

## Models with partial differential equations

### ( Material balances)

The death of the fish in a lake where is at the top of a high mountain is due to freezing of the surface resulting reduced oxygen levels. At the end of the winter following the melting of ice, concentration of oxygen at the lake was found to be  $C_{A0}=4 \times 10^{-5} \text{ kmol/m}^3$ . The **stagnant lake** became enriched by  $O_2$  at spring because it had been contact with air. Considering the stagnant lake is at 2500 m altitude and  $5^\circ\text{C}$

**Note:**  $O_2$  concentration at the interface is assumed to be at equilibrium with air in contact and can be taken

$C_A^* = 4 \times 10^{-4} \text{ kmol/m}^3$ . Diffusion coefficient is  $2 \times 10^{-9} \text{ kmol/m}^3$ . Oxygen is only transferred **one dimensional (z direction)**.

Use 
$$y = \frac{C_A - C_{A0}}{C_A^* - C_{A0}}$$

For calculation of the  $O_2$  concentration ( $C_A$ ) 5 cm deep for the 1st day is required mathematical expression of this system

### Material balances;

$$N_A A|_z - N_A A|_{z+\Delta z} = \frac{\partial}{\partial t}(C_A \cdot V); \quad V = A \cdot \Delta z$$

divide by  $A \cdot \Delta z$  and  $\lim \Delta z \rightarrow 0$ ,

$$-\frac{\partial(N_A)}{\partial z} = \frac{\partial C_A}{\partial t}$$

$$N_A = -D_{AB} \frac{\partial C_A}{\partial z} + v_z C_A \quad \text{Because of stagnant lake, convective transport.}$$

is negligible with respect to diffusion.

$$N_A = -D_{AB} \frac{\partial C_A}{\partial z}$$

$$D_{AB} \frac{\partial^2 C_A}{\partial z^2} = \frac{\partial C_A}{\partial t}$$

$$y = \frac{C_A - C_{A0}}{C_A^* - C_{A0}}$$

$$D_{AB} \frac{\partial^2 y}{\partial z^2} = \frac{\partial y}{\partial t}$$

## The initial and boundary conditions

$$\text{IC: } t=0 \quad C_A=C_{A0} \quad y=0$$

$$\text{BC1: } z=0 \quad C_A=C_A^* \quad y=1$$

$$\text{BC2: } z \rightarrow \infty \quad C_A=C_{A0} \quad y=0$$