Lecture 4a: Systematic (computer) aided model generation

ICAS - ModDev

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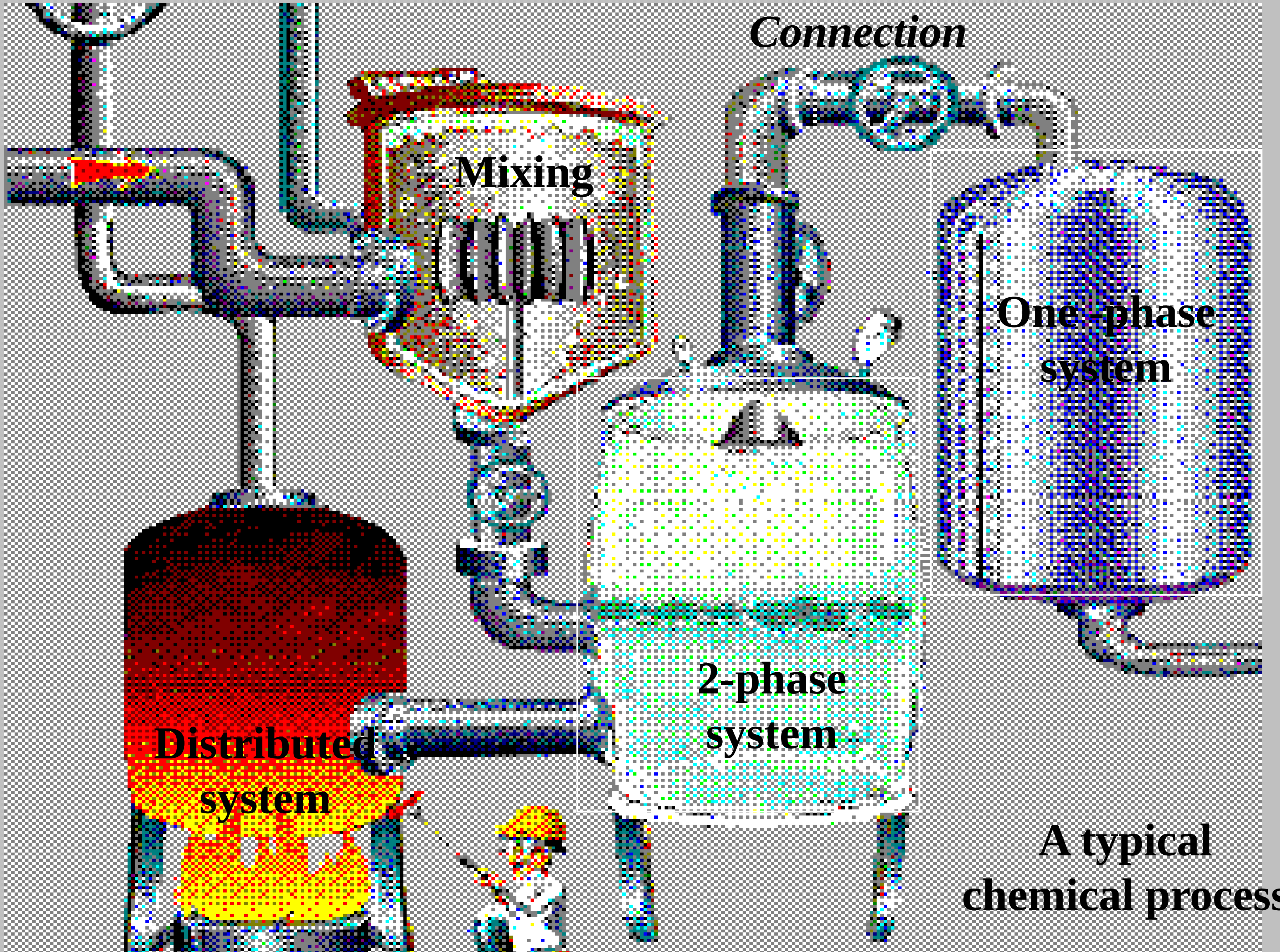
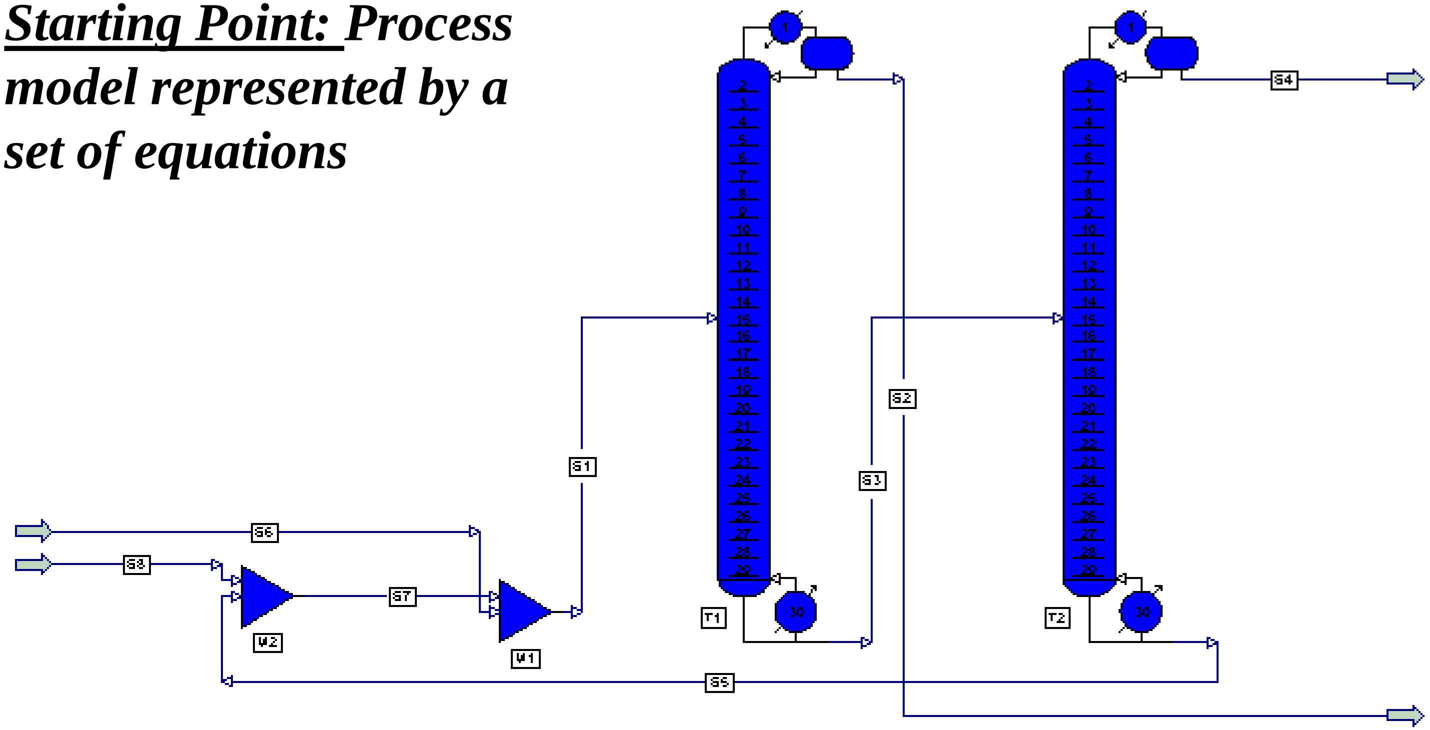

Connection
Mixing
One-phase system
2-phase system
Distributed system
A typical chemical process

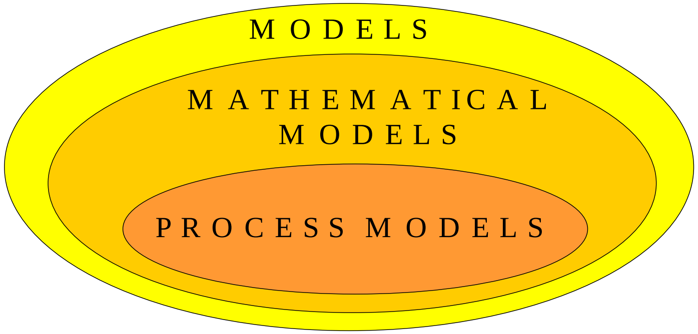
Model Construction: Separation System

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

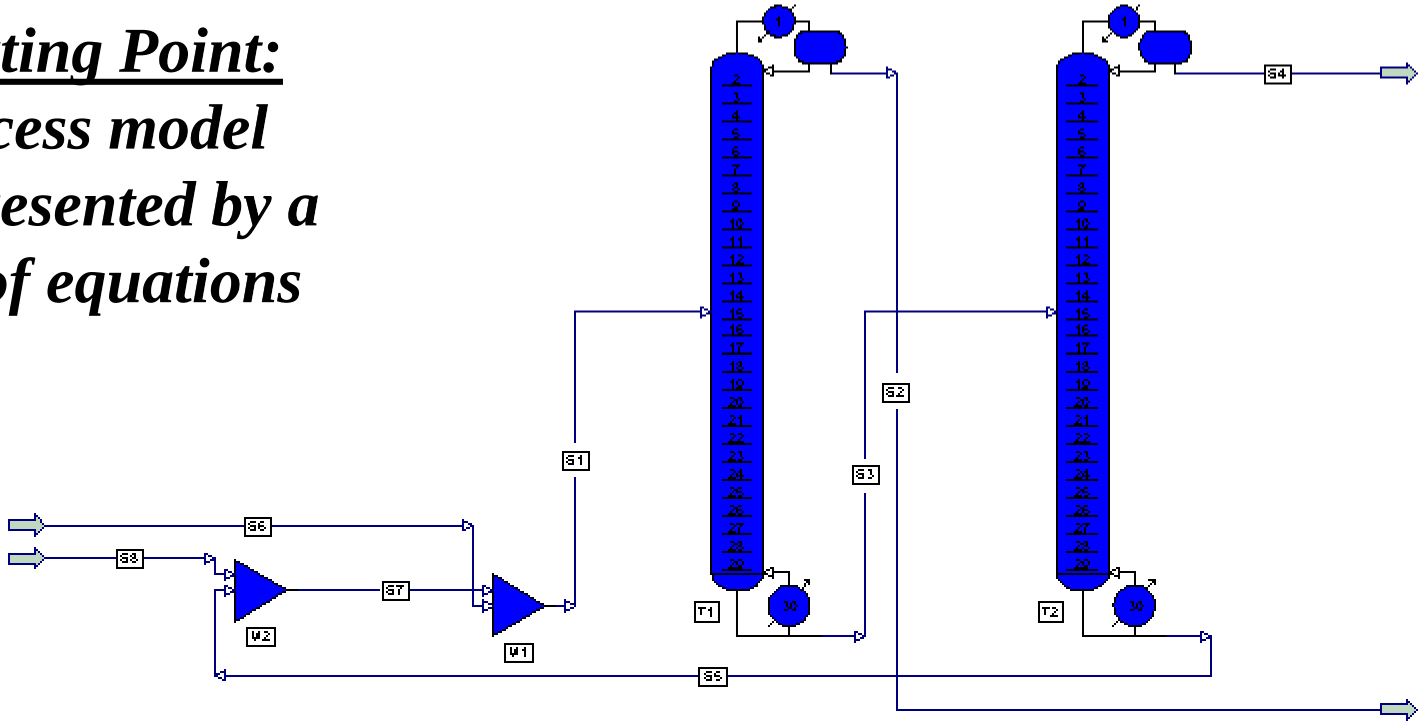
Model Construction Steps



- **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

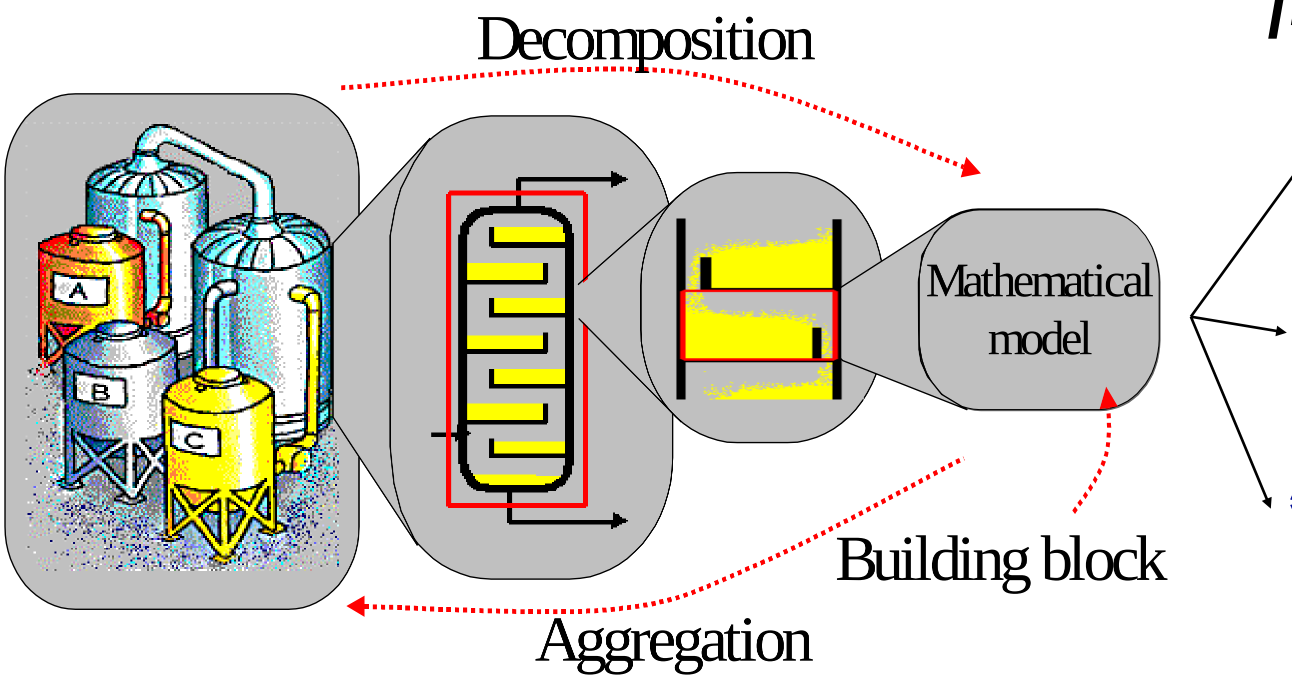
Starting Point:
Process model represented by a set of equations



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



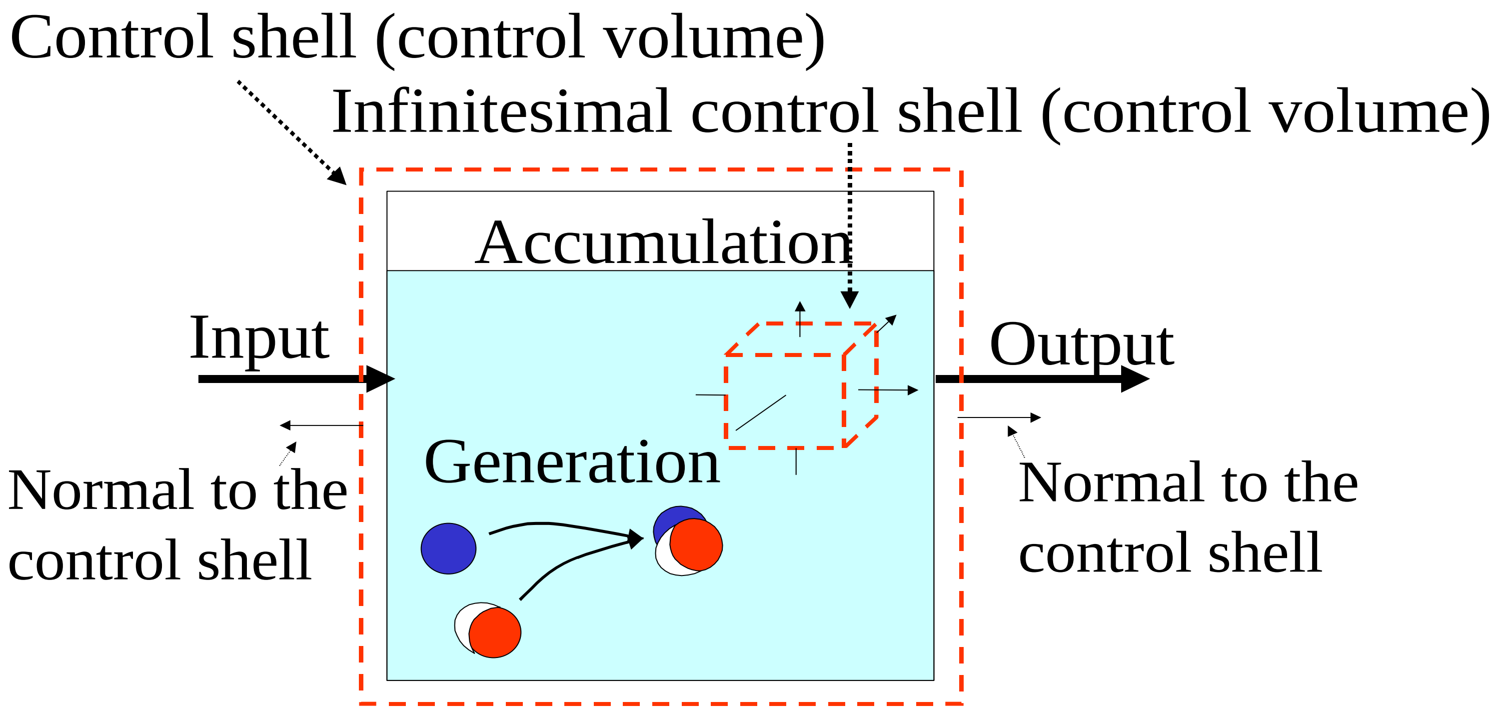
*** Balance Equations**

***Constraint Equations**

***Constitutive Equations**

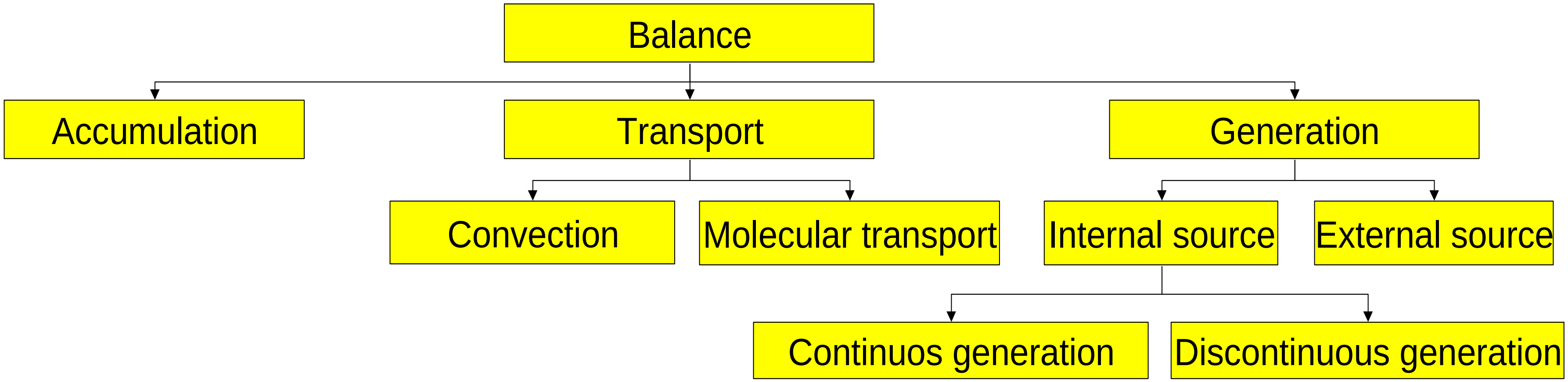
1.Define Boundary **2.Describe System** **3.Identify Building Blocks**

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



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

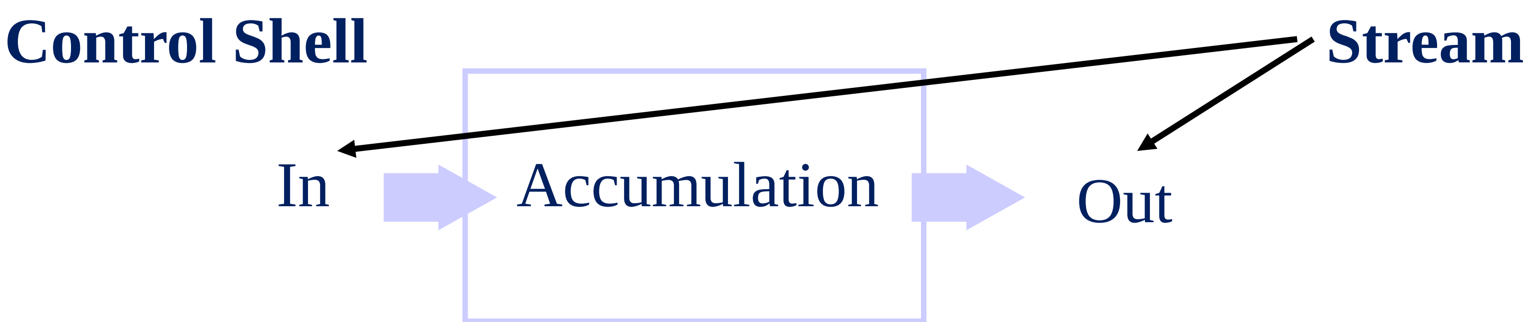
Each model building block is either represented by a *Reference Model* or a generic (*Created Model)* building block (model)

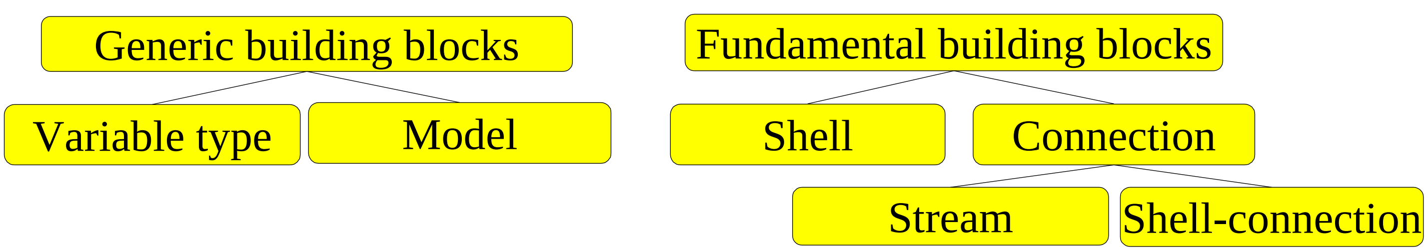
Model equations available in the knowledge base

Model equations not available in the knowledge base

Process ↔ Model Equations

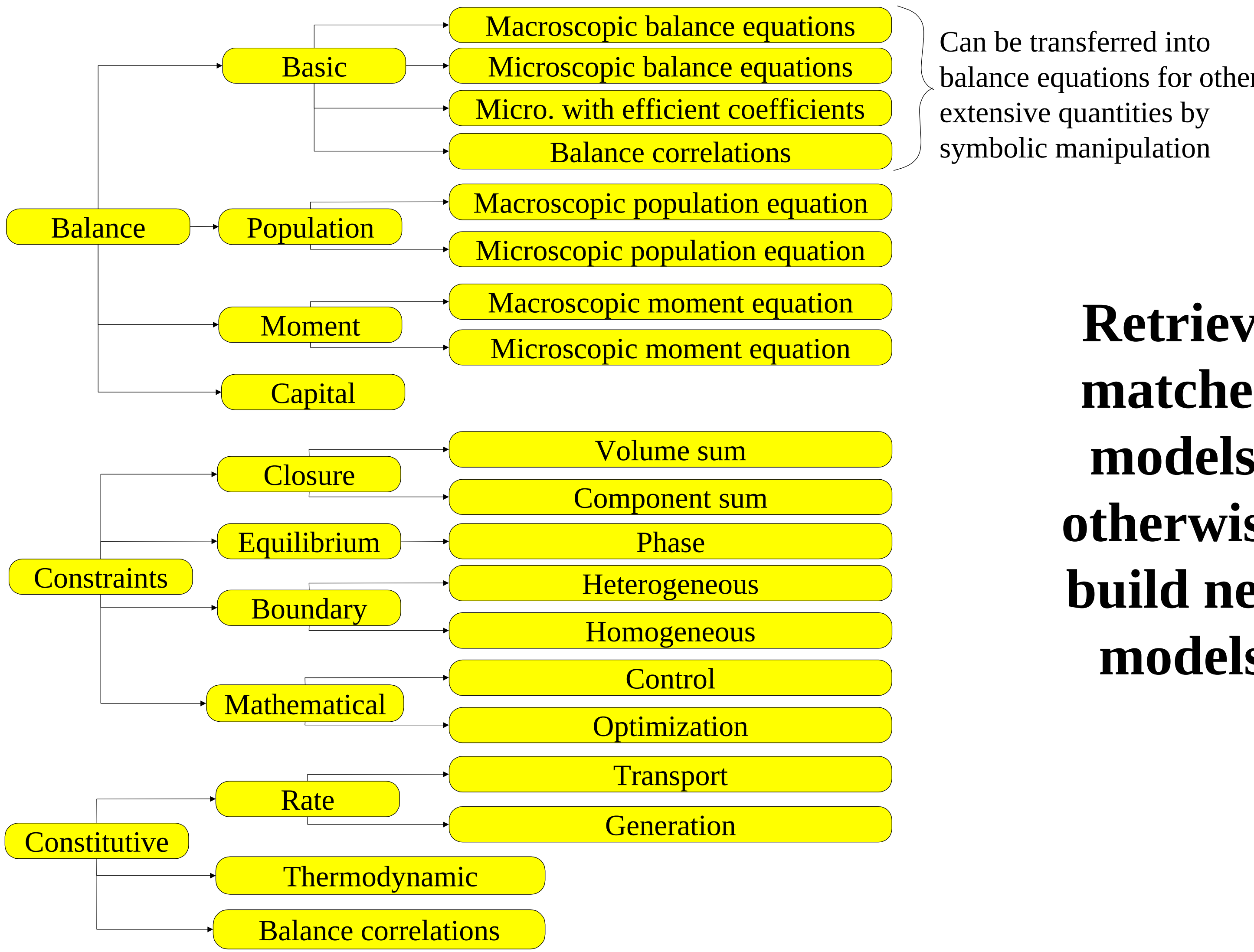
Relationship between process and model equation is established through descriptions of control shells (system boundaries) and connections





(a) (b)

Generation of model equations for control shells

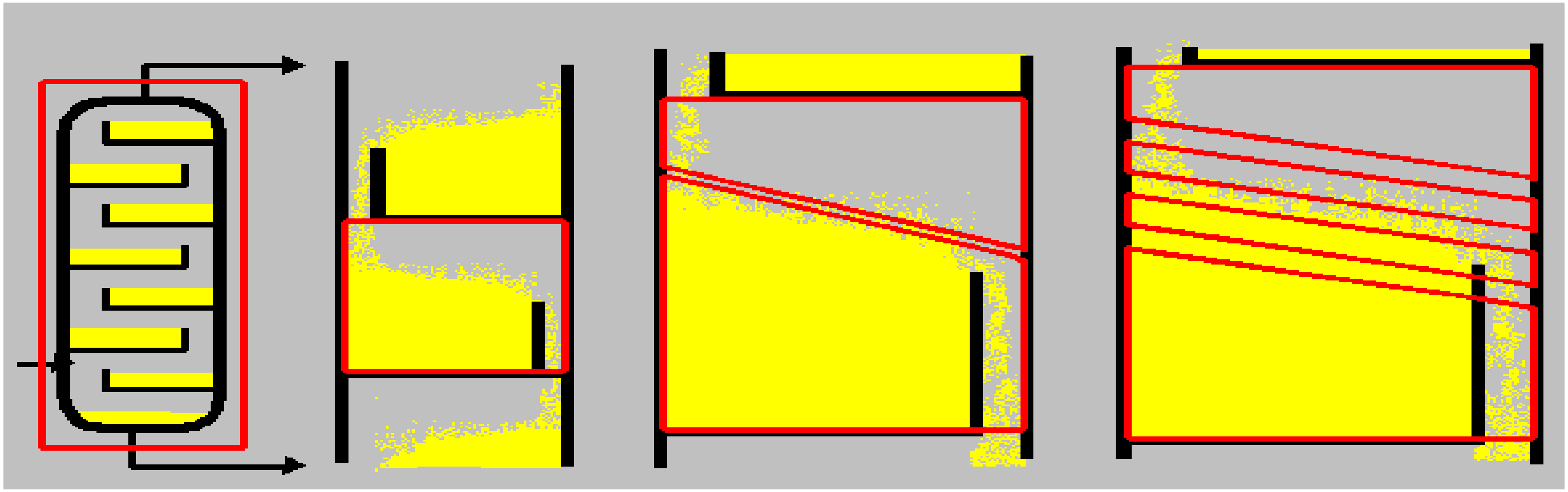


Retrieve matched models; otherwise, build new models

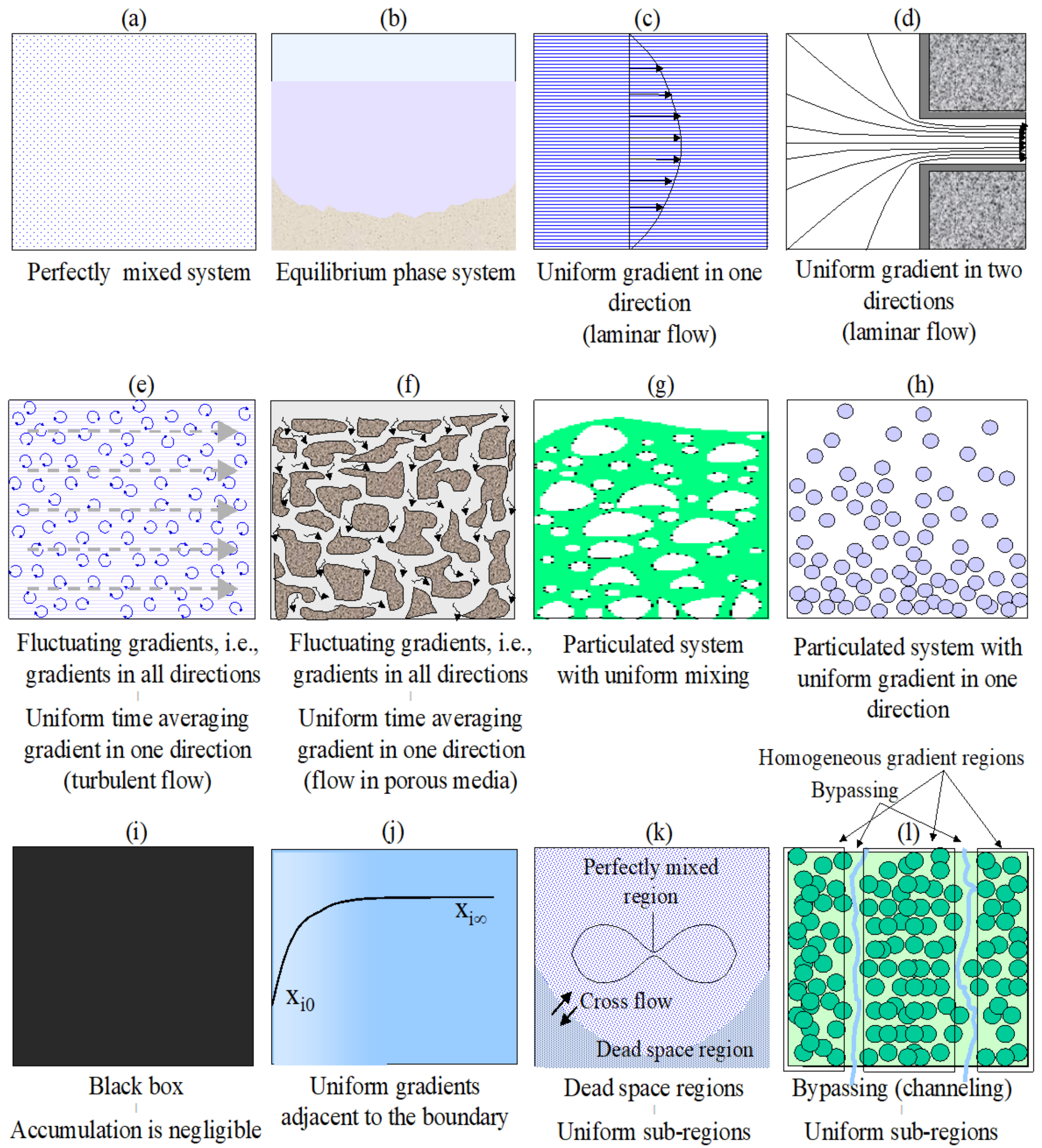
Describe control shells & connections

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 - Figure2.4l 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

Process Models

Balance Equations

$dx/dt = f(x, y, p, d, t)$

Constraint Equations

$0 = g_2(x, y, p, d)$

Constitutive Equations/ Phenomena Models

$0 = g_1(x, y) - \theta$

Conceptual variables - cannot be measured directly

$\underline{\theta}$

Intensive variables - can be measured

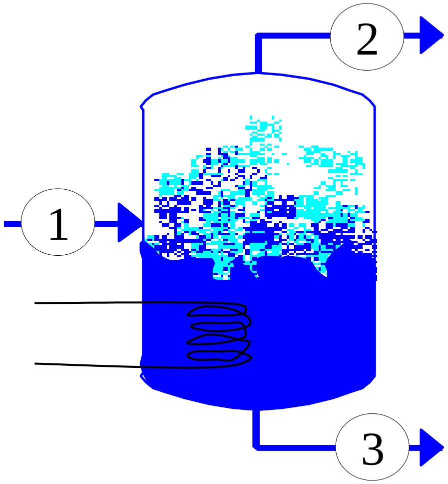
T, P, $\underline{x}$; Ñ, species

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})

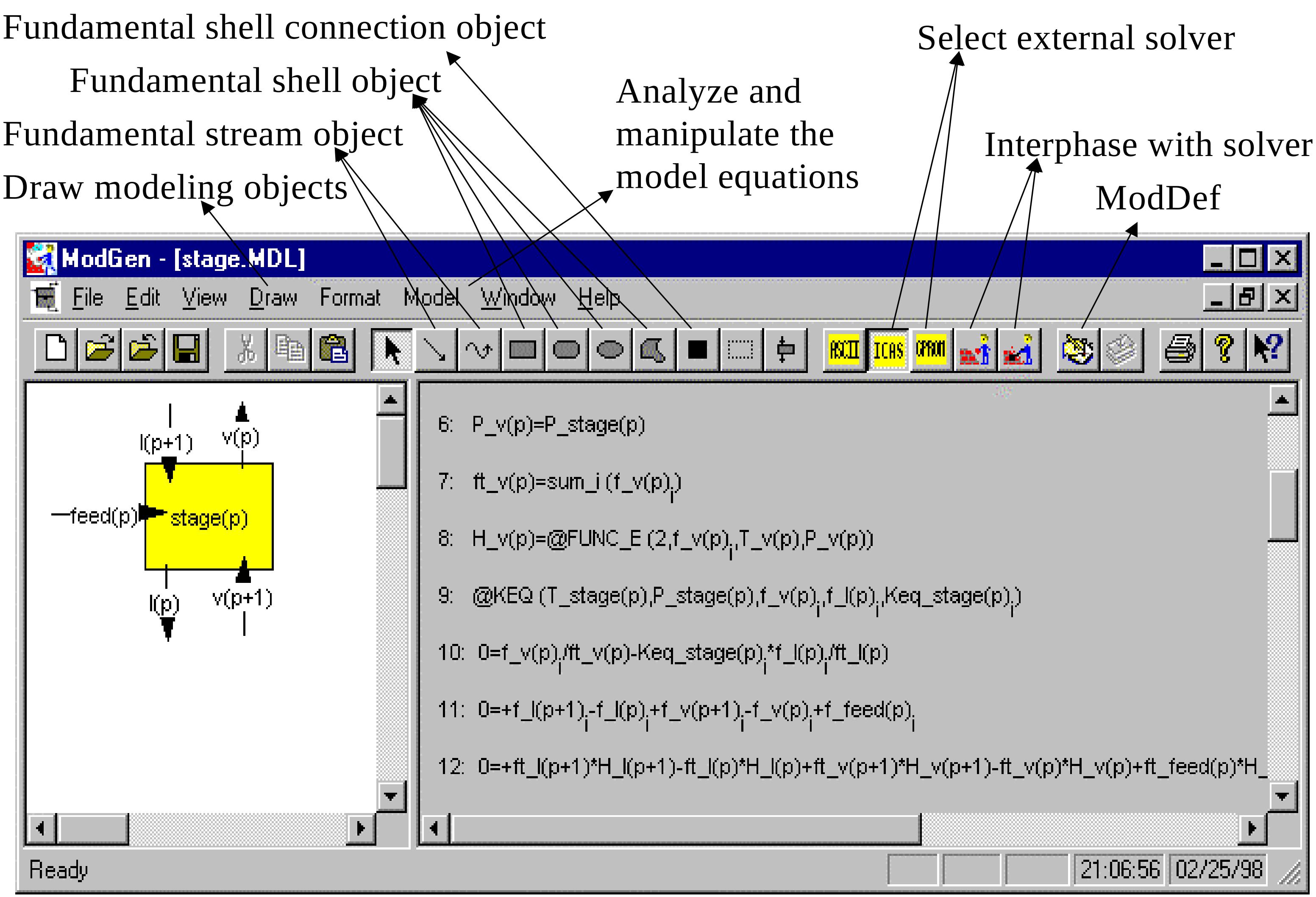
SHELL CONNECTION OBJECT
Name: *heater*
Connection models:
Energy connection: $Q_{heater}=Q_{flash}$

Model generation through ICAS-ModDev

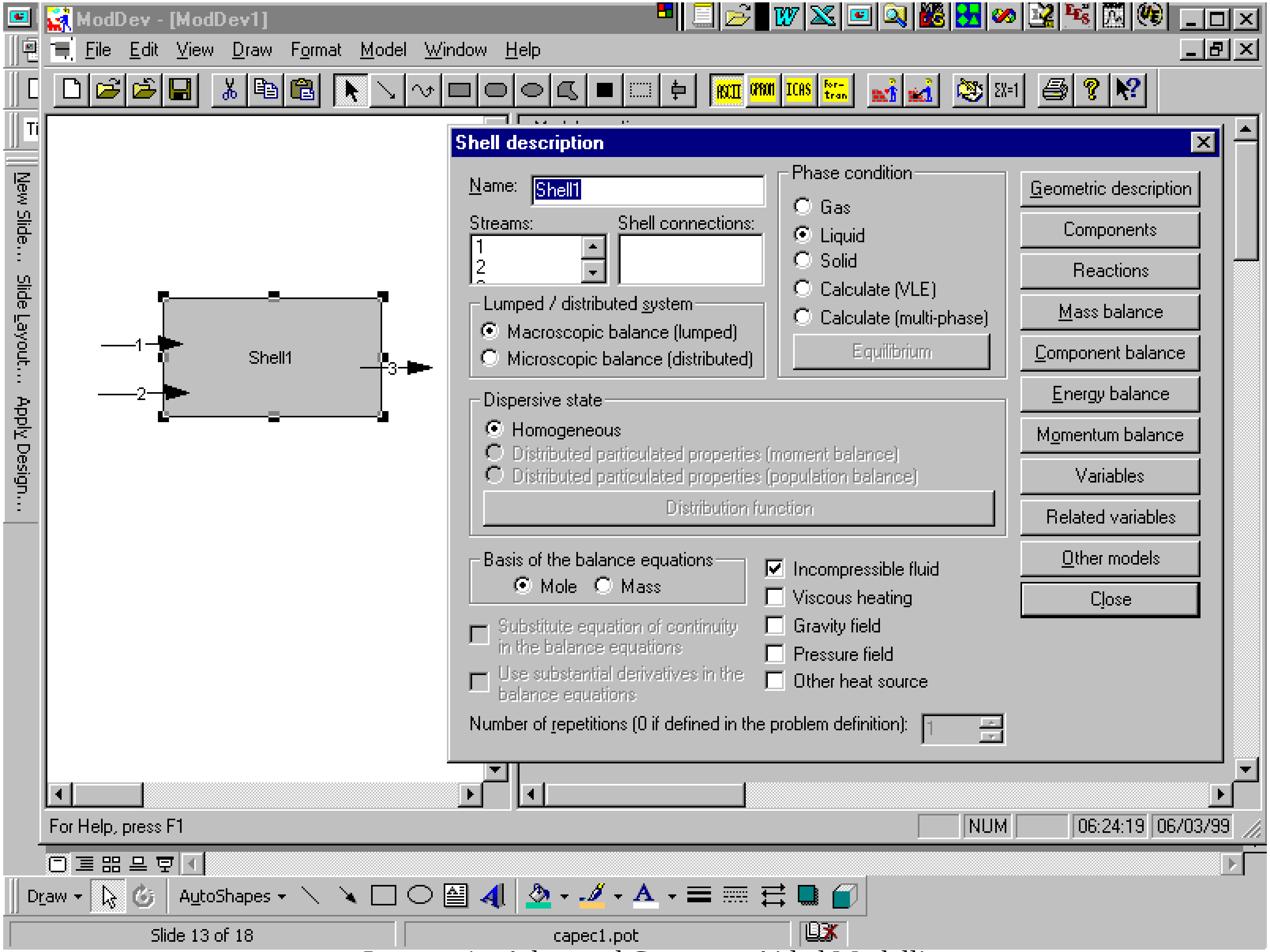
Describe the shell and connections of the processes to be modelled through ModDev, which will then generate the necessary model equations.

Note that for constitutive models, if the appropriate model is not present in the library, a user-supplied model would be necessary. Álso, 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

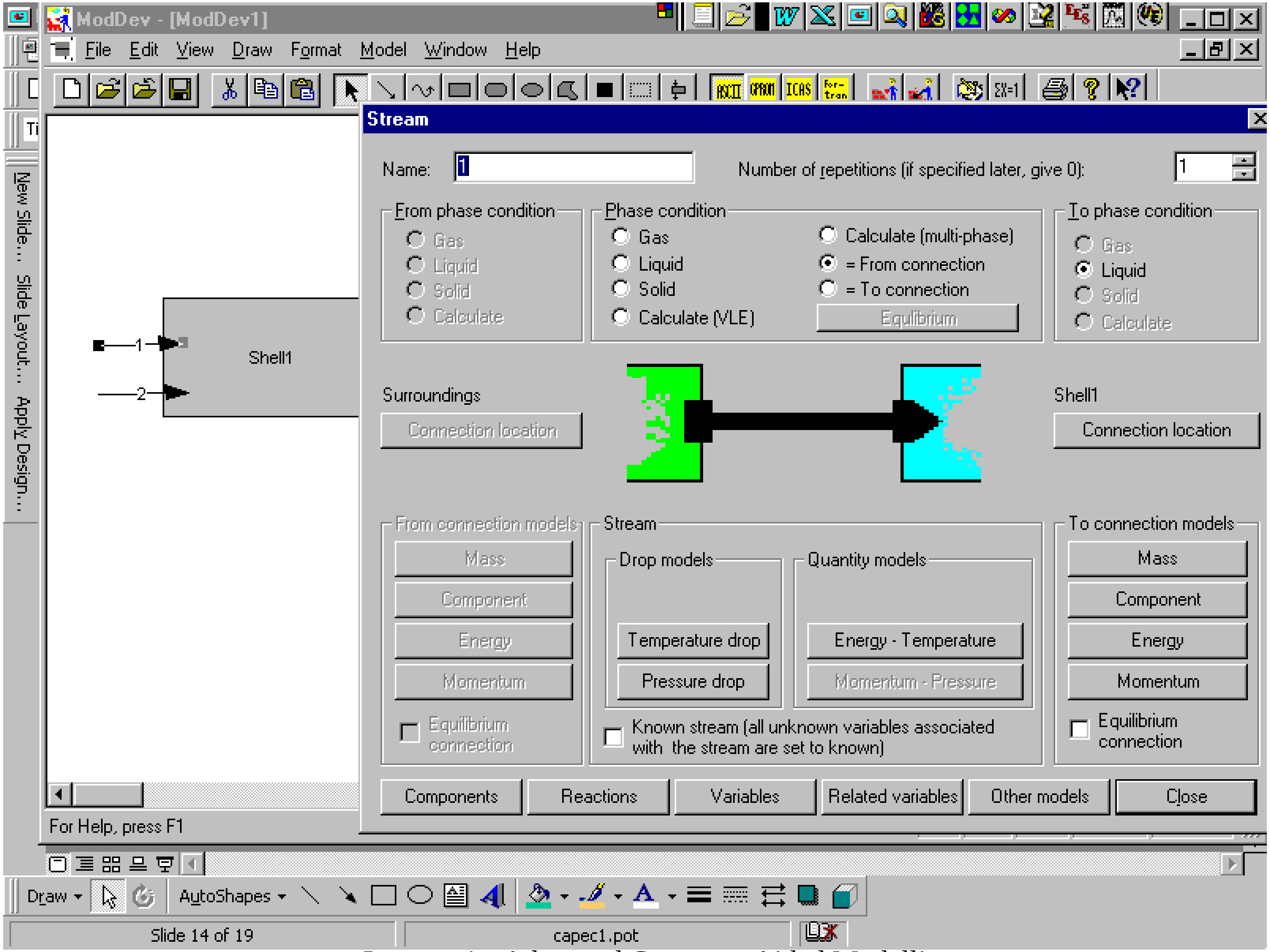
Tools & options in ModDev (ModGen)



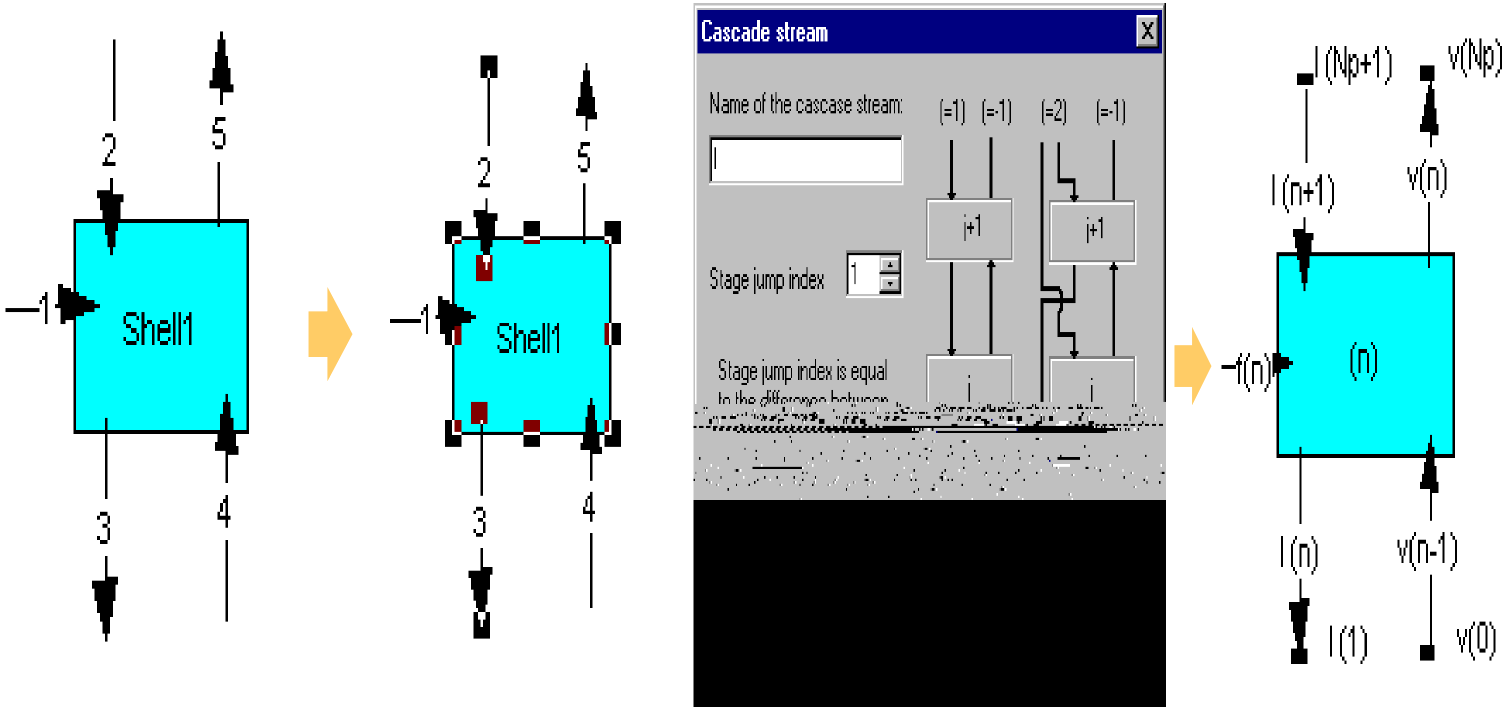
Tools & options in ModDev (ModGen) - define shell



Tools & options in ModDev (ModGen) -define stream



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

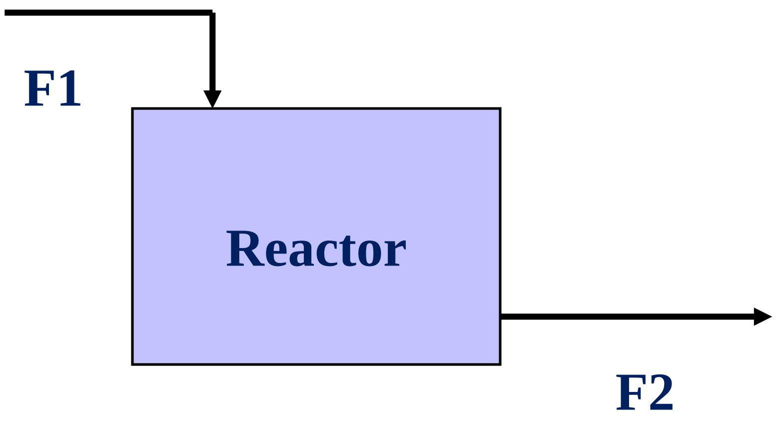
Equations	No.	Type
$d = f_{1i}\,(x_i, y_i, z_i, F, L, V);\ i=1,NC$	(1)	Balance Equations
$D = f_2\,(F, L, V, h_F, h, H, Q)$	(2)	
$0 = g_1\,(x, y, K)$	(3)	Constraint Equations
$K_i = g_{2i}\,(y, x, T, P)\ ;\ i=1,NC$	(4)	Constitutive Models
$h = g_3\,(x, T, P)$	(5)	
$H = g_4\,(y, T, P)$	(6)	

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

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

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

Construction of an operation model



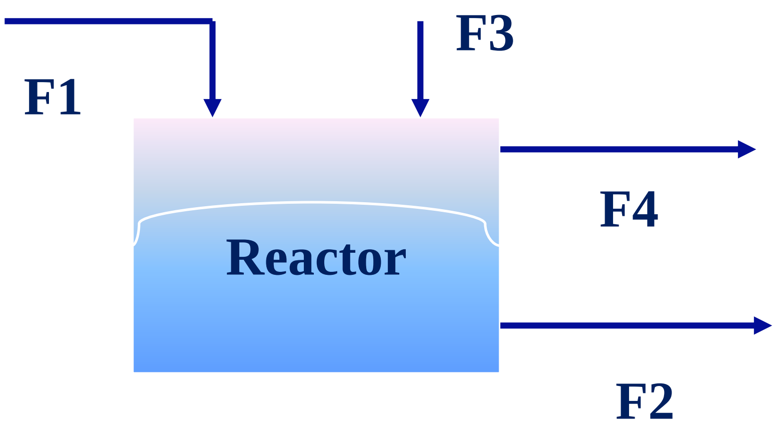
Reaction : $A \rightarrow B$

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 ≥ 0.9
6. …….

Construction of an operation & design model



Reaction : A $\rightarrow$ B

Maximum conversion of 50% A at T = 340 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 tutoria-4-II.pdf, extension to a CSTR is included.