:** Shell1
- Streams:** 1, 2
- Shell connections:** (empty)
- Phase condition:**
  - Gas
  - Liquid
  - Solid
  - Calculate (VLE)
  - Calculate (multi-phase)
- Equilibrium:** (button)
- Geometric description:** (button)
- Components:** (button)
- Reactions:** (button)
- Mass balance:** (button)
- Component balance:** (button)
- Energy balance:** (button)
- Momentum balance:** (button)
- Variables:** (button)
- Related variables:** (button)
- Other models:** (button)
- Close:** (button)
- Lumped / distributed system:**
  - Macroscopic balance (lumped)
  - Microscopic balance (distributed)
- Dispersive state:**
  - Homogeneous
  - Distributed particulated properties (moment balance)
  - Distributed particulated properties (population balance)
- Distribution function:** (button)
- Basis of the balance equations:**
  - Mole
  - Mass
- Incompressible fluid
- Viscous heating
- Gravity field
- Pressure field
- Other heat source
- Substitute equation of continuity in the balance equations
- Use substantial derivatives in the balance equations
- Number of repetitions (0 if defined in the problem definition):** 1

The status bar at the bottom indicates 'Slide 13 of 18', 'capec1.pot', and the date '06/03/99'.

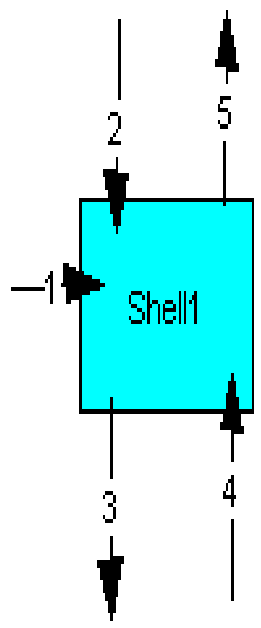
# Tools & options in ModDev (ModGen) -define stream

The screenshot shows the ModDev software interface with the 'Stream' dialog box open. The dialog box is titled 'Stream' and contains the following fields and options:

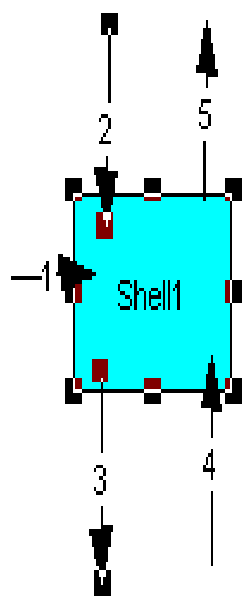
- Name:** 1
- Number of repetitions (if specified later, give 0):** 1
- From phase condition:**
  - Gas
  - Liquid
  - Solid
  - Calculate
- Phase condition:**
  - Gas
  - Liquid
  - Solid
  - Calculate (VLE)
  - Calculate (multi-phase)
  - = From connection
  - = To connection
- To phase condition:**
  - Gas
  - Liquid
  - Solid
  - Calculate
- Equilibrium:** [Button]
- Surroundings:** [Connection location] [Diagram showing a stream between two shells, Shell1 and Shell2, with a green background on the left and a cyan background on the right.]
- From connection models:**
  - [Mass]
  - [Component]
  - [Energy]
  - [Momentum]
  - Equilibrium connection
- Stream:**
  - Drop models:**
    - [Temperature drop]
    - [Pressure drop]
  - Quantity models:**
    - [Energy - Temperature]
    - [Momentum - Pressure]
  - Known stream (all unknown variables associated with the stream are set to known)
- To connection models:**
  - [Mass]
  - [Component]
  - [Energy]
  - [Momentum]
  - Equilibrium connection
- Buttons:** Components, Reactions, Variables, Related variables, Other models, Close

The background shows a diagram of a 'Shell1' with two input streams labeled '1' and '2'. The software interface includes a menu bar (File, Edit, View, Draw, Format, Model, Window, Help), a toolbar, and a status bar at the bottom indicating 'Slide 14 of 19' and 'capec1.pot'.

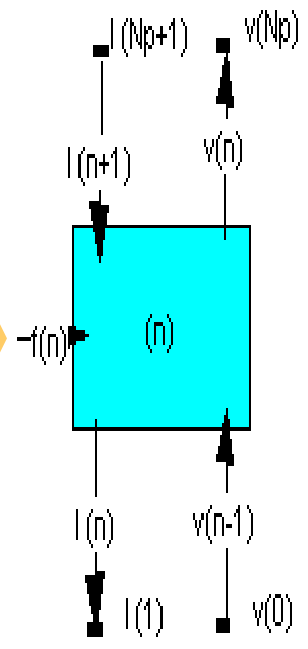
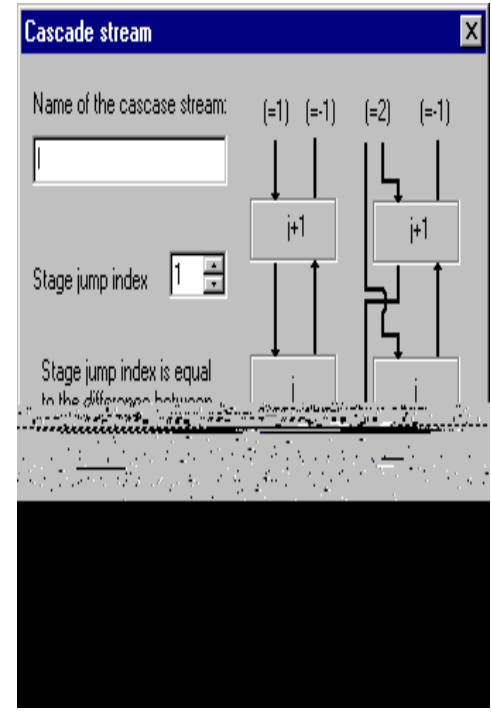
# Generation of cascade models



(a)



(b)



(c)

Variables					
	Mass	Energy	Momentum	Geometric	Other
Implicit Equations	2*NC	2	0	0	0
Unknown Var. to Specify	1	-1	0	0	0
Unknown Variables	f_3[i],ft_4,f_5[i]	T_Jacket			
Known Variables	f_1[i],f_2[i],alpha_CSTR[m],Key[m],x_4[i]	H_1,H_2,H_4,T_CSTR,EU_Wall	P_CSTR,P_Jacket		
Parameters	nu[i][m]				
Explicit Variables	ft_1,ft_2,ft_3,f_4[i],ft_5,RC_CSTR[i],RR_CSTR[m]	H_3,H_5,T_3,T_5,Q_Wall	P_3,P_5		

# Model Generation -II: Vaporiser/distillation

$$d = f_{1i}(x_v, y_v, z_v, F, L, V); i=1, NC \quad (1)$$

$$D = f_2(F, L, V, h_F, h, H, Q) \quad (2)$$

$$0 = g_1(x, y, K) \quad (3)$$

$$K_i = g_{2i}(y, x, T, P); i=1, NC \quad (4)$$

$$h = g_3(x, T, P) \quad (5)$$

$$H = g_4(y, T, P) \quad (6)$$

Balance Equations

Constraint Equations

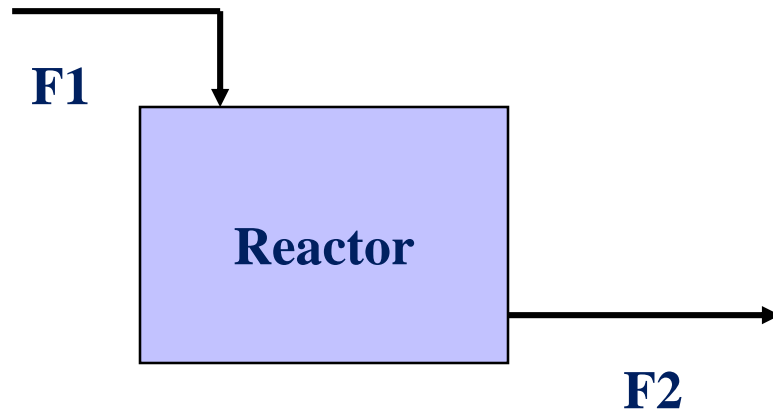
Constitutive Models

$$y_i = \frac{\alpha_{ij} x_i}{1 + x_i (\alpha_{ij} - 1)}$$

$$K_i = \frac{\gamma_i P_i^S}{P}; \gamma_i = f(\underline{A}_i, \underline{\tau}_{ij}, \underline{x}, T)$$

**System identification; Constitutive model parameter estimation (generate custom models from reference)**

# Construction of an operation model



**Reaction :  $A \rightarrow B$**

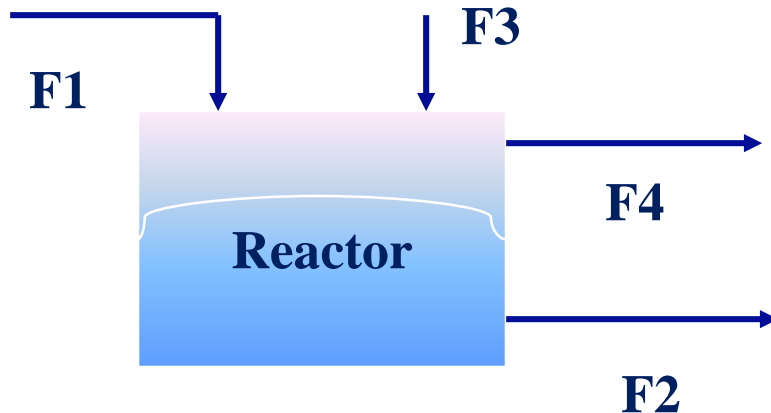
**High conversion at  
temperature = 340 K**

## 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  
 $\geq 0.9$**
- 6. ....**



# Construction of an operation & design model



**Reaction :  $A \rightarrow B$**

**Maximum conversion  
of 50% A at  $T = 340\text{ K}$**

**Extract B from reactor  
with solvent!**

*Solvent ID and effects  
need to be modeled*

## 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. **.....**

## Modelling exercise - 4: ModDev

Use tutorial document (tutorial-4-I.pdf) to generate a steady state mixer model; followed by a dynamic model. In tutorial-4-II.pdf, extension to a CSTR is included.