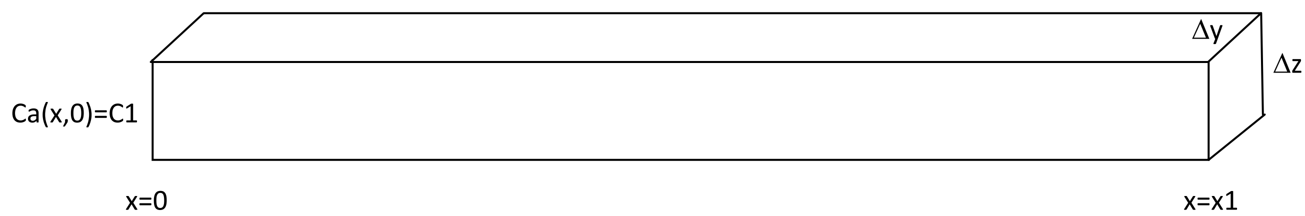
A chemical reaction (A-> B) is occurring while the reactant diffuses down a rectangular channel.



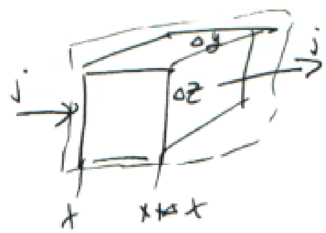
Prior to t=0 the reactant concentration in the channel is uniform at Ca(x,0)=Co. At t=0, at x=0, the end concentration is raised to C(0,0)=C1 and held there. Develop a finite difference model for Ca(x,t).

The reactant moves down the channel by diffusion, i.e. flux = -*D**(area)*(dCa(x,t)/dx) and reacts in a 1st order reaction, i.e. r = -k*Ca.

Notes:
Flux has dimensions of mass/time
D has dimensions of L^2/time.
k has dimensions of 1/time.
r has dimensions of mass/L^3-t.

Suggestion: Use a component mass balance on A for a differential element of size Δx.

Chem rxn $r = kC_A$ Diffusive flux $= j = \mathcal{D}\frac{dC_A}{dX}$
$A \rightarrow B$



$$Aj\Big|_x - Aj\Big|_{x+\Delta x} - Vr = V\frac{dC_A}{dt}$$

$A = \Delta y \Delta z$
$V = \Delta x \Delta y \Delta z$

$$\lim_{\Delta x \to 0} \frac{j\big|_x - j\big|_{x+\Delta x}}{\Delta x} - r = \frac{dC_A}{dt}$$

$$\frac{dj}{dx} - r = \frac{dC_A}{dt}$$

$j = \mathcal{D}\frac{dC_A}{dx}$
$r = kC_A$

$$\mathcal{D}\frac{d^2C_A}{dx^2} - kC_A = \frac{dC_A}{dt}$$

$$\frac{d^2C}{dx^2} = \frac{C_{m+1}^{p} - 2C_m^{p} + C_{m-1}^{p}}{\Delta x^2}$$

$$\left[\frac{C_{m+1}^{p} - 2C_m^{p} + C_{m-1}^{p}}{\Delta x^2}\right] - kC_m^{p} = \frac{C_m^{p+1} - C_m^{p}}{\Delta t}$$

$C = C_m^{p}$

$$\frac{dC}{dt} = \frac{C_m^{p+1} - C_m^{p}}{\Delta t}$$

$$C_m^{p+1} = \mathcal{D}\Delta t\left[\frac{C_{m+1}^{p} - 2C_m^{p} + C_{m-1}^{p}}{\Delta x^2}\right] - k\Delta t\, C_m^{p} + C_m^{p}$$