Modelling Water Scrubbing Biogas Based Technology

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Why do we need a model?

- Description of real life situations
- Tool to help design and operate a system
- Provide predictions on how a system will behave under different conditions
- "Everything should be made as simple as possible, but not simpler"- Albert Einstein

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Modelling Approach

Equilibrium Based Models

- Empirical design
- HETP and HTU/NTU

Rate Based Models

- 1D, 2D or 3D
- Steady state or dynamic model
- CFD

Modelling Assumptions

- Well mixed system with negligible directional concentration gradients
- Ideal Gas Law and ideal liquid flow
- Isothermal reactor
- Chemical reaction
- Which species should mass transfer consider
- Mass transfer liquid or gas side dominant?

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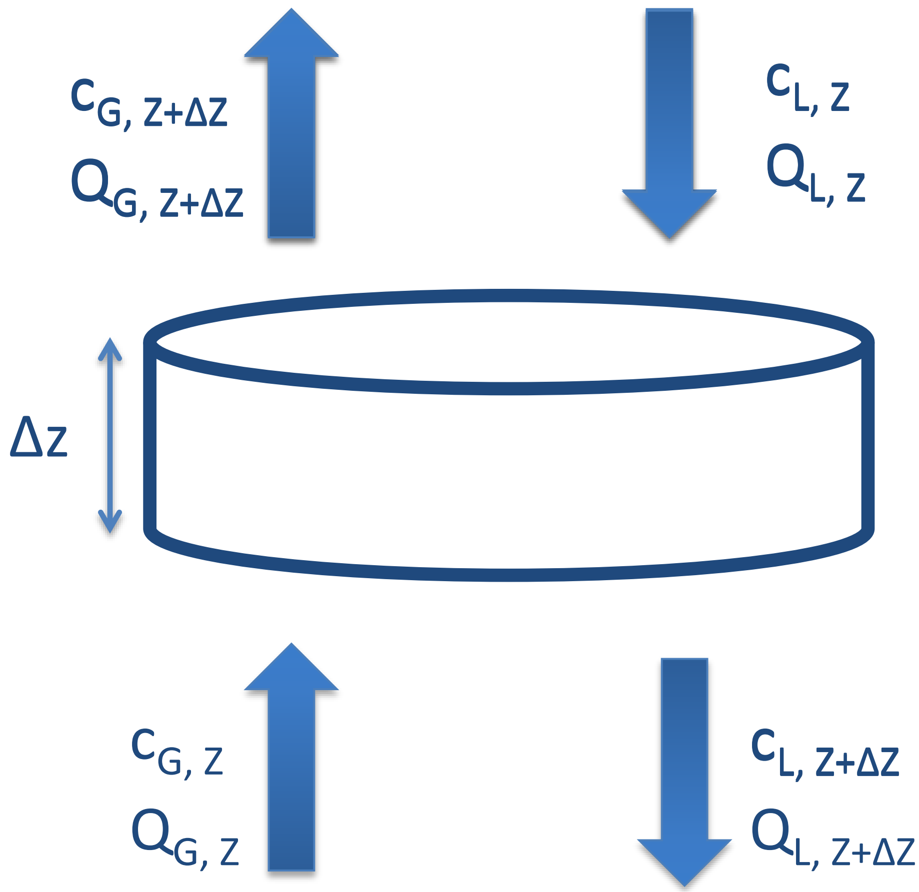
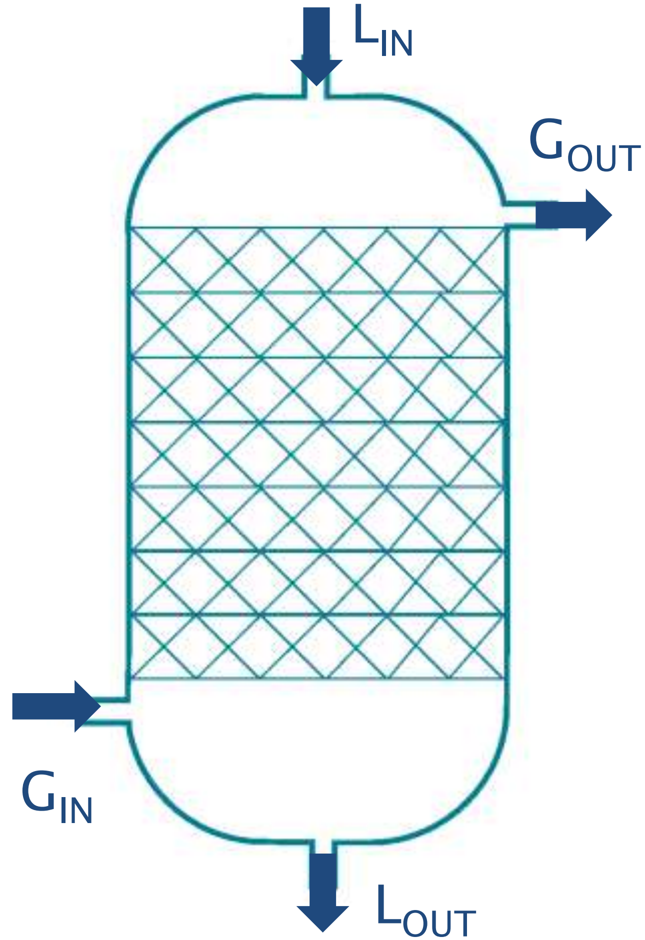
Model Derivation





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Plug Flow Reactor

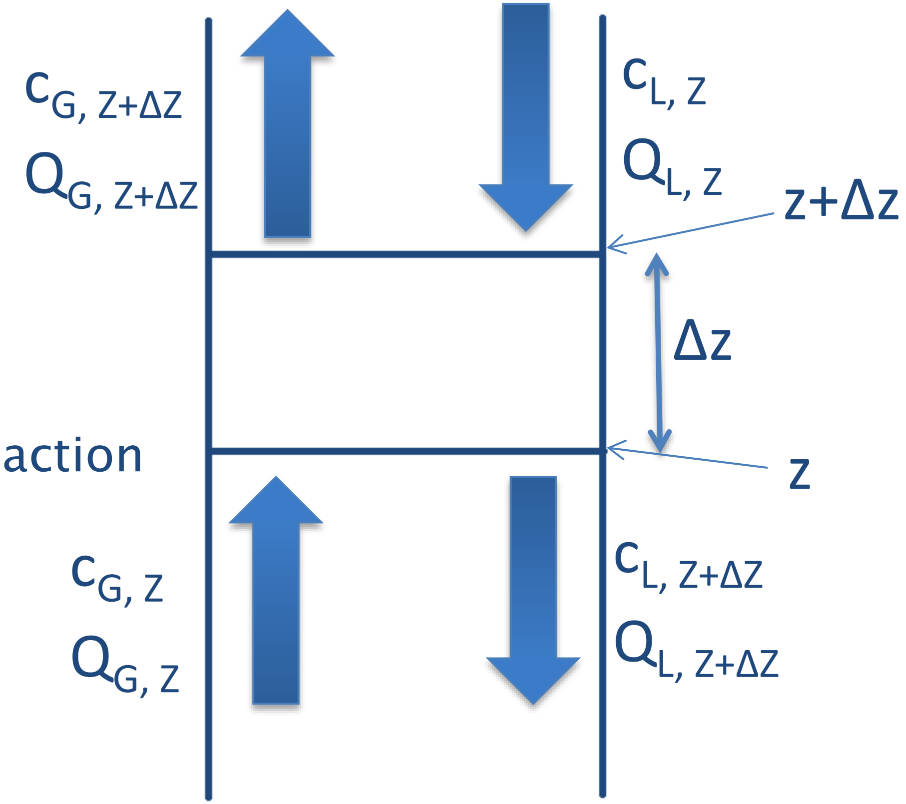
- Mass Balance:

$$\frac{\partial c_A}{\partial t} = Qc_A(z) - Qc_A(z + \Delta z) - r_A$$

Accumulation = input – output – reaction

$$\frac{\partial c_A}{dt} = -\frac{\partial (uc_A)}{\partial z} + r_A$$

- No axial mixing
- Perfect radial mixing



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Axial Dispersion Model

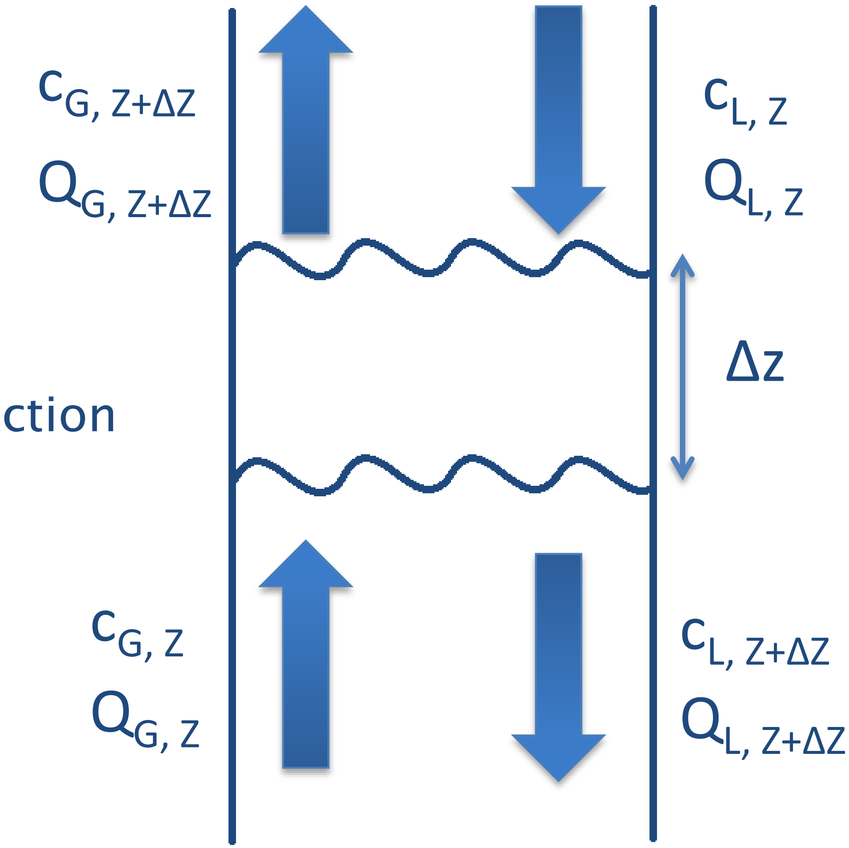
- Mass Balance:

$$\frac{\partial c_A}{\partial t} = D_A \frac{\partial^2 c_A}{\partial z^2} - \frac{\partial (u c_A)}{\partial z} - r_A$$

Accumulation = input – output – reaction

- Considers back mixing
- Peclet number

$$Pe = \frac{Lu}{D_A}$$



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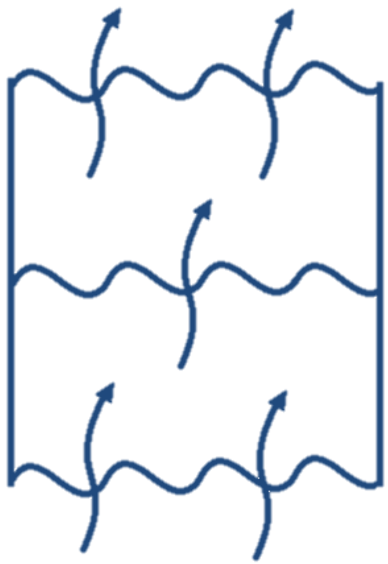
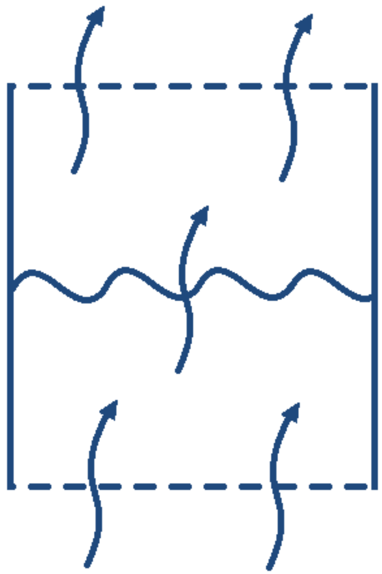
Boundary Conditions

Open - Open



Closed - Closed

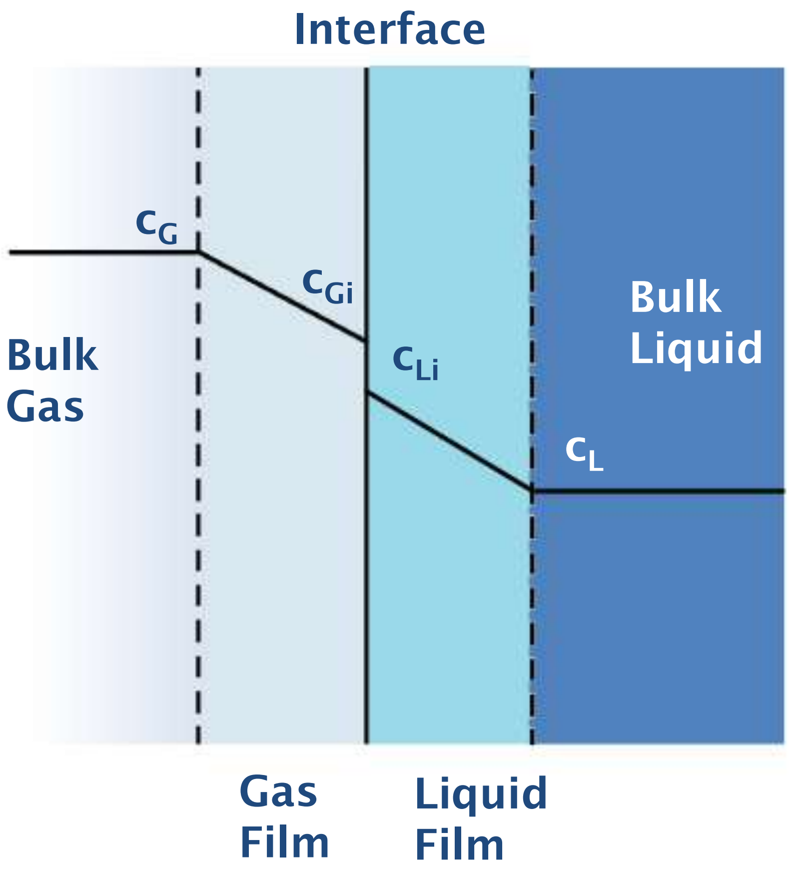


Mass Transfer Theory

- Two – Film Theory

$$k_L = \frac{D_L}{\delta f}$$

- Film thickness
- Proportional to diffusion coefficient
- $N_A = k_L(c_G - c_{Gi})$



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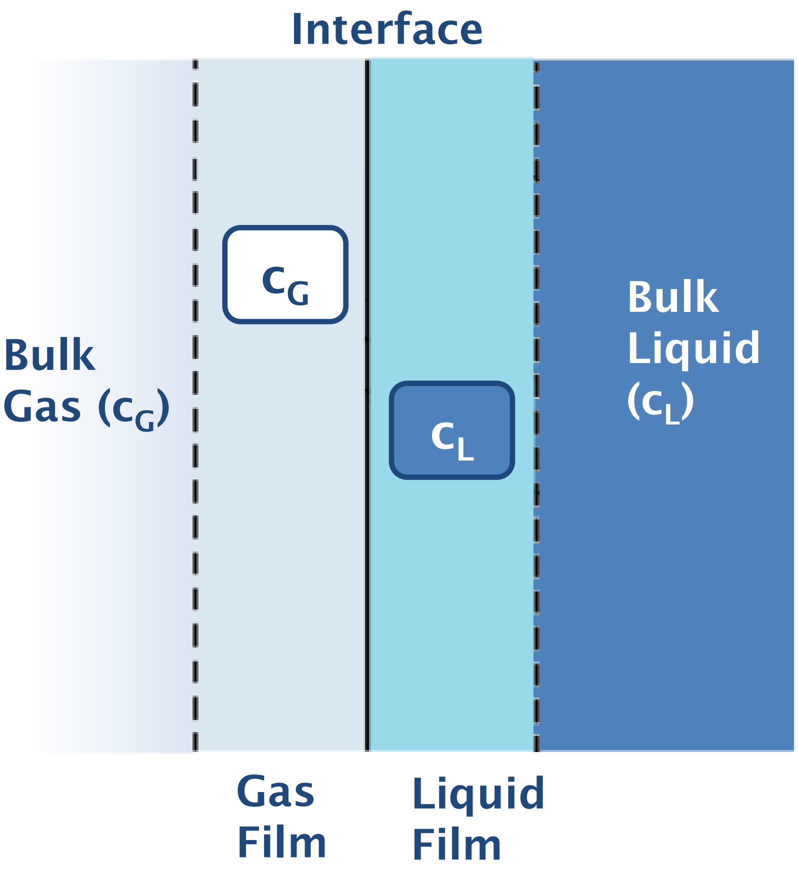
Mass Transfer Theory

- Surface Renewal Theory

$$k_L = \sqrt{\frac{D_L}{t}}$$

- Contact time ‘packets’ in contact with interface
- Proportional to square root of diffusion coefficient



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Empirical Correlations

- Henry's Law
- Mass transfer coefficients
- Interfacial area
- Pressure drop
- Gas/ liquid holdup

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Finite Difference

- Numerical solution to ode and pde's.
- Explicit or implicit schemes
- Discretisation techniques
  - Upwind scheme: $\frac{dc}{dz} = \left(\frac{c_{i+1} - c_i}{\Delta z}\right)$
- Multiphase counter-current flow
  - Gauss Seidel iteration

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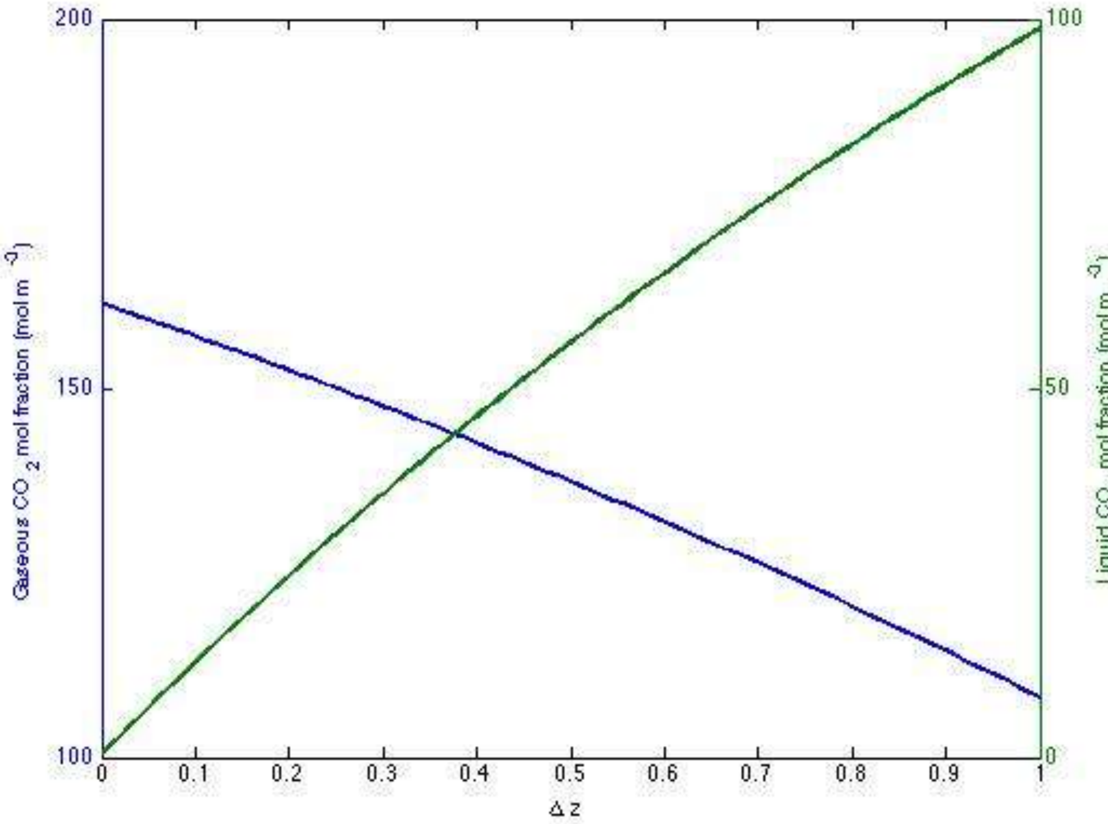
Finite Difference



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Summary

- Simple models often out perform more detailed models
- Assumptions need to be taken with care

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Thank you for listening

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