Lecture 4b: Modelling of Distributed Parameter Systems

Rafiqul Gani
(Plus material from Ian Cameron)

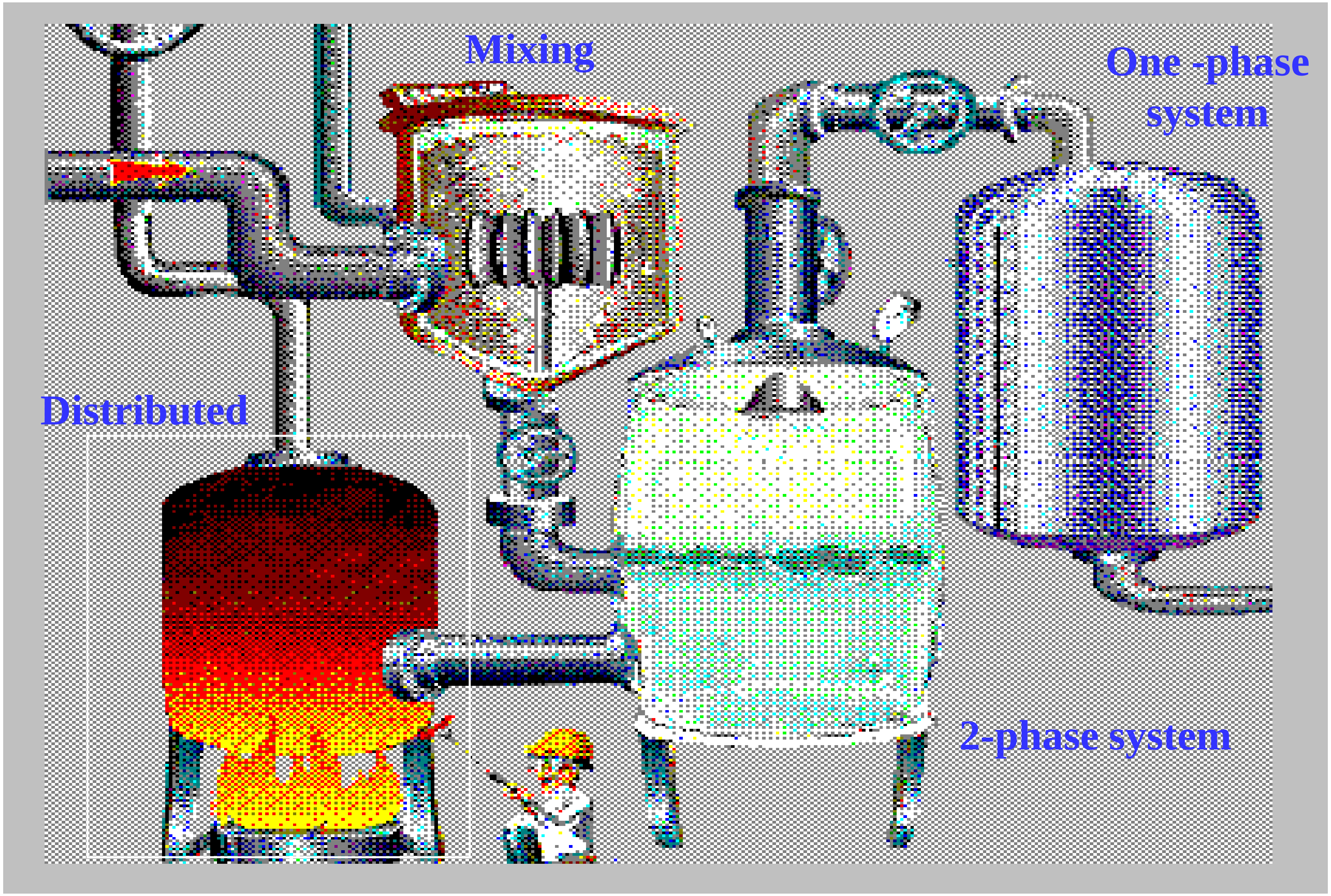
PSE for SPEED
Skyttemosen 6, DK-3450 Allerod, Denmark
rgani2018@gmail.com

www.pseforspeed.com

Overview of lecture 4b

- Origin of DPS models
- Modelling of DPS
  - Balance volumes
  - Conservation balances
  - Boundary and initial conditions
- Classification of DPS model equations
- Lumped parameter models for DPS
- Examples

The Origin of DPS Models



The Origin of DPS Models: Differential form of conservation balances

For a conserved extensive quantity Φ and its related potential φ

Flow terms:

- convective flows: $J_C = v\,\Phi$
- diffusive flows: $J_D = -D\ \textit{grad}\ \varphi$
  (assume D=constant and no cross-effect)

Co-ordinate system independent form:

$$\frac{\partial\hat{\Phi}}{\partial t} = D(\nabla^2\varphi(r,t)) - \nabla\bullet(\hat{\Phi}(r,t)v(r,t)) + \hat{q}(r,t)$$

Conservation in rectangular co-ordinates

Differential operator, rectangular co-ordinate system

$$\frac{\partial \hat{\Phi}}{\partial t} = D\left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2}\right) - \left(\frac{\partial \hat{\Phi}}{\partial x} v_x + \frac{\partial \hat{\Phi}}{\partial y} v_y + \frac{\partial \hat{\Phi}}{\partial z} v_z\right) + \hat{q}$$

"dynamic" "diffusion" "convection" "source"

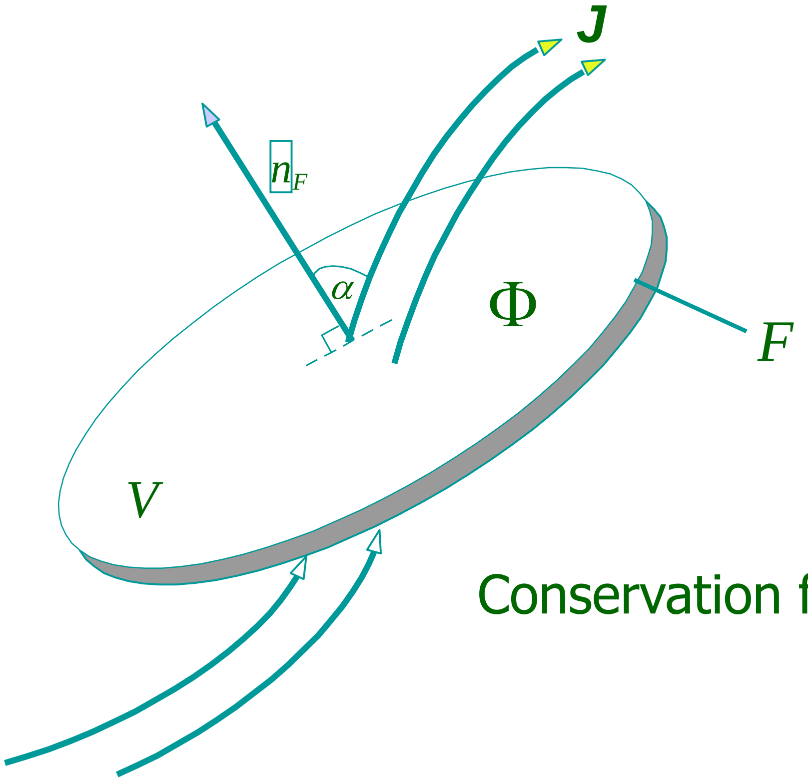
- Parabolic partial differential equation

- Induced algebraic equations
  - extensive-intensive relations
  - rate equations (transfer and reaction)

Balance volumes for DPSs

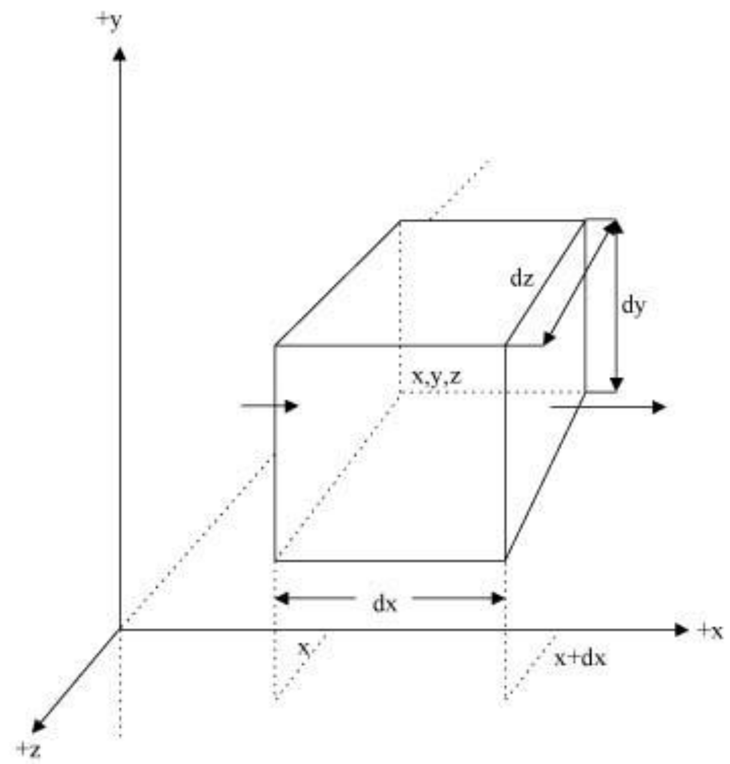
- "Distributed" balance volumes
  - uniform phase
  - uniform flow pattern
- Size of the balance volume
- Shape of the balance volumes
  - co-ordinate system
    - rectangular
    - cylindrical
    - spherical

Balance or "control" volume

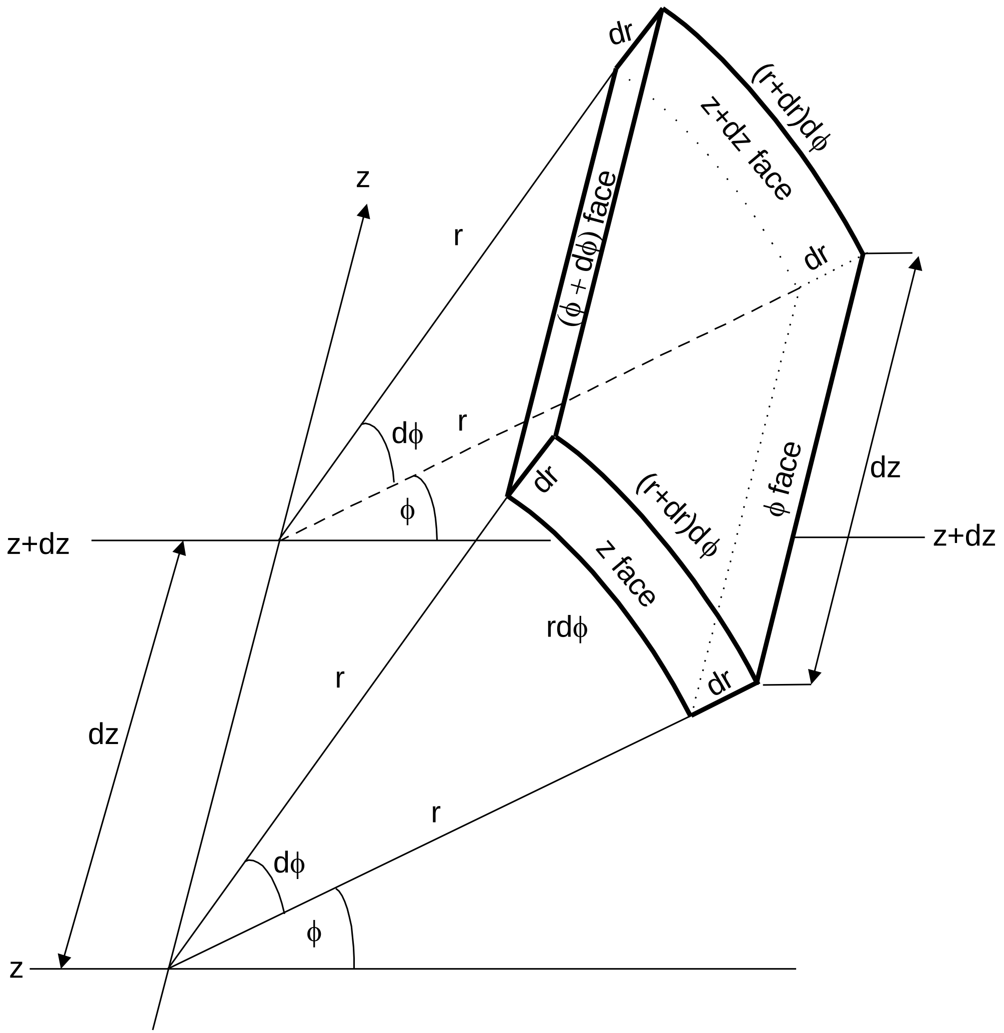


Conservation for the general balance volume

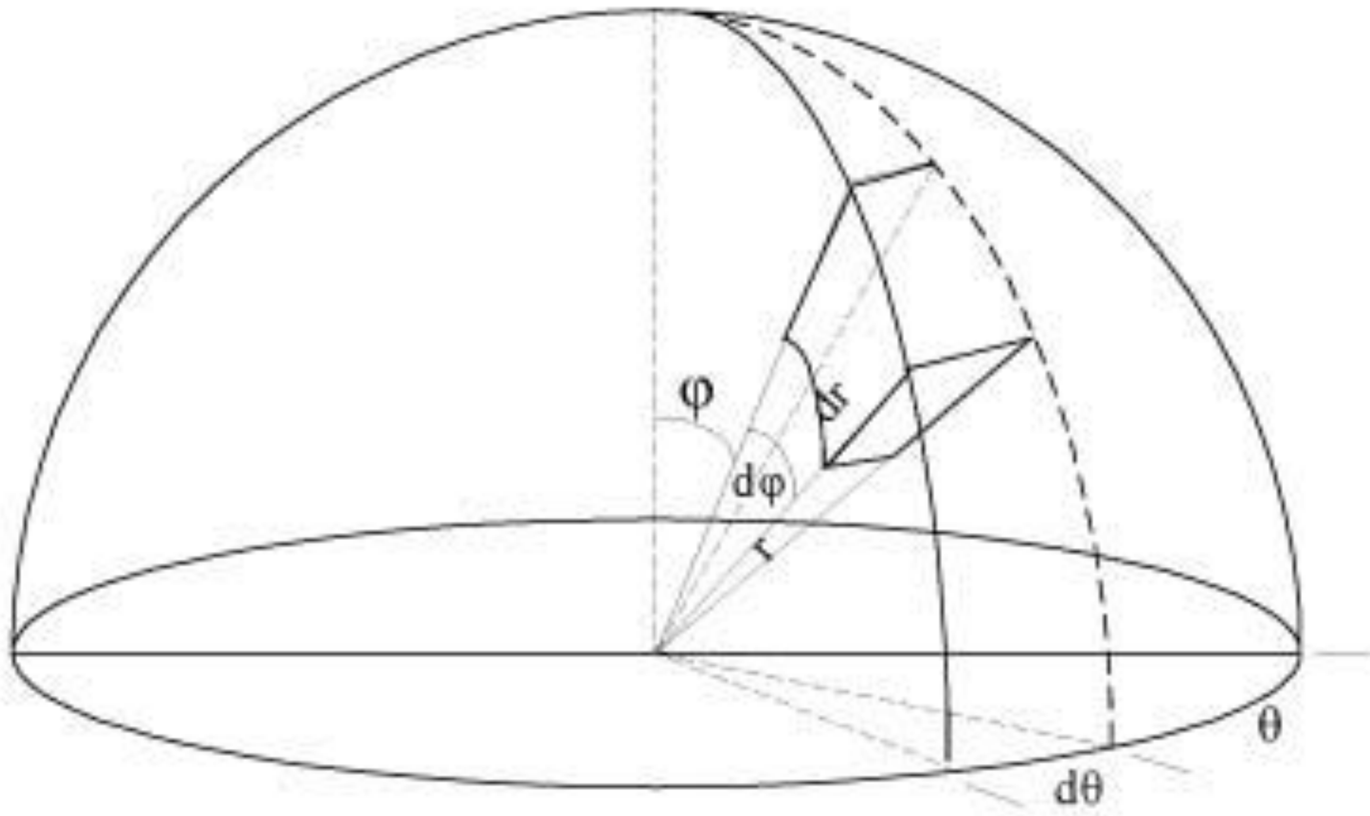
Balance Volume in rectangular co-ordinates



Balance volume in cylindrical co-ordinates



Balance volume in spherical co-ordinates



Derivation of DPS models – using microscopic balances

- Use of an arbitrary finite volume.
- Consider volume reduced to a point.
- Applicable to all geometries.
- Transformation to other co-ordinate systems is possible.

Mass balance in rectangular co-ordinates

Balance volume: $dV = dx.dy.dz$

Mass conservation within dV:

$$\frac{\partial(M)}{\partial t} = \frac{\partial(\rho.dx.dy.dz)}{\partial t} = (\rho v_x - \rho v_{x+dx}).dy.dz + (\rho v_y - \rho v_{y+dy}).dx.dz + (\rho v_z - \rho v_{z+dz}).dx.dy$$

x-direction y-direction z-direction

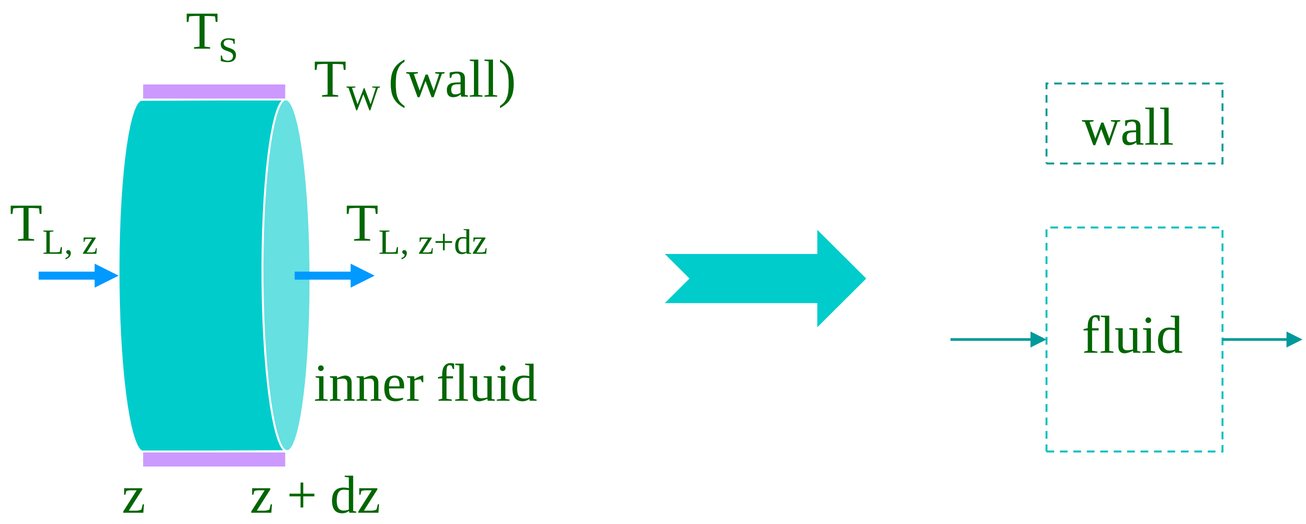
Divide by dx.dy.dz:

$$\frac{\partial(M)}{dV\partial t} = \frac{\partial \rho}{\partial t} = \frac{(\rho v_x - \rho v_{x+dx})}{dx} + \frac{(\rho v_y - \rho v_{y+dy})}{dy} + \frac{(\rho v_z - \rho v_{z+dz})}{dz}$$

In the limit:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x}\rho v_x - \frac{\partial}{\partial y}\rho v_y - \frac{\partial}{\partial z}\rho v_z = -\nabla.\rho v$$

Double pipe heat exchanger



Fluid energy conservation:

$$\frac{\partial E_L}{\partial t} = \frac{\partial (A_f \rho c_p T_L dz)}{\partial t} = F\hat{h}_{L,z} - F\hat{h}_{L,z+dz} + Q_{WL} = u\rho_L c_{PL}(T_z - T_{z+dz}) + U_L A_L dz(T_W - T_L)$$

In the limit: $$\rho_L A_f c_L \frac{\partial T_L}{\partial t} = -u\rho_L A_f c_L \frac{\partial T_L}{\partial z} + U_L A_L (T_W - T_L)$$

Double pipe heat exchanger (cont.)

Wall energy conservation:

$$\frac{\partial E_W}{\partial t} = \frac{\partial (M_W c_{pw} T_W dz)}{\partial t} = Q_{SW} - Q_{WL} = h_{SW} A_S dz(T_S - T_W) + h_{WL} A_L dz(T_W - T_L)$$

In the limit:

$$M_W c_{pw} \frac{\partial (T_W)}{\partial t} = h_{SW} A_S (T_S - T_W) + h_{WL} A_L (T_W - T_L)$$

Final:

$$\frac{\partial T_L}{\partial t} = -u \frac{\partial T_L}{\partial z} + \frac{1}{\tau_L}(T_W - T_L)$$

$$\frac{\partial T_W}{\partial t} = \frac{1}{\tau_{SW}}(T_S - T_W) - \frac{1}{\tau_{WL}}(T_W - T_L)$$

BCs & ICs

$$T_L(z,0) = f_1(z) \;;\; T_W(z,0) = f_2(z)$$

$$T_L(0,t) = T^{(i)}(t) \quad t \geq 0$$

$$T_W(0,t) = T^{w}(t) \quad t \geq 0$$

Packed-bed catalytic reactor

Assumptions (balances and constitutive equations)

- plug flow
- first order $A \rightarrow B$ reaction
- liquid bulk phase
- solid phase catalyst
- uniform in cross-section
- constant physico-chemical properties
- bulk temperature constant

Packed-bed catalytic reactor

Model equations

Component mass

$$\frac{\partial C_A}{\partial t} = D\frac{\partial^2 C_A}{\partial x^2} - F\frac{\partial C_A}{\partial x} - r_A$$

Energy

$$\frac{\partial \hat{U}}{\partial t} = \kappa\frac{\partial^2 \hat{U}}{\partial x^2} - F\frac{\partial \hat{U}}{\partial x} - \Delta H r_A - q_{tr}$$

Constitutive equations

$$\hat{U} = c_P \rho T \qquad r_A = k_0 e^{-\frac{E}{RT}} C_A$$

$$q_{tr} = K(T - T_w)$$

Spherical catalyst pellet

Assumptions (balances & constitutive equations)

- overall mass and volume is constant
- first order $A \rightarrow B$ reaction
- no convection
- uniform in all directions
- constant physico-chemical properties

Spherical catalyst pellet

Model equations in spherical co-ordinate system

Component mass
$$\frac{\partial c}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c}{\partial r}\right) - k_0 c e^{\frac{E}{RT}}$$

Energy
$$\frac{\partial T}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right) - k_0 c e^{\frac{E}{RT}} \Delta H_R$$

Note: Constitutive equations are substituted

Initial conditions

Set the values of the states at the initial time ($t = 0$)

Given as a modelling assumption

Examples:

$$T(x,0) = f_1(x) \qquad (f_1(x) \text{ is given})$$

$$c_A(x,0) = c_0 \qquad (c_0 \text{ is given})$$

Boundary conditions

- Relevant assumptions
  - conditions on the boundaries
  - balance volume shape (coordinate system)
  - balance volume size (infinite)
- Number of independent boundary conditions
  - along a co-ordinate direction
  - equal to the order of partial derivatives

Boundary condition types

Dirichlet (1st type) condition

value set on boundary: $c_A(0,t) = c_*$

Neumann (2nd type) condition $$\frac{\partial c_A}{\partial x}(0,t) = 0$$

flux set on boundary

Robbins (3rd type) condition

convective transfer $$\frac{\partial c_A}{\partial x}(x_M,t) = K\left(c^* - c_A(x_M,t)\right)$$

Packed-bed catalytic reactor

Additional **assumptions**

- initial distribution uniformly constant
- "very long" reactor

Initial condition $C_A(x,0) = C^*\ ,\ T(x,0) = T^*$

Boundary conditions

$$\frac{\partial C_A}{\partial x}(L,0) = 0 \quad , \quad C_A(0,t) = C_A^{(i)}$$

$$\frac{\partial T}{\partial x}(L,0) = 0 \quad , \quad T(0,t) = T^{(i)}$$

Spherical catalyst pellet

Additional **assumptions**

- given initial conditions
- heat and mass transfer on the surface

Boundary conditions

at the centre

$$\frac{\partial c}{\partial x} = \frac{\partial T}{\partial x} = 0$$

at the surface

$$-\frac{\partial T}{\partial x} = \frac{Nu}{2}(T - g_1(t))$$

$$-\frac{\partial c}{\partial x} = \frac{Sh}{2}(c - g_2(t))$$

Initial conditions $T(x,0) = h_1(x)$, $c(x,0) = h_2(x)$

Classification of DPS models

Partial differential part of the conservation equation

$$\frac{\partial \hat{\Phi}}{\partial t} = D\left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2}\right) - \left(\frac{\partial \hat{\Phi}}{\partial x} v_x + \frac{\partial \hat{\Phi}}{\partial y} v_y + \frac{\partial \hat{\Phi}}{\partial z} v_z\right) + \hat{q}$$

Associated algebraic equation

$$t = D x^2 + D y^2 + D z^2 - v_x x - v_y y - v_z z$$

Geometry of the 2nd order curve

- parabola: $D \neq 0$
- hyperbola (degenerate): $D=0, v \neq 0$
- ellipse: steady-state, $D \neq 0$

Lumped parameter models for DPSs

Conceptual steps in **lumping:**

- divide balance volume into sub-volumes
- lump each sub-volume using perfect mixing
- convection → in- and out-flows of lumps
- diffusion → multidirectional in- and out-flows
- same sources for every lump
- balance equations for every lump
- boundary conditions → in- and outflows of lumps on system boundary

DPS model of a double-pipe heat exchanger

Model equations

Variables $0 \leq z \leq L \;\; , \;\; 0 \leq t \;\; , \;\; T_L(z,t) \;\; , \;\; T_w(x,t)$

Energy balances

$$\rho_L A_L c_f \frac{\partial T_L}{\partial t} = -u \rho_L A_f c_L \frac{\partial T_L}{\partial z} + h_L A_L (T_w - T_L)$$

$$M_w c_w \frac{\partial T_w}{\partial t} = h_s A_s (T_s - T_w) - h_L A_L (T_w - T_L)$$

Initial conditions

$$\begin{aligned} T_L(z,0) &= f_1(z) \\ T_w(z,0) &= f_2(z) \end{aligned}$$

Boundary condition $T_L(0,t) = T^{(i)}(t) \quad \text{for all t} \geq 0.$

Lumped model of a double-pipe heat exchanger

Model equations

Variables $\left(T_L^{(k)}(t)\ ,\ T_w^{(k)}(t)\ ,\ k=1,2,3\right)\quad,\quad 0\leq t$

Energy balances

$$\frac{dT_L^{(k)}}{dt}=3u\left(T_L^{(k-1)}-T_L^{(k)}\right)+\frac{1}{\tau_L}\left(T_w^{(k)}-T_L^{(k)}\right)$$

$$k=1,2,3\quad,\quad T_L^{(0)}(t)=T_L^{(i)}(t)$$

$$\frac{dT_w^{(k)}}{dt}=\frac{1}{\tau_{sw}}\left(T_s-T_w^{(k)}\right)-\frac{1}{\tau_{wL}}\left(T_w^{(k)}-T_L^{(k)}\right)$$

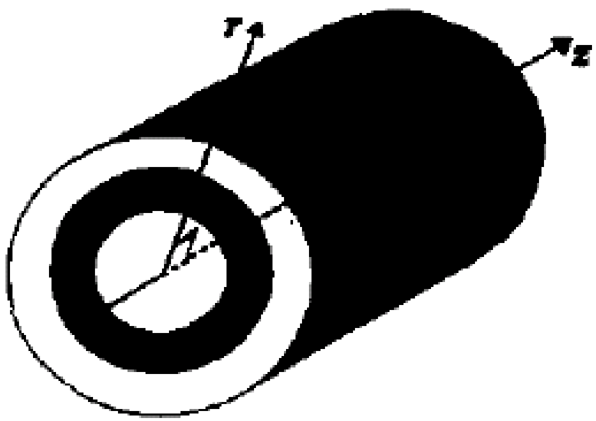
$$k=1,2,3$$

Initial conditions

$$T_L^{(k)}(0)=f_1^{(k)}\quad,\quad k=1,2,3$$

$$T_w^{(k)}(0)=f_2^{(k)}\quad,\quad k=1,2,3$$

Modelling exercise – 4b: DPS model for a cylindrical catalyst (Problem II – home exercise)



Step 2: Retrieve the general form of the balance volume equations:

- Select coordinate system
- Write conservation equation (in derivative form) for the corresponding coordinate system

Step 1: Identify the phenomena to be considered:

- Conduction of mass and energy
- Reaction
- Single phase
- No accumulation

Step 3: Generate final form of the model:

- Remove the terms not needed
- Retrieve from library the needed terms
- Add constitutive models
- Add initial and boundary conditions

$$\frac{\partial \hat{\Phi}}{\partial t} = D\left(\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{\partial \mathrm{f}}{\partial \mathrm{r}}\right) + \frac{1}{r^2}\frac{\partial^2 \mathrm{f}}{\partial \varphi^2} + \frac{\partial^2 \mathrm{f}}{\partial \mathrm{z}^2}\right) - \left(\left(\frac{\partial \hat{\Phi}}{\partial \mathrm{r}}\right)\hat{r} + \left(\frac{1}{r}\frac{\partial \hat{\Phi}}{\partial \varphi}\right)\hat{\varphi} + \frac{\partial \hat{\Phi}}{\partial \mathrm{z}}\hat{z}\right) + \hat{q}$$