Lecture 5a: Model Analysis - Lumped Parameter & DPS Models

Rafiqul Gani
(Plus material from Ian Cameron)

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

www.pseforspeed.com

Key issues to consider

- **Must analyze before solving**
  - Degrees of freedom analysis
  - Incidence matrix; singularity of equation system; index-number
  - Stability of the model

Degrees of freedom analysis - 1

Classify equations

Algebraic equations (AEs)

- **explicit (a = b*x + c with b, c, x as known)**
- **implicit (0 = b*x(a) + c – a with b, c as known)**

Ordinary differential equations (ODEs)

- **first order ODEs ($d\underline{y}/dt = f(\underline{y}, t)$)**

Partial differential equations (PDEs)

- **time plus one-three spatial directions for different coordinate systems**

Note: Mathematical model can have any combination of above

Degrees of freedom analysis - 2

Classify variables

- **Known**
  - **variables fixed by system**
  - **variables fixed by problem**
  - **variables fixed by model**
- **Unknown**
  - **dependent (differential)**
  - **dependent (partial differential)**
  - **implicit (algebraic)**
  - **explicit (algebraic)**
- **Independent**
  - **time, length, ..**

Degrees of freedom analysis - 3

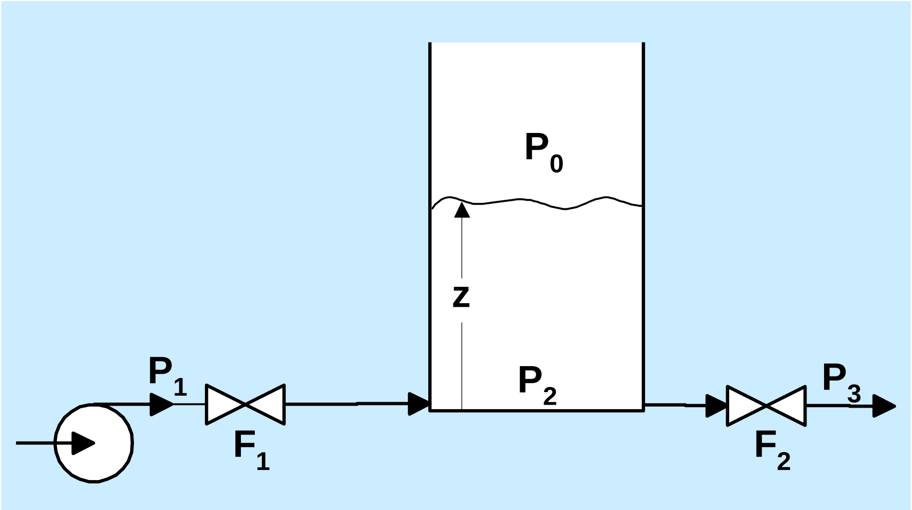
Definition (N_{DF} or N_S; degrees of freedom or number of variables to specify):

$$N_{DF} = N_V - N_E \quad \textbf{OR} \quad N_S = N_V - N_U$$

- N_V = total number of variables (not counting independent variables)
- N_U = number of unknown variables
- N_E = number of independent equations

Assign dependent (partial) to PDEs; dependent (differential) to ODEs; implicit & explicit algebraic to AEs

Example DoF analysis



Introduction to MoT

- **Model construction**
- **Model analysis**

Model

$$\frac{dz}{dt} = \frac{(F_1 - F_2)}{A}$$

$$F_1 - C_V\sqrt{P_1 - P_2} = 0$$

$$F_2 - C_V\sqrt{P_2 - P_3} = 0$$

$$P_2 - P_0 - \rho g z = 0$$

DOF analysis

State (dependent-differential) variable $= z$

Algebraic variables $= F_1, F_2, P_0, P_1, P_2, P_3$

Parameters $= \mathrm{C_V}, A, \rho$

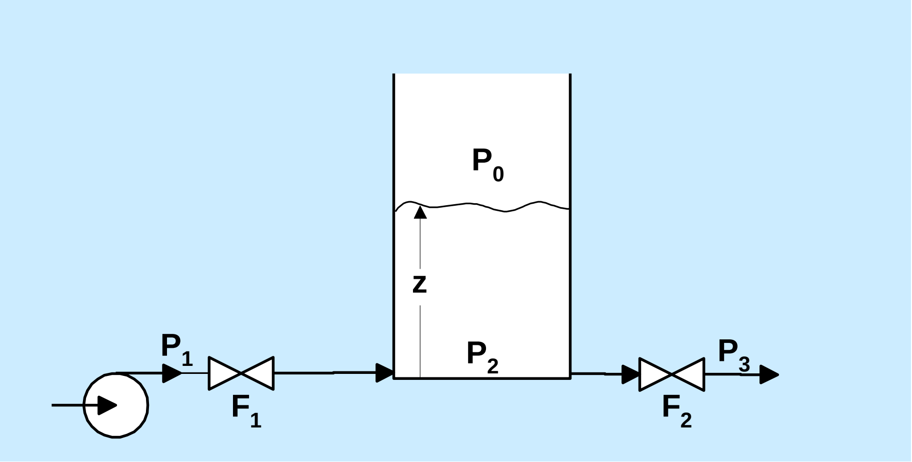
Constants $= g$

Equations $= 1 + 3$

$N_{DF} = N_V - N_E = 11 - 4 = 7$

Assign *z* to ODE; *C_v*, *A*, *ρ*, *g* as fixed by system; select 3 variables from ”algebraic” as fixed & 3 as unkown

Different specifications (DoF selection)



Select 3 variables from "algebraic" as fixed, making the remaining 3 as unknown and assigned to the AEs

Specification 1

$$S_1 = [P_0, P_1, P_3]$$

	F_1	F_2	P_2
g_1	x		x
g_2		x	x
g_3			x

Specification 2

$$S_2 = [P_0, P_1, P_2]$$

	F_1	F_2	P_3
g_1	x		
g_2		x	x
g_3			

Unsolvable system?

High index DAEs

- Only for Differential-algebraic equations (for PDEs, first discretize the PDEs)
- Pure ODE systems are index 0
- Many index 1 DAE solvers
- Few higher index solvers
- Ensure index 1 models are used

DAE index definition

- The "index" of the DAE system is the number of times the algebraic sub-system must be differentiated to give a set of ODEs.

General DAE system

General system

$$\frac{dy}{dt} = f(y,z,t)$$
$$0 = g(y,z,t)$$

Differentiate the algebraic equations

$$0 = g_y \frac{dy}{dt} + g_z \frac{dz}{dt}$$
$$0 = g_y f + g_z \frac{dz}{dt}$$
$$\frac{dz}{dt} = -g_z^{-1} g_y f \qquad iff \quad g_z \quad full\, rank$$

What is full rank?

High index example

Case 1

$$\dot{y}_1 = y_1 + y_2 + z_1$$
$$\dot{y}_2 = y_1 - y_2 - z_1$$
$$0 = y_1 + 2y_2 - z_1$$

Differentiate once

$$\dot{z}_1 = \dot{y}_1 + 2\dot{y}_2$$
$$\dot{z}_1 = 3y_1 - y_2 - z_1$$

index 1 model!

Case 2

$$\dot{y}_1 = y_1 + y_2 + z_1$$
$$\dot{y}_2 = y_1 - y_2 - z_1$$
$$0 = y_1 + 2y_2$$

Differentiate once

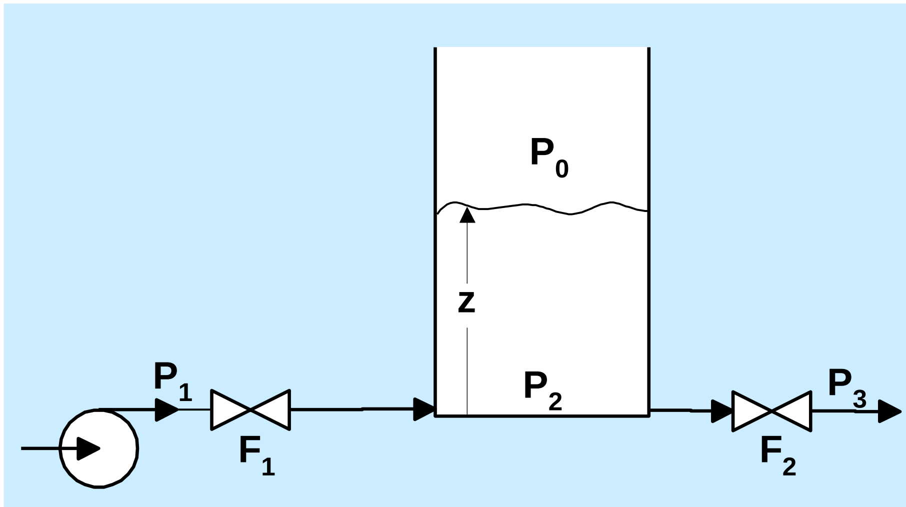
$$0 = \dot{y}_1 + 2\dot{y}_2$$
$$0 = 3y_1 - y_2 - z_1$$

and again ...

$$0 = 3\dot{y}_1 - \dot{y}_2 - \dot{z}_1$$
$$\dot{z}_1 = 2y_1 + 4y_2 + 4z_1$$

index 2 model!

What is the index of this model?



Specification 1

$$S_1 = \left[P_0, P_1, P_3\right]$$

	F_1	F_2	P_2
g_1	x		x
g_2		x	x
g_3			x

Model

$$\frac{dz}{dt} = \frac{(F_1 - F_2)}{A}$$

$$F_1 - C_V\sqrt{P_1 - P_2} = 0$$

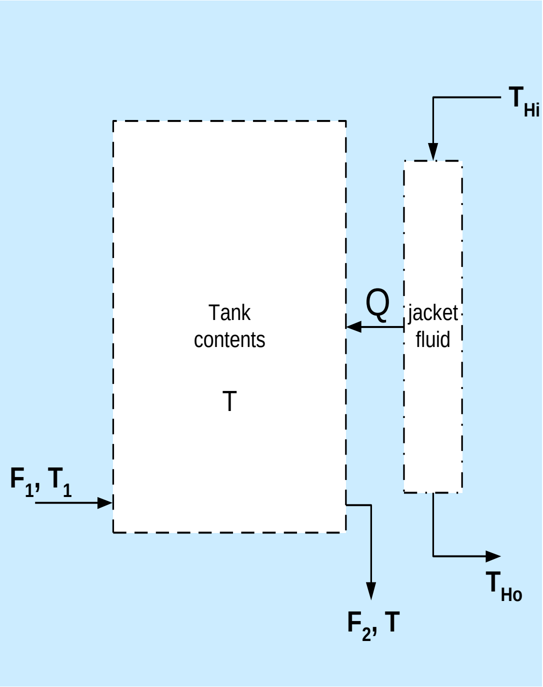
$$F_2 - C_V\sqrt{P_2 - P_3} = 0$$

$$P_2 - P_0 - \rho g z = 0$$

- **Insert F1 and F2 into Eq. 1**
- **Differentiate Eq. 4 with respect to t**
- **What happens if P_0, P_1, P_2 are specified?**

Exercise - 4 : What is the index of this model?

System



Tank

Conservation

$$\frac{dH}{dt} = Q + F_1\hat{h}_1 - F_2\hat{h}_2$$

Constitutive

$$Q = UA(T_H - T)$$

$$\hat{h}_1 = f(T_1, P)$$

$$\hat{h}_2 = f(T_2, P)$$

$$H = Mc_PT$$

$$A = \pi Dz$$

Jacket

Conservation

$$\frac{dH_J}{dt} = F_H\hat{h}_{Hi} - F_H\hat{h}_{Ho} - Q$$

Constitutive

$$Q = F_H c_{PH}(T_{Hi} - T_{Ho})$$

$$\hat{h}_{Hi} = f(T_{Hi}, P)$$

$$\hat{h}_{Ho} = f(T_{Ho}, P)$$

$$H_J = M_{HJ}c_{PH}T_H$$

$$T_H = (T_{Hi} + T_{Ho})/2$$

Stability of the model

❖ Indicated by the dynamic modes

- time constants of the system

$$\tau_i \propto \frac{1}{\lambda_i}$$

- related to physico-chemical phenomena
  - •fluid flow (generally fast)
  - •mass transfer rates (can be slow)
  - •heat transfer (usually slow)
  - •reaction kinetics (very fast to very slow)

Linear model analysis

Linear equation system

$$y' = Ay + \phi$$

$$\begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \begin{pmatrix} -2000 & 999.75 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \begin{pmatrix} 1000.25 \\ 0 \end{pmatrix}$$

Solution given by

$$y_1(t) = -1.449e^{-0.5t} + 0.499e^{-2000.5t} + 1$$

$$y_2(t) = -2.999e^{-0.5t} - 0.0025e^{-2000.5t} + 1$$

Slow mode (component)   Fast mode (component)

Computing eigen-values of the J-matrix

- In MoT, write the ODE system; and then ask for calculation of the eigen-values
- For problem of slide 13, the solution is:

Two eigen-values
(-2000.5, -0.5)

Solution with MATLAB

```
» A=[-2000 999.75;1 -1];
» b=eig(A)

b =

  1.0e+003 *

   -2.0005
   -0.0005
```

General linear system analysis

$$\frac{dx}{dt} = Ax, \qquad x(0) = x^0$$

Linear set of equations

$$x(t) = Z\exp(\lambda t)$$

Solution to the equations

$$x_i(t) = \sum_{j=1}^{n} Z_{ij} e^{\lambda_j t}$$

Individual component solution to the equations
– note the eigenvalues !
– note the eigenvectors !

$$where:$$

$$Z_{ij} = \sum_{k=1}^{n} V_{ij} \left(V^{-1}\right)_{jk} x_k^0$$

The eigen-values contain the stability information

Eigen-value analysis

- Dynamic modes determined by eigen-values of the linear system

- Nonlinear problems must be linearised first to get Jacobian J(y,t) on the trajectory

- Eigen-values of Jacobian computed using MoT or MATLAB eig(A) or similar function.

Behaviour of linear systems

- Phase plane analysis illustrates motion of system
- Second order systems plot $y_1 \text{ vs } y_2$ or $\dot{y} \text{ vs } y$
- Typical second order system (cf. valve actuator) :

$$\ddot{y} + a\dot{y} + by = 0$$

$$with$$

$$\lambda_1 = \left\{-a + \sqrt{\left(a^2 - 4b\right)}\right\}/2$$

$$\lambda_2 = \left\{-a - \sqrt{\left(a^2 - 4b\right)}\right\}/2$$

Set $y_1 = dy/dt = \dot{y}$

$y_2 = dy_1/dt = d^2y/dt = \ddot{y}$

So,

$y_2 + a\, y_1 + by = 0$

Therefore,

$dy/dt = y_1$

$dy_1/dt = -\,(a\, y_1 + by)$

Phase plane analysis

- Several cases dependent on eigen-values

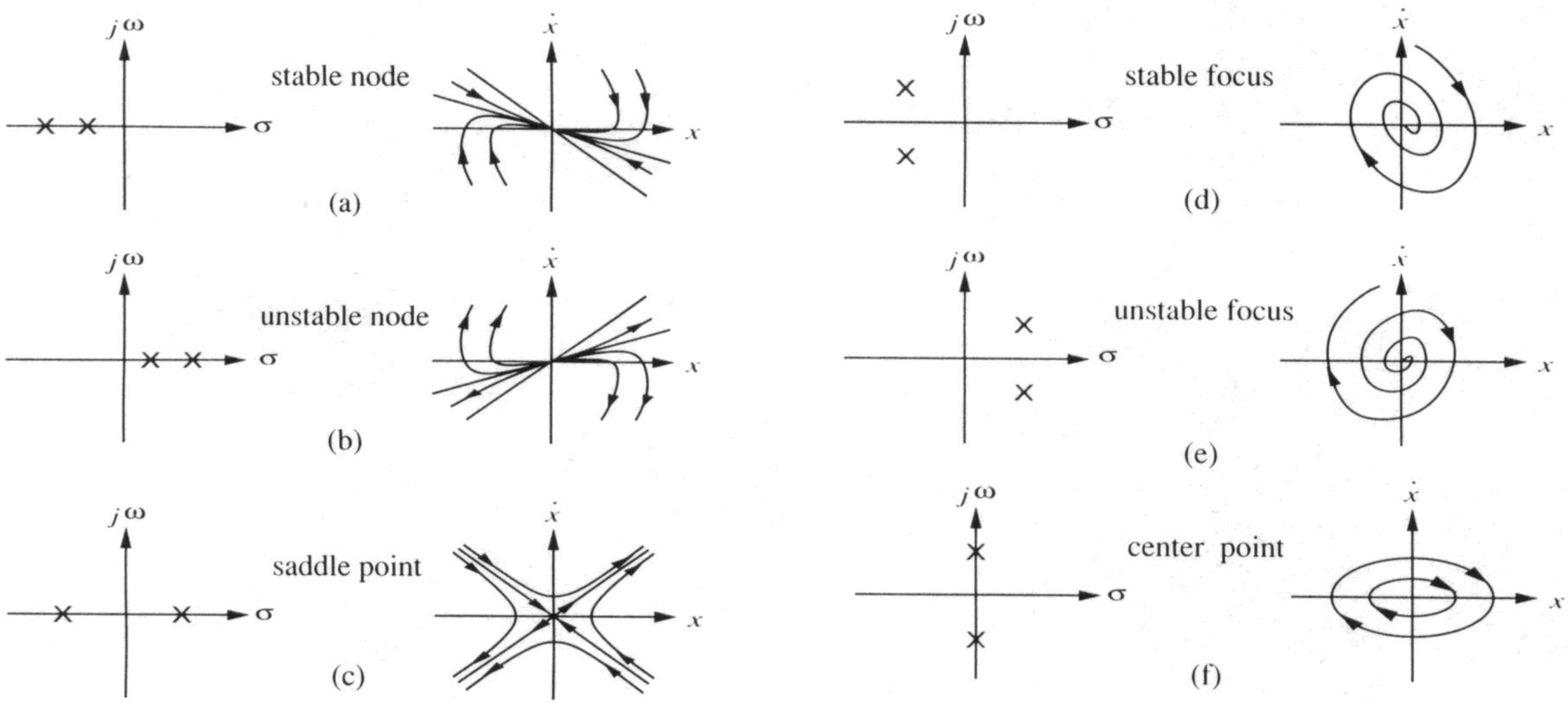
λ_1 and λ_2 both real and same sign

λ_1 and λ_2 both real but opposite sign

λ_1 and λ_2 complex conjugates with non-zero real parts

λ_1 and λ_2 complex conjugates with zero real parts

Phase plane diagrams



General nonlinear model

- Linearize at some point $y' = f(y,t)$

- Obtain linear model $y' = A(y - g(t)) + f(t, g(t))$

- Solution is $y(t) = \sum_{i=1}^{n} c_i e^{\lambda_i t} v_i + g(t)$

Derive the linear model and solution for:
$dy_1/dt = y_1 * y_2 + (y_1)^2$
$dy_2/dt = y_1 + (y_2)^2$

Stability cases

- Stable model $\lambda_i \leq 0 \text{ for all i}$
- Unstable model $\text{Some } \lambda_{\mathrm{i}} \text{ will be} > 0$
- Ultra-stable (“stiff”)

$$\lambda_i \leq 0$$

$$\text{Some } \lambda_{\mathrm{i}} \text{ "small"}$$

$$\text{Some } \lambda_{\mathrm{i}} \text{ "large"}$$

Stability implications for numerical solution

- The problem determines the choice of numerical method
- "Stiff" problems need special attention
- All simple explicit methods have limitations on allowable step lengths

$$h_{\max} = \frac{\text{method stability bound}}{\lambda_{i_{\max}}}$$

Multiscale, lumping, simplification, stability: Example

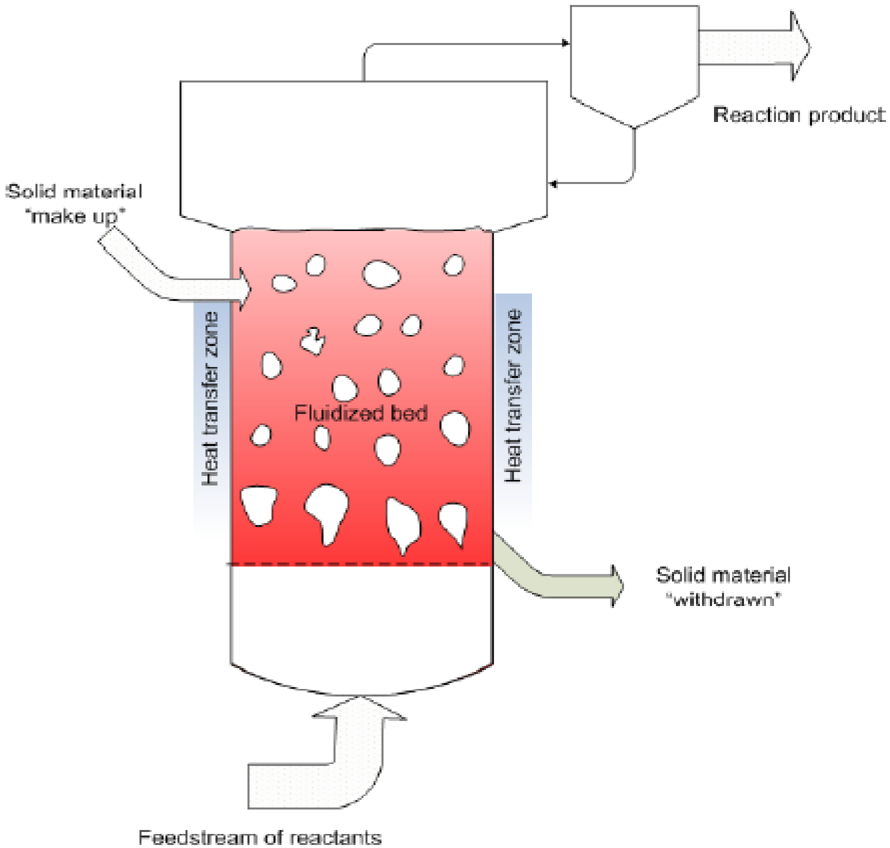


Figure 4.1 Catalytic fluidized bed reactor.

- Fluid zone
- Particle zone
- Heat transfer zone
- Catalyst recovery zone

Luss, D. and Amudson, N.R. (1968). Stability of Batch Catalytic Fluidized Beds. *AIChE Journal*. 14, 211.

Multiscale, lumping, simplification, stability: Example

Multiscale balance relations

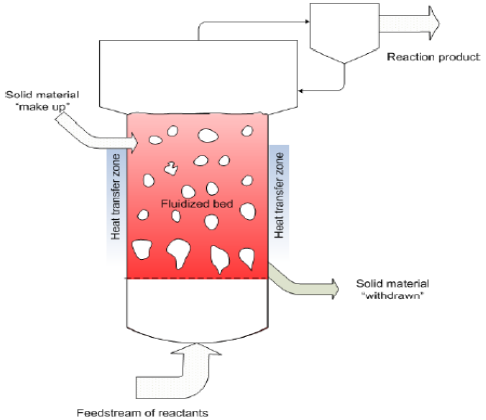


Figure 4.1 Catalytic fluidized bed reactor.

$$f_1\left(p_p, p\right)=\frac{dp}{d\tau}=p-p_e+H_g\left(p_p-p\right) \qquad 4.7$$

$$f_2\left(T_p, T\right)=\frac{dT}{d\tau}=T_e-T+H_w\left(T_w-T\right)+H_T\left(T_p-T\right) \qquad 4.8$$

$$f_3\left(p_p, p, T_p\right)=A\frac{dp_p}{d\tau}=H_g\left(p-p_p\right)-H_gKkp_p \qquad 4.9$$

$$f_3\left(T, p_p, T_p\right)=C\frac{dT_p}{d\tau}=H_T\left(T-T_p\right)+H_TFKkp_p \qquad 4.10$$

Multiscale, lumping, simplification, stability: Example

Constitutive relations

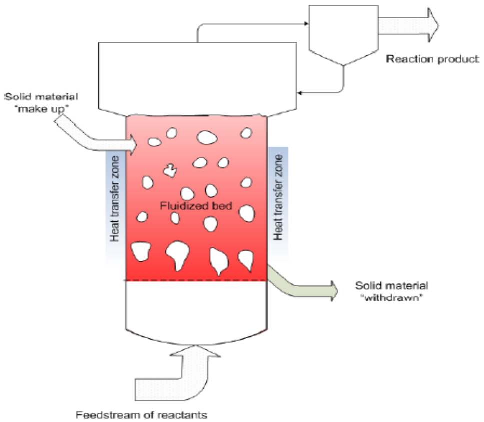


Figure 4.1 Catalytic fluidized bed reactor.

$$A = \frac{\alpha v_p a_v}{\varepsilon s_p} \qquad C = \frac{a_v c_s v_p \rho_s}{\varepsilon s_p c_g \rho_g}$$

$$F = \frac{(-\Delta H) k_g}{h_g} \qquad H_g = \frac{a_v k_g MPV}{q}$$

$$H_T = \frac{a_v h_g V}{q c_g} \qquad H_w = \frac{2 h_w V}{r c_g q}$$

$$K = \frac{\alpha v_p}{s_p k_g} \qquad \tau = \frac{q\theta}{\varepsilon \rho_g V}$$

$$(1-\varepsilon)\frac{s_p}{v_p} = a_v \qquad k = k_0 \exp\left(\frac{-\Delta E}{R T_p}\right)$$

Multiscale, lumping, simplification, stability: Example

$$f_1(p_p, p) = \frac{dp}{d\tau} = p - p_e + H_g(p_p - p)$$

$$f_2(T_p, T) = \frac{dT}{d\tau} = T_e - T + H_w(T_w - T) + H_T(T_p - T)$$

p_p

T_p

Micro-scale

Meso-scale

p

T

$$f_3(p_p, p, T_p) = A\frac{dp_p}{d\tau} = H_g(p - p_p) - H_g K k p_p$$

$$f_3(T, p_p, T_p) = C\frac{dT_p}{d\tau} = H_T(T - T_p) + H_T F K k p_p$$

Figure 4.3 Data-flow for the batch catalytic fluidized bed reactor.

Multiscale, lumping, simplification, stability: Example

Stability analysis

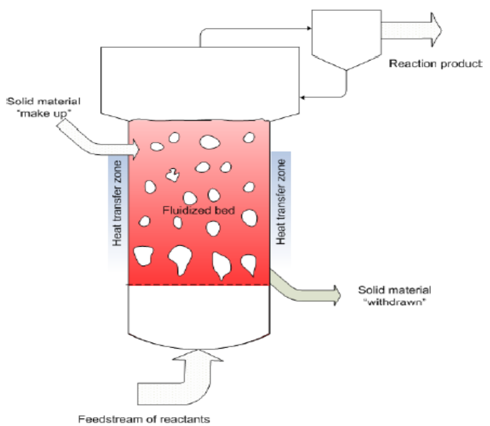


Figure 4.1 Catalytic fluidized bed reactor.

- 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