Lecture 5b: Analysis of Process Models

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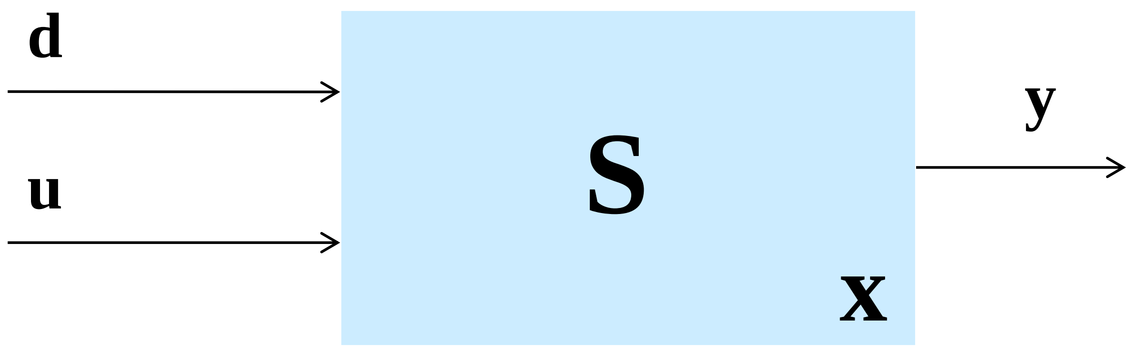
Overview: Topics to be covered

- Model analysis
  - LTI
  - Stability analysis
- Model reduction
- Model simplification

Model analysis: Problem statement

- **Clear statement of inputs, outputs and goal.**
  - algorithmic problem statement used:
    - GIVEN input data, model, …
    - FIND/COMPUTE outputs, characteristics, …
    - USING a chosen method or procedure
- **Classes of problems**
  - Decision problem (Yes/No)
  - Search problem (compute)

The Process System



- Inputs, **u**
- Outputs, **y**
- States, **x**
- Disturbances, **d**
- **y = S[u,d]**
- SISO, MIMO
- SS or dynamic
- lumped or distributed

Experimental Design for Parameter Estimation

Data acquisition & analysis

Static models

- number of measurements
- test point spacing
- test point sequencing

Dynamic models (…in addition)

- sampling time selection
- Excitation level (frequency content)

Input-Output Models

- Contains only **input** and **output** variables and their derivatives

- For an LTI* system we may use:
  - linear differential equations. (higher order)
  - impulse response function
  - transfer function (frequency domain)

**** LTI: Linear Time Invariant***

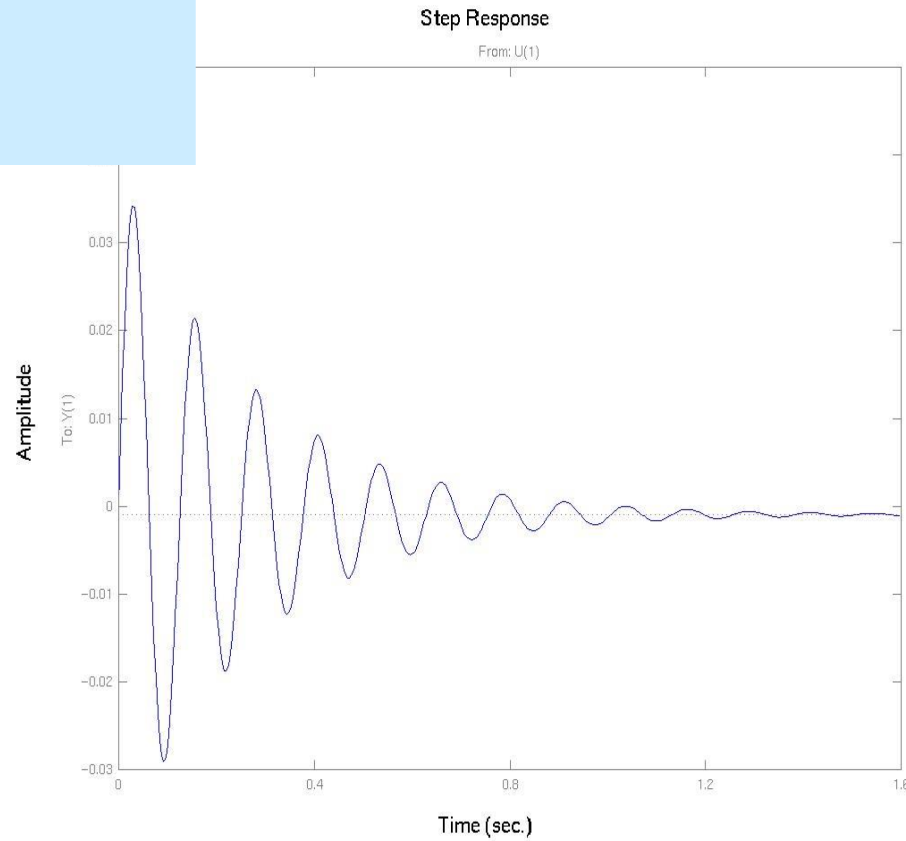
Example of step test of model

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -7.1847 & -50.0415 \\ 50.0415 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \end{bmatrix} u$$

$$y_1 = \begin{bmatrix} 1.9558 & -0.04761 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Model

Set-up the above DAE model to obtain the response shown on the right



Linear System Models

Advantages:

- Superposition concept applies
- Wealth of powerful mathematical tools
- Initial conditions zero when written in terms of deviation variables
- Simpler to analyze and solve

LTI State-Space Models

$$\dot{x}(t) = Ax(t) + Bu(t) + Ed(t)$$
$$y(t) = Cx(t) + Du(t) + Fd(t)$$

Linear model

A = nxn state matrix
B = nxr input matrix
C = mxn output matrix
D = mxr input-to-output coupling matrix
E = nxv disturbance input matrix
F = mxv disturbance output matrix
with constant matrices
(A,B,C,D,E,F) is a realization (which is **not** unique)

Multivariable Linearization

1. Original model:

$$\frac{dx}{dt} = f(x)$$

or

$$\frac{dx_1}{dt} = f_1(x_1,\ldots,x_n)$$
$$\frac{dx_2}{dt} = f_2(x_1,\ldots,x_n)$$
$$\frac{dx_n}{dt} = f_n(x_1,\ldots,x_n)$$

2. Expand ODEs about $(x_{1_0}, x_{2_0},\ldots, x_{n_0})$

$$\frac{dx_1}{dt} \cong f_1(x_0) + \frac{\partial f_1}{\partial x_1}\Big|_{x_0}(x_1 - x_{1_0}) + \ldots + \frac{\partial f_1}{\partial x_n}\Big|_{x_0}(x_n - x_{n_0})$$
$$= f_1(x_0) + \sum_{j=1}^{n} \frac{\partial f_1}{\partial x_j}\Big|_{x_0}(x_j - x_{j_0})$$
$$\frac{d\hat{x}_1}{dt} = \sum_{j=1}^{n} \frac{\partial f_1}{\partial x_j}\Big|_{x_0}\hat{x}_j$$

3. Final form:

$$\frac{d\hat{x}_1}{dt} = \sum_{j=1}^{n} \frac{\partial f_i}{\partial x_j}\Big|_{x_0}\hat{x}_j$$

$$\mathrm{i} = 1,\ldots,\mathrm{n}$$

$$\frac{d\hat{x}}{dt} = J\hat{x}$$

$$J = \left(\frac{\partial f_i}{\partial x_j}\right)$$
$$i, j = 1,\ldots n$$

Linearized Nonlinear State Space Models

General nonlinear model:

$$\frac{dx}{dt} = f(x(t), u(t), p)$$

$$y(t) = g(x(t), u(t), p)$$

Note: The structure of the model is defined by the structure of matrices ([A],[B],[C],[D])

Linearized model:

$$\dot{x}(t) = Ax(t) + Bu(t)$$

$$y(t) = Cx(t) + Du(t)$$

$$A_{ij} = \left(\frac{\partial f_i}{\partial x_j}\right), \quad B_{ij} = \left(\frac{\partial f_i}{\partial u_j}\right)$$

$$C_{ij} = \left(\frac{\partial g_i}{\partial x_j}\right), \quad D_{ij} = \left(\frac{\partial g_i}{\partial u_j}\right)$$

Stability of systems - overview

- Two stability notions
  - bounded input bounded output (BIBO)
  - asymptotic stability

- Testing asymptotic stability of LTI systems
- MATLAB functions (e.g. eig(A))
- Stability of nonlinear process systems
  - Lyapunov's principle

BIBO Stability

A system is said to be “bounded input, bounded output (BIBO) stable” if it responds with a bounded output signal to any bounded input signal, i.e.

Actuator (manipulated or design) variable

$$\text{if} \quad y = \mathbf{S}[u] \quad \text{then}$$

$$\| u \| \Rightarrow \| y \|$$

where $\| . \|$ is a signal norm.

Measured (controlled or process) variable

BIBO stability is external stability

Asymptotic Stability

A system is said to be "asymptotically stable" if for a "small" deviation in the initial state the resulting "perturbed" solution goes to the original solution in the limit, i.e.

$$\text{whenever } \| x_0 - x_0^0 \| \leq \delta \text{ then}$$

$$\| x(t) - x^0(t) \| \to 0 \text{ if } t \to \infty$$

where $\| . \|$ is a vector norm.

asymptotic stability is internal stability

Asymptotic Stability of LTI Systems

A LTI system with state space realization matrices (A,B,C) is asymptotically stable if and only if all the eigen-values of the state matrix A have negative real parts, i.e.

$$\mathrm{Re}\{\lambda_{\mathrm{i,A}}\} < 0 \;\; \text{for all} \;\; i$$

asymptotic stability is a system property

Example

Model equations

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -7.1847 & -50.0415 \\ 50.0415 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \end{bmatrix} u$$

$$y_1 = \begin{bmatrix} 1.9558 & -0.04761 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Analysis

$$A = [-7.1847\ -50.0415;\ 50.0415\ 0];$$

$$eig(A)$$

$$-3.5924 + 49.9124i$$

$$-3.5924 - 49.9124i$$

Stable!

Model (Simplification and) Reduction

LTI models with state space representation

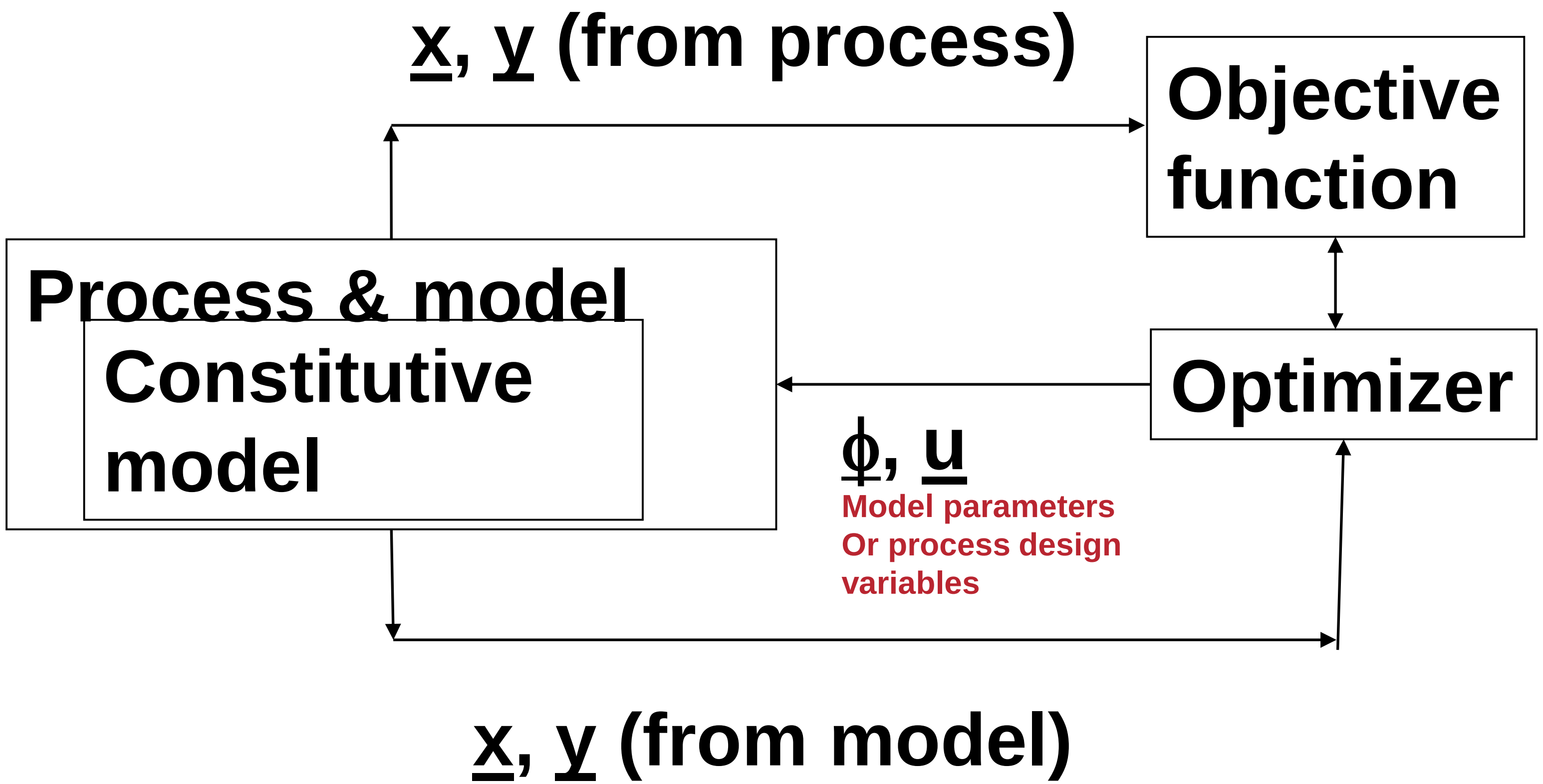
$$\frac{dx}{dt} = \mathbf{A}x + \mathbf{B}u \quad , \quad y = \mathbf{C}x$$

States can be classified into:

- **slow** modes ("small" negative eigenvalues)
  states essentially constant
- **fast** modes ("large" negative eigenvalues)
  go to steady state rapidly
- **medium** modes

Modeling issues -3

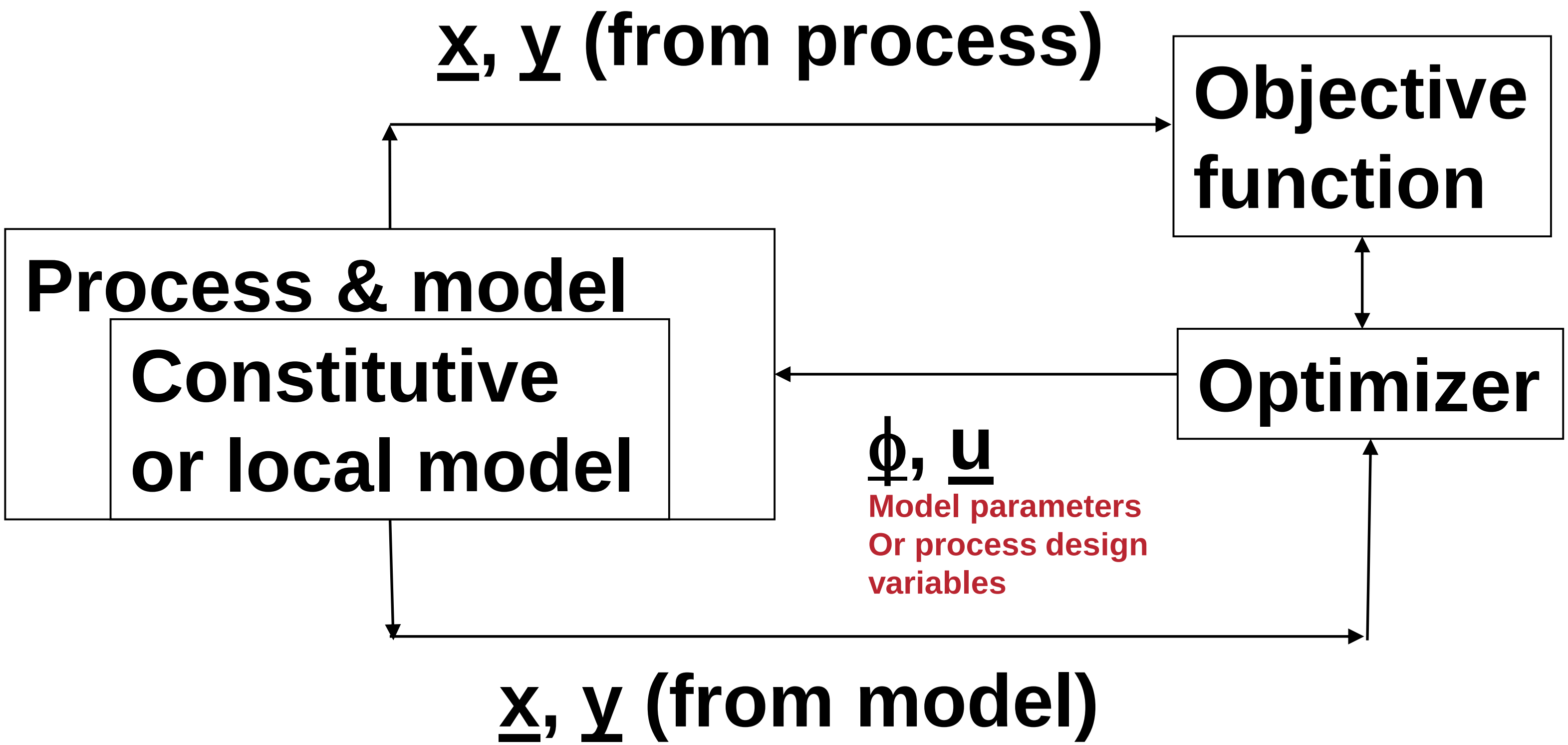
Identification & use of models



$\underline{\phi}$ **(optimization variables for parameter estimation – data driven modeling);** $\underline{u}$ **(design variables for process optimization)**

Modeling issues - 4

Local models

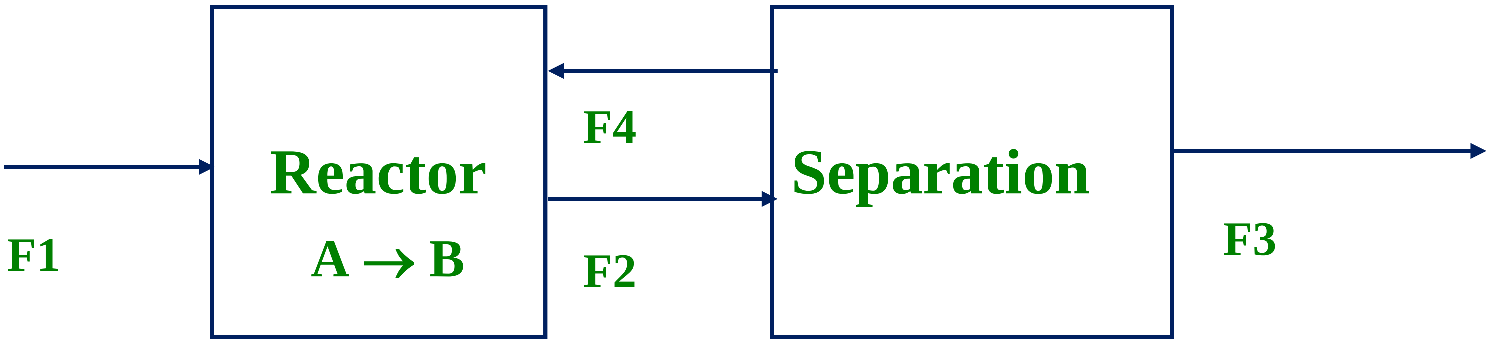


Local model used only for (in inner loop to reduce time)

$\Delta y = J^{-1}F$

In 1980s by Macchietto; Hertzberg; Gani

Model Simplification



$$F_2 = \frac{F_1(x_{4i} - x_{3i})V_R k}{x_{4i}V_R k - F_1(x_{1i} - x_{3i})} = \frac{x_{2i}V_R k + F_1(x_{4i} - x_{1i})}{x_{4i} - x_{2i}}$$

$$F_2 = \frac{F_1 V_R k}{V_R k - F_1} = \frac{x_{2A} V_R k}{1 - x_{2A}}$$

Set $D_a = (V_R k) / F_1$

$$\frac{F_2}{F_1} = \frac{(V_R k) / F_1}{(V_R k) / F_1 - 1}$$

$$F_2 = \frac{F_1 D_a}{D_a - 1}$$

Note: For a fixed value of D_a close to 1, a small disturbance in F_1 produces a large change in F_2

Model Reduction

Reduce the number of equatons representing the model by:

- by neglecting some effects
- by reducing the number of discretization points
- by lumping of variables and equations

Side effects:

Equation set may become more sensitive;

Model reduction: Example

Stability analysis

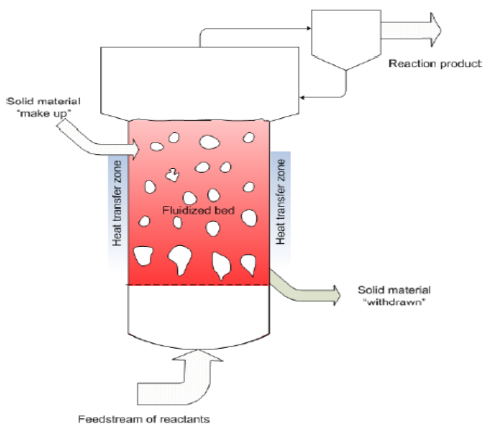
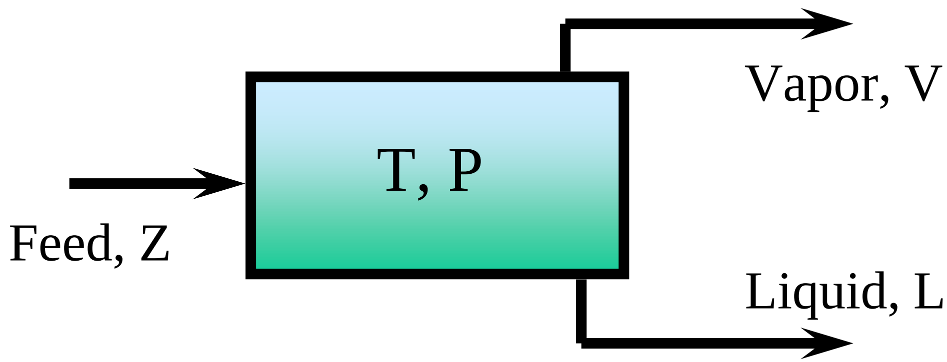


Figure 4.1 Catalytic fluidized bed reactor.

- Multiple steady states
- Unstable state

	1st SS	2nd SS	3rd SS
p_p	0.0935	0.06694	0.00653
p	0.09352	0.06704	0.00682
T_p	690.72	759.167	915.13
T	690.45	758.35	912.8
λ_1	-2187.2494513	-2189.306306	-2258.0244252
λ_2	-270.55715028	-270.5775586	-270.60246532
λ_3	-0.9120340679	-1.256116493	-12.560859964
λ_4	-6.4105069E-03	5.6925189E-03	-7.379499E-03

Model Reduction – 2 (example)



$$x_i\, \varphi_i^L = y_i\, \varphi_i^V \qquad i = 1,\ldots.NC$$

$$\Sigma_i\, x_i = \Sigma_i\, y_i = \Sigma_i\, z_i = 1$$

$$Z\, z_i = V\, y_i + L\, x_i \quad i = 1,\ldots.NC$$

The constitutive model provides the fugacity coefficients and derivatives

Model Reduction – 2 (SRK EOS)

$$P = RT/(V-b) - a/[(V + \varepsilon\, b)(V + \sigma b)]\ \text{, or,}$$

$$Z = V/(V-b) - (a\, V)/[RT(V + \varepsilon\, b)(V + \sigma b)]$$

a & b are parameters that need to be defined through mixing rules eg.,

$$a = \Sigma_i \Sigma_j x_i x_j a_{ij};\quad b = \Sigma_i\, x_i b_i\,;\ m_i = m(\omega)$$

$$a_{ij} = (a_{ii} a_{jj})^{1/2}(1 - k_{ij})\quad ;\ b_i = \psi_B\, RT_{ci}/P_{ci}$$

$$a_{ii} = \psi_A\, (R^2\, T_{ci}^{\,2}/P_{ci})[1 + m_i\, (1 - T_{ri})^{1/2}]^2$$

ψ_A, ψ_B, $m(\omega)$, ε, & σ also need to be defined (these values are different for different EOS)

ln φ_i (fugacity coefficient) is computed from T, P & $\underline{x}$ or, independent of $\underline{x}$ in terms of a and b parameters

Model Reduction – 3 (reduction method)

*** Verify if constitutive variables can be estimated independent of compositions using the operators**

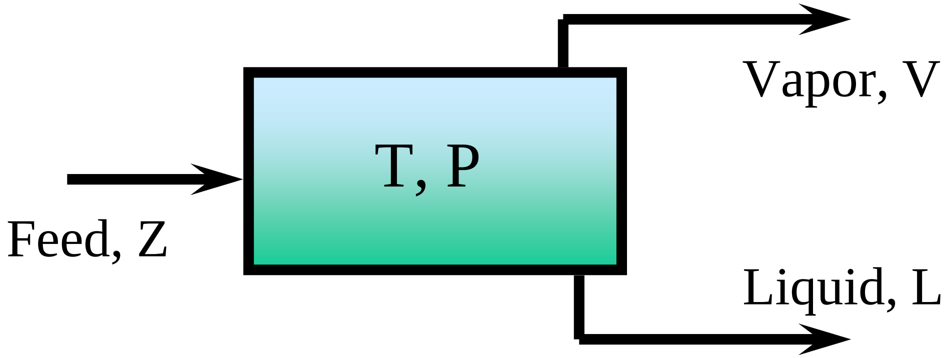
a $= \sum x_i \alpha_i$; **b** $= \sum x_i \beta_i$; ……..

- **multiply balance equations with the pure component parameters α_i ;**
- **sum for all components;**
- **replace summation term with operator a. Repeat for all operators**

*** Using only the operators a & b, NS(NC+2) equations is replaced by NS(2+2) equations independent of the number of components in the system (NS = number of stages; NC = number of compounds)**

Gani & O'Connell (2001)

Model Reduction – 4 (new reduced model)



Known: a_z, $\underline{z}$, T, P, $\underline{\alpha}$, $\underline{b}$

Solve Eqs 1-3 for

a_x, b_x & β

$$x_i\,\varphi_i^L = y_i\,\varphi_i^V \qquad i = 1,\ldots.NC$$

$$\Sigma_i\, x_i = \Sigma_i\, y_i = \Sigma_i\, z_i = 1$$

$$Z\, z_i = V\, y_i + L\, x_i \qquad i = 1,\ldots.NC$$

NC+1 equatons reduced to 2+1 equations (not counting energy balance)

$$a_Z - \beta\, a_y - (1-\beta)\, a_x = 0 \qquad (1)$$

$$b_Z - \beta\, b_y - (1-\beta)\, b_x = 0 \qquad (2)$$

$$\sum (K_i - 1) z_i \,/\, (1 + \beta\,(K_i - 1)) = 0 \qquad (3)$$