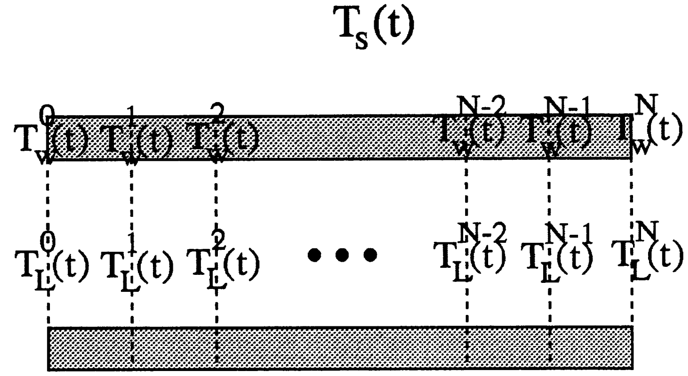
In Finite Difference Method, a grid is established in the direction of spatial variation



$$\begin{aligned} T_L^j(t) &= T_L(z,t)\big|_{z=j\Delta z} \\ T_w^j(t) &= T_w(z,t)\big|_{z=j\Delta z} \end{aligned}$$

Now note that <u>each</u> $T_L^j(t)$ and $T_w^j(t)$ depends only on time and therefore are not distributed parameters. In return, we have $2N+2$ variables in place of the two distributed parameters.

Q: What should be the grid size?

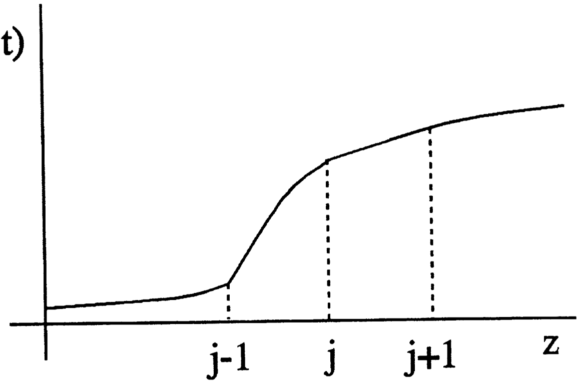
The finer the grid, the more information and the better the approximation. However, it also means more equations.

$$\begin{aligned} \frac{\partial T_L}{\partial t} &= -\,v\frac{\partial T_L}{\partial z} + \frac{1}{\tau_{HL}}(T_w - T_L) \\ \frac{\partial T_w}{\partial t} &= \frac{1}{\tau_{sw}}(T_s - T_w) + \frac{1}{\tau_{wL}}(T_L - T_w) \end{aligned}$$

with $T_s(t)$, $T_L(0,t)$, $T_L(z,0)$, $T_w(z,0)$ given, we would like to solve the above at every grid point.

One complication is what to do with the term $\partial T_L/\partial z$.

Finite Difference Approximation



Backward Difference Approximation

$$\left.\frac{\partial T_L}{\partial z}\right|_{z=j\Delta z} \approx \frac{T_L^j(t) - T_L^{j-1}(t)}{\Delta z}$$

Forward Difference Approximation

$$\left.\frac{\partial T_L}{\partial z}\right|_{z=j\Delta z} \approx \frac{T_L^{j+1}(t) - T_L^j(t)}{\Delta z}$$

Average Approximation

$$\left.\frac{\partial T_L}{\partial z}\right|_{z=j\Delta z} \approx \frac{\frac{T_L^j(t)-T_L^{j-1}(t)}{\Delta z} + \frac{T_L^{j+1}(t)-T_L^j(t)}{\Delta z}}{2}$$

$$= \frac{T_L^{j+1}(t) - T_L^{j-1}(t)}{2\Delta z}$$

$$\begin{aligned}\frac{\partial T_L(z,t)}{\partial t} =& - v\frac{\partial T_L(z,t)}{\partial z} + \frac{1}{\tau_{HL}}(T_w(z,t) - T_L(z,t))\\ \frac{\partial T_w(z,t)}{\partial t} =& \frac{1}{\tau_{sw}}(T_s(t) - T_w(z,t)) + \frac{1}{\tau_{wL}}(T_L(z,t) - T_w(z,t))\end{aligned}$$

$$\Downarrow \textbf{FDM}$$

At $z = j\Delta z$ (j^{th} grid point)

$$\begin{aligned}\frac{dT_L^j(t)}{dt} =& - v\frac{T_L^{j+1}(t) - T_L^{j-1}(t)}{2\Delta z} + \frac{1}{\tau_{HL}}(T_w^j(t) - T_L^j(t))\\ \frac{dT_w^j(t)}{dt} =& \frac{1}{\tau_{sw}}(T_s(t) - T_w^j(t)) + \frac{1}{\tau_{wL}}(T_L^j(t) - T_w^j(t))\end{aligned}$$

Note that we converted 2 PDEs into 2N ODEs:

$$\begin{aligned}\frac{dT_L^1(t)}{dt} =& - v\frac{T_L^2(t) - T_L^0(t)}{2\Delta z} + \frac{1}{\tau_{HL}}(T_w^1(t) - T_L^1(t))\\ \vdots\quad & \quad\vdots\\ \frac{dT_L^N(t)}{dt} =& - v\frac{T_L^N(t) - T_L^{N-1}(t)}{\Delta z} + \frac{1}{\tau_{HL}}(T_w^N(t) - T_L^N(t))\\ \frac{dT_w^1(t)}{dt} =& \frac{1}{\tau_{sw}}(T_s(t) - T_w^1(t)) + \frac{1}{\tau_{wL}}(T_L^1(t) - T_w^1(t))\\ \vdots\quad & \quad\vdots\\ \frac{dT_w^N(t)}{dt} =& \frac{1}{\tau_{sw}}(T_s(t) - T_w^N(t)) + \frac{1}{\tau_{wL}}(T_L^N(t) - T_w^N(t))\end{aligned}$$

Dependent Variables: $T_L^1, \cdots, T_L^N, T_w^1, \cdots, T_w^N$
Independent Variables: T_s, T_L^0

Comments:

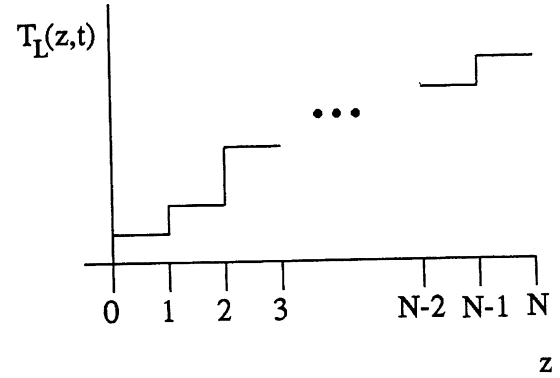
1. For $2N$ ODEs,
   dependent variables are $T_L^1, \cdots, T_L^N, T_w^1, \cdots, T_w^N$
   independent variables are T_s, T_L^0

   Note that T_L^0 is given by the required boundary condition $T_L(0, t)$ for PDE. So, the boundary condition gets translated to an additional independent variable when discretized.

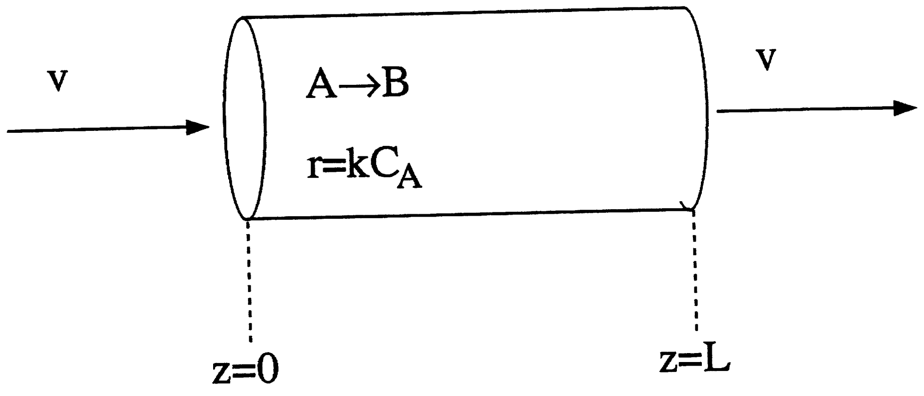
   Of course, to solve the ODEs, the initial conditions $T_L^1(0), \cdots, T_L^N(0), T_w^1(0), \cdots, T_w^N(0)$ must be given. They come from the initial condition of the PDE $T_L(z, 0)$ and $T_w(z, 0)$.

2. One does not obtain the complete profile, but only values at discrete (grid) points. However, if N is large enough, this will be sufficient. In addition, note that as N increases, the finite difference approximation of the derivatives gets better.

3. Would FDM be equivalent to assuming CST for each segment established by the grids?



C. Isothermal Fixed Bed Reactor



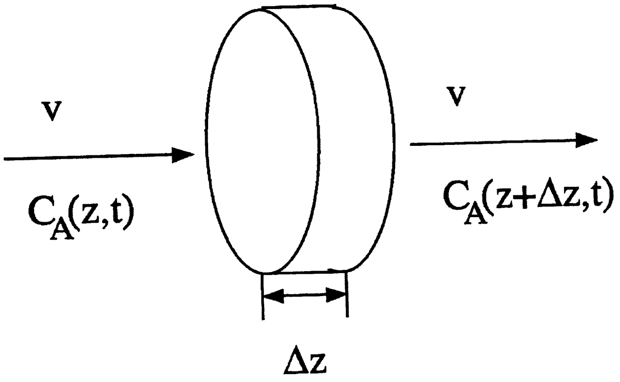
Assumptions:

- Isothermal Operation ⇒ no need for energy balance
- No radial dispersion ⇒ no radial concentration variation
- constant velocity plug flow ⇒ no need for total mass balance
- Axial dispersion (due to molecular diffusion and eddy diffusion)

$$\text{Molar Flux} = -\mathcal{D}_{\mathcal{L}} \frac{\partial C_A}{\partial z}$$

Independent Variables: $v, C_A(0,t), C_B(0,t)$
Dependent Variables: $C_A(z,t), C_B(z,t)$

- **Shell balance**



Component A Balance

$$\frac{d(C_A(z+\Delta z,t)A\Delta z}{dt} = vAC_A(z,t) - vAC_A(z+\Delta z,t)$$

$$+\left(-A\mathcal{D}_{\mathcal{L}}\frac{\partial C_A}{\partial z'}\bigg|_{z'=z}\right) - \left(-A\mathcal{D}_{\mathcal{L}}\frac{\partial C_A}{\partial z'}\bigg|_{z'=z+\Delta z}\right) - A\Delta z k C_A$$

Divide both sides by $A\Delta z$

$$\frac{dC_A(z+\Delta z,t)}{dt} = -v\frac{C_A(z+\Delta z,t) - C_A(z,t)}{\Delta z}$$

$$+\mathcal{D}_{\mathcal{L}}\frac{\left(\frac{\partial C_A}{\partial z'}\Big|_{z'=z+\Delta z} - \frac{\partial C_A}{\partial z'}\Big|_{z'=z}\right)}{\Delta z} - kC_A$$

Let $\Delta z \to 0$

$$\boxed{\frac{\partial C_A(z,t)}{\partial t} = -v\frac{\partial C_A(z,t)}{\partial z} + \mathcal{D}_{\mathcal{L}}\frac{\partial^2 C_A}{\partial z^2} - kC_A}$$

We obtain a second order partial differential equation. In order to solve the above equation, we need the following conditions.

1. Initial Condition (first order wrt time ⇒ one condition)
   $C_A(z,0)$ (i.e., initial concentration profile across the reactor) must be specified
2. Boundard Condition (second order wrt z ⇒ two conditions)
   - $C_A(0,t)$ (i.e., reactor inlet concentration) must be specified
   - $\left.\frac{\partial C_A}{\partial z}\right|_{z=L} = 0$ (no axial dispersion at exit) is another condition typically used.

- **Discretization via FDM**

Divide the reactor into N segments. Approximate

$$\left.\frac{\partial C_A}{\partial z}\right|_{z=j\Delta z} \approx \frac{C_A^{j+1}(t) - C_A^{j-1}(t)}{2\Delta z}$$

$$\begin{aligned}\left.\frac{\partial^2 C_A}{\partial z^2}\right|_{z=j\Delta z} &\approx \frac{\left.\frac{\partial C_A}{\partial z}\right|_{z=(j+\frac{1}{2})\Delta z} - \left.\frac{\partial C_A}{\partial z}\right|_{z=(j-\frac{1}{2})\Delta z}}{\Delta z} \\ &\approx \frac{\frac{C_A^{j+1}(t)-C_A^{j}(t)}{\Delta z} - \frac{C_A^{j}(t)-C_A^{j-1}(t)}{\Delta z}}{\Delta z} \\ &= \frac{C_A^{j+1}(t) - 2C_A^{j}(t) + C_A^{j-1}(t)}{\Delta z^2}\end{aligned}$$

$$\boxed{\begin{aligned}\frac{\partial C_A}{\partial t} &= -v\frac{\partial C_A}{\partial z} + \mathcal{D}_{\mathcal{L}}\frac{\partial^2 C_A}{\partial z^2} - kC_A \\ &\Downarrow \\ \frac{dC_A^j}{dt} &= -v\frac{C_A^{j+1} - C_A^{j-1}}{2\Delta z} + \mathcal{D}_{\mathcal{L}}\frac{C_A^{j+1} - 2C_A^{j} + C_A^{j-1}}{\Delta z^2} - kC_A^j \\ & j = 1, \cdots, N\end{aligned}}$$

The final system of equations is N coupled ODEs:

$$\frac{dC_A^1}{dt} = -\,v\frac{C_A^2 - C_A^0}{2\Delta z} + \mathcal{D}_{\mathcal{L}}\frac{C_A^2 - 2C_A^1 + C_A^0}{\Delta z^2} - kC_A^1$$

$$\vdots \qquad \vdots$$

$$\frac{dC_A^N}{dt} = -\,v\frac{C_A^{N+1} - C_A^{N-1}}{2\Delta z} + \mathcal{D}_{\mathcal{L}}\frac{C_A^{N+1} - 2C_A^N + C_A^{N-1}}{\Delta z^2} - kC_A^N$$

Initial Condition

$C_A(z,0)$ **provides** $C_A^j(0)$ **for** $j = 1, \cdots, N$

Boundary Conditions

$C_A(0,t)$ **provides** $C_A^0(t)$ **which appears as an independent variable in the above.**

$$\left.\frac{\partial C_A}{\partial z}\right|_{z=L} = 0 \;\Rightarrow\; \frac{C_A^{N+1} - C_A^{N-1}}{2\Delta z} \approx 0$$

$C_A^{N+1} \approx C_A^{N-1}$. **This enables us to get rid of the extra variable** C_A^{N+1} **that appears in the above.**