Problem 1 An engineer consultant is hired to help in the design of a new F1-car front-wing air-foil. The back part of the air-foil is in contact with the car nose (chassis) and the outer part is in contact with flowing air. At first, the engineer needs to know the temperature profile across the wing as the temperature of chassis is at 200^{o}C and the ambient air temperature is at 20^{o}C. Heat loss in the tip of the air-foil is assumed negligible. The engineer also assumed that air is incompressible and that the nose and air temperatures are constant. The temperature across the air-foil can be expressed as an 1-D elliptic partial differential equation,

$$\frac{\partial^2 T}{\partial x^2} - \alpha T = -\alpha T_{\text{amb}}$$

where $\alpha = 20$ °C.m^{-2} and T_{amb} is the temperature of the flowing air. Estimate the temperature profile at 4 nodes equally spaced in the air-foil of length $L = 0.30$m.

Problem 2 Define the 3 types of boundary conditions used to solve PDEs.

Problem 3 A particular case of PDE's is

$$u_t + \alpha u_x = \kappa u_{xx}$$

that represents advection-diffusion problems (with constant coefficients α and κ) with a number of applications in fluid and solid mechanics. Demonstrate that the advection term (in 1D and assuming regular grid) is

$$\frac{\partial u}{\partial x} = \frac{u_{i+1} - u_i}{\Delta x_i} + \mathcal{O}\left(\Delta x\right)$$

using Taylor's expansion.

Problem 4 A team of process chemical engineers is tasked to design a stirred tank with optimal mixing performance to synthetise product-$\mathcal{X}$. The team initially needs to understand the flow dynamics of Newtonian and incompressible fluids in the tank by solving advection-diffusion transport equations with a commercial CFD. In order to validate the initial assumptions of the fluid and the problem, they decided to perform a hand-calculation in a 1D system. Chemical species are advected at velocity $u_x = 0.50$ m/s with time-step size (Δt) of 3s through 60 m. Discretising the transport equation in space and time the concentration can be calculated, using FDM, as

$$\mathcal{C}_i^{j+1} = \mathcal{C}_i^j - \frac{u\Delta t}{\Delta x}\left(\mathcal{C}_{i+1}^j - \mathcal{C}_i^j\right)$$

where $i \in \{1, 2, ..., N_x\}$ and $j \in \{0, 1, ..., k\}$ are spatial- and time-increment indexes, respectively. The system is initially at rest. Assume:

- The domain is divided into $N_x = 4$ nodes;
- Initial condition is given by,

$$\mathcal{C}\left(x, t=0\right) = \begin{cases} 0.1 & \text{for } x < 20 \\ 0.075 + e^{-0.01(x-45)^2} & \text{for } 20 \leqslant x \leqslant 40 \\ 0.0 & \text{elsewhere.} \end{cases}$$

- The *ghost-node*: $x_{N_x+1} = x_{N_x}$

Calculate $\mathcal{C}_i^1$ (i.e., at $j = 1$ – a-d).

i	1	2	3	4
x_1				
$\mathcal{C}_i^0$				
$\mathcal{C}_i^1$	(a)	(b)	(c)	(d)

Problem 5 The same engineering team decided that the most efficient way to synthetise product-$\mathcal{X}$ is to use a series of CSTRs (continuous stirred tank reactor). For the initial assessment prior to the CSTR design, they decided to investigate the flow dynamics in one CSTR assuming constant inlet and outlet mass flows (Fig. 1). The system is assumed adiabatic (thus no heat transfer to the surroundings). In the reactor, a fluid A (pure at liquid phase) reacts with a fluid B (pure at gas phase) producing $\mathcal{X}$ with reaction rate of $\mathcal{R}$ until the system reach equilibrium with equilibrium constant of K_e,

$$\mathrm{A(l)} + \mathrm{B(g)} \xrightleftharpoons{\mathrm{K}_e} \mathcal{X}(l) \tag{C 1}$$

Fluid mixing is a key aspect in the design of a high-performace CSTR, therefore 4 baffles and a stirrer are included in the system. Before the reactor (and required associated facilities) design stage starts, the team needs to determine a few key-variables profiles (spatial and temporal): $\mathbf{u}\left(\underline{x}, t\right)$, $P\left(\underline{x}, t\right)$, $T\left(\underline{x}, t\right)$ and $\mathcal{C}_i\left(\underline{x}, t\right)$ (where $i \in \{1, 2, \cdots\}$ corresponds to the different chemical species in solution). Describe the mathematical and physical formulations for the problem with all the necessary assumptions. This must include all steps from the initial formulation, and pre-processing to the begining of the simulation.

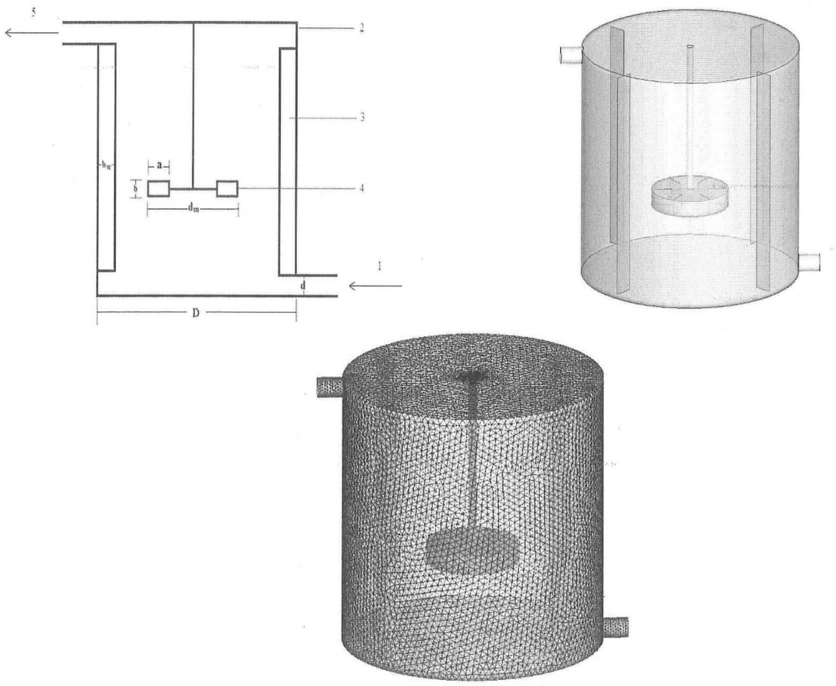


Figure 1: Schematics of the CSTR (**Problem 5**.)

P1: $$\frac{\partial^2 T}{\partial x^2} - \alpha T = -\alpha T_{amb}$$

For: $\alpha = 20\,°C/m^2$; $T_{wall} = 200\,°C$

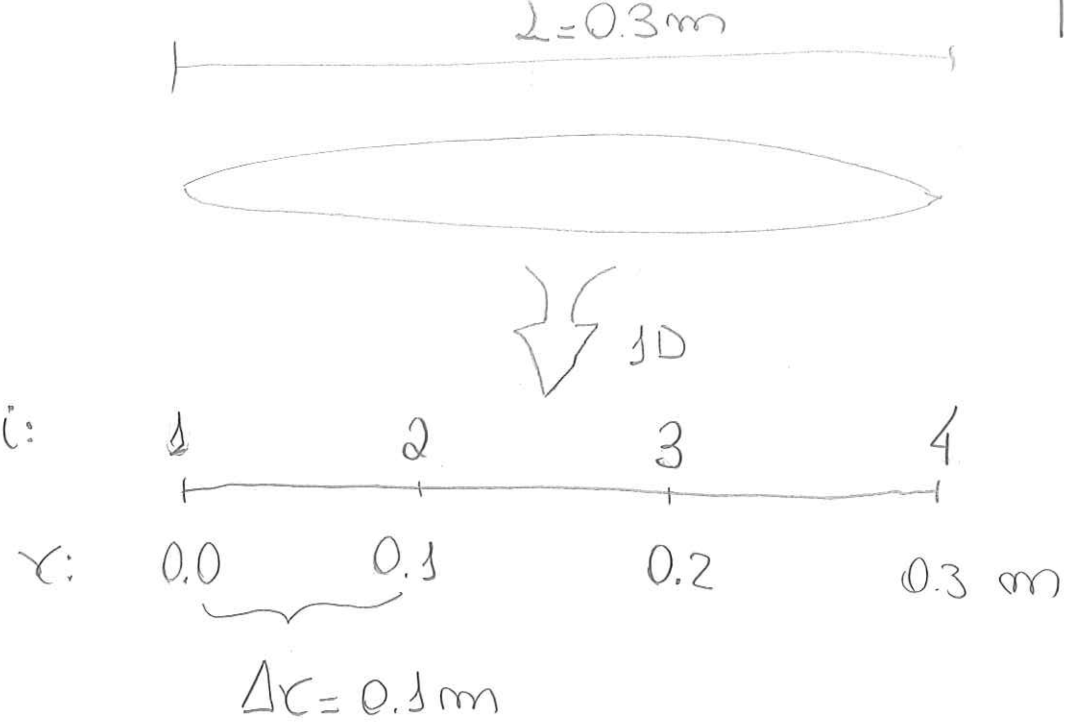
$L = 0.3\,m$; $T_{amb} = 20\,°C$

$0 \le x \le L$

BC:

$T(x=0) = T_{wall}$

$\partial T / \partial x \,(x = L) = 0$



Using central-difference scheme for the second-order derivative:

$$\frac{T_{i+1} - 2T_i + T_{i-1}}{(\Delta x)^2} - \alpha T_i = \overbrace{-\alpha T_{amb}}^{\beta \text{ (constant)}} \qquad i = 1, 2, \ldots \qquad (1)$$

Rearranging this eqn.:

$$\frac{1}{(\Delta x)^2} T_{i-1} - \left[\frac{2}{(\Delta x)^2} + \alpha\right] T_i + \frac{1}{(\Delta x)^2} T_{i+1} = -\beta \qquad (2)$$

- For mode $i=2$

$$\frac{1}{(\Delta x)^2} T_1 - \left[\frac{2}{(\Delta x)^2} + \alpha\right] T_2 + \frac{1}{(\Delta x)^2} T_3 = -\beta \qquad (3)$$

- For mode $i=3$

$$\frac{1}{(\Delta x)^2} T_2 - \left[\frac{2}{(\Delta x)^2} + \alpha\right] T_3 + \frac{1}{(\Delta x)^2} T_4 = -\beta \qquad (4)$$

For these 2 modes, there are $\underline{\underline{4}}$ unknowns and $\underline{\underline{2}}$ equations. However $\underline{T(x=0) = T_1 = T_{wall}}$.

And for the second boundary conditions,

$$\frac{\partial T}{\partial x}(x=L) = 0 \qquad (5)$$

we can discretise with backward difference scheme as,

$$\frac{\partial T}{\partial x} = \frac{T_i - T_{i-1}}{\Delta x} = 0 \qquad (6)$$

where $i=4$:

$$\frac{T_4 - T_3}{\Delta x} = 0 \therefore -\frac{1}{\Delta x} T_3 + \frac{1}{\Delta x} T_4 = 0 \qquad (7)$$

Now rearranging Eqns. 3, 4 and 7 in matricial form:

$$\begin{cases} -\left[\frac{2}{(\Delta x)^2} + \alpha\right] T_2 + \frac{1}{(\Delta x)^2} T_3 = -\beta - \frac{1}{(\Delta x)^2} T_1 \\ \frac{1}{(\Delta x)^2} T_2 - \left[\frac{2}{(\Delta x)^2} + \alpha\right] T_3 + \frac{1}{(\Delta x)^2} T_4 = -\beta \\ -\frac{1}{\Delta x} T_3 + \frac{1}{\Delta x} T_4 = 0 \end{cases}$$

$$\begin{pmatrix} -\gamma & 1/(\Delta x)^2 & 0 \\ 1/(\Delta x)^2 & -\gamma & 1/(\Delta x)^2 \\ 0 & -1/\Delta x & 1/\Delta x \end{pmatrix} \begin{pmatrix} T_2 \\ T_3 \\ T_4 \end{pmatrix} = \begin{pmatrix} -\beta - 1/(\Delta x)^2 T_1 \\ -\beta \\ 0 \end{pmatrix}$$

where $\gamma = 2/(\Delta x)^2 + \alpha$

Now replacing the symbols representing constants:

$$\gamma = \frac{2}{0.1^2} + 20 = 220$$

$$1/(\Delta x)^2 = 1/0.1^2 = 100 \qquad 1/\Delta x = 1/0.1 = 10$$

$$\beta = \alpha T_{amb} = 20 \times 20 = 400$$

$$-\beta - \frac{T_1}{(\Delta x)^2} = -400 - \frac{200}{(0.1)^2} = -20400$$

$$\begin{pmatrix} -220 & 100 & 0 \\ 100 & -220 & 100 \\ 0 & -10 & 10 \end{pmatrix} \begin{pmatrix} T_2 \\ T_3 \\ T_4 \end{pmatrix} = \begin{pmatrix} -20400 \\ -400 \\ 0 \end{pmatrix}$$

$$\begin{cases} T_2 = 151.71\,^\circ C \\ T_3 = 129.76\,^\circ C \\ T_4 = 129.76\,^\circ C \end{cases}$$

P2:

(a) In Dirichlet BC, one prescribes the value of a variable at the boundary,

$$C = C_D \text{ on } \Gamma_D$$

↳ constant

(b) In Newmann BC, one prescribes the gradient normal to the boundary of a variable at the boundary,

$$\underline{n} \cdot \nabla C = C_N \text{ on } \Gamma_N$$

↳ constant

(c) In mixed (or Robin) BC, a function of the form

$$\underline{n} (\underline{u} C - D \nabla C) = C_R \text{ on } \Gamma_R$$

is imposed at the boundary, when C_R and D are constants.

P3: Demonstrate that the advection term is given by

$$\frac{\partial u}{\partial x} = \frac{u_{i+1} - u_i}{\Delta x_i} + O(\Delta x)$$

using Taylor's expansion.

Expanding a function $\underline{u}$ at x_{i+1} about the point x_i (assuming regular grid):

$$u(x_i + \Delta x_i) = u(x_i) + \Delta x_i \left.\frac{\partial u}{\partial x}\right|_{x_i} + \frac{(\Delta x_i)^2}{2!}\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} + \frac{(\Delta x_i)^3}{3!}\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \dots$$

The Taylor's expansion can be rearranged as,

$$\frac{u(x_i + \Delta x_i) - u(x_i)}{\Delta x_i} - \left.\frac{\partial u}{\partial x_i}\right|_{x_i} = \frac{\Delta x_i}{2!}\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} + \frac{(\Delta x_i)^2}{3!}\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \dots$$

The rhs of the equation is the truncation error of the series and the eqn. can be rewritten as:

$$\left.\partial u/\partial x\right|_{x_i} = \frac{u_{i+1} - u_i}{\Delta x} + O(\Delta x)$$

P4: $$C_i^{j+1} = C_i^j - \frac{u\Delta t}{\Delta x}\left(C_{i+1}^j - C_i^j\right)$$

$i \in \{1, 2, \dots, N_x\}$

$j \in \{0, 1, \dots, K$

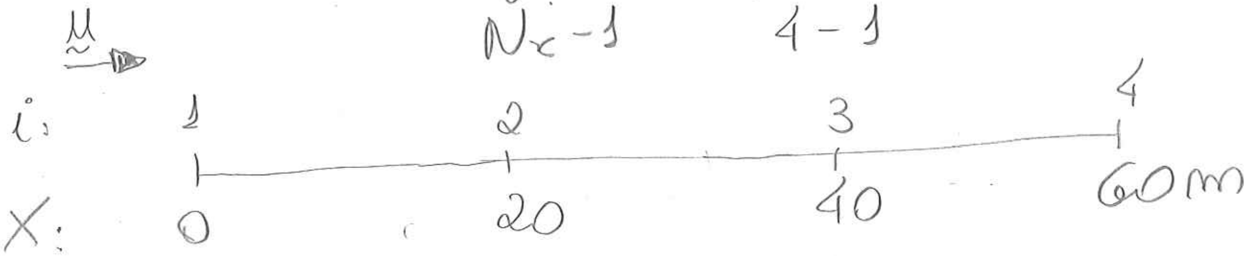
$N_x = 4$ modes

$$C(x, t=0) = \begin{cases} 0.075 + \exp\left[-0.01(x-45)^2\right] & ; \ 20 \le x \le 40 \\ 0.1 & ; \ x < 20 \\ 0.0 & ; \ \text{elsewhere} \end{cases}$$

Ghost-mode : $x_{N_x+1} = x_{N_x}$

Let's first calculate Δx

$$\Delta x = \frac{X_3 - X_0}{N_x - 1} = \frac{60 - 0}{4 - 1} = 20$$



Now solving for concentration at time $j = 0$,

$$C_i^{j+1} = C_i^j - \frac{u\Delta t}{\Delta x}\left(C_{i+1}^j - C_i^j\right)$$

$$\left.\begin{aligned}
i=1:&\quad C_1^1 = C_1^0 - \frac{0.5\times 3}{20}\left(C_2^0 - C_1^0\right) \\
i=2:&\quad C_2^1 = C_2^0 - \frac{0.5\times 3}{20}\left(C_3^0 - C_2^0\right) \\
i=3:&\quad C_3^1 = C_3^0 - \frac{0.5\times 3}{20}\left(C_4^0 - C_3^0\right) \\
i=4:&\quad C_4^1 = C_4^0 - 0.5\times 3/20\left(C_5^0 - C_4^0\right)
\end{aligned}\right\} \quad (\#)$$

where:

$$C_1^0 = C(x=0, t=0) = 0.1$$

$$C_2^0 = C(x=20, t=0) = 0.075 + \exp[-0.01(20-45)^2]$$
$$= 7.6930\times10^{-2} \ g/l$$

$$C_3^0 = C(x=40, t=0) = 0.075 + \exp[-0.01(40-45)^2]$$

$$= 8.5380\times10^{-1} \ g/l$$

ghost-cell: $x_{N_x+1} = x_{N_x}$

$$C_4^0 = C(x=60, t=0) = 0$$

$$C_5^0 = C(x=80, t=0) = C(x=60, t=0) = 0$$

Replacing in (#):

$$C_1^1 = 0 - \frac{0.5\times3}{20}(7.693\times10^{-2} - 0.1) = 1.7303\times10^{-3} \ g/l$$

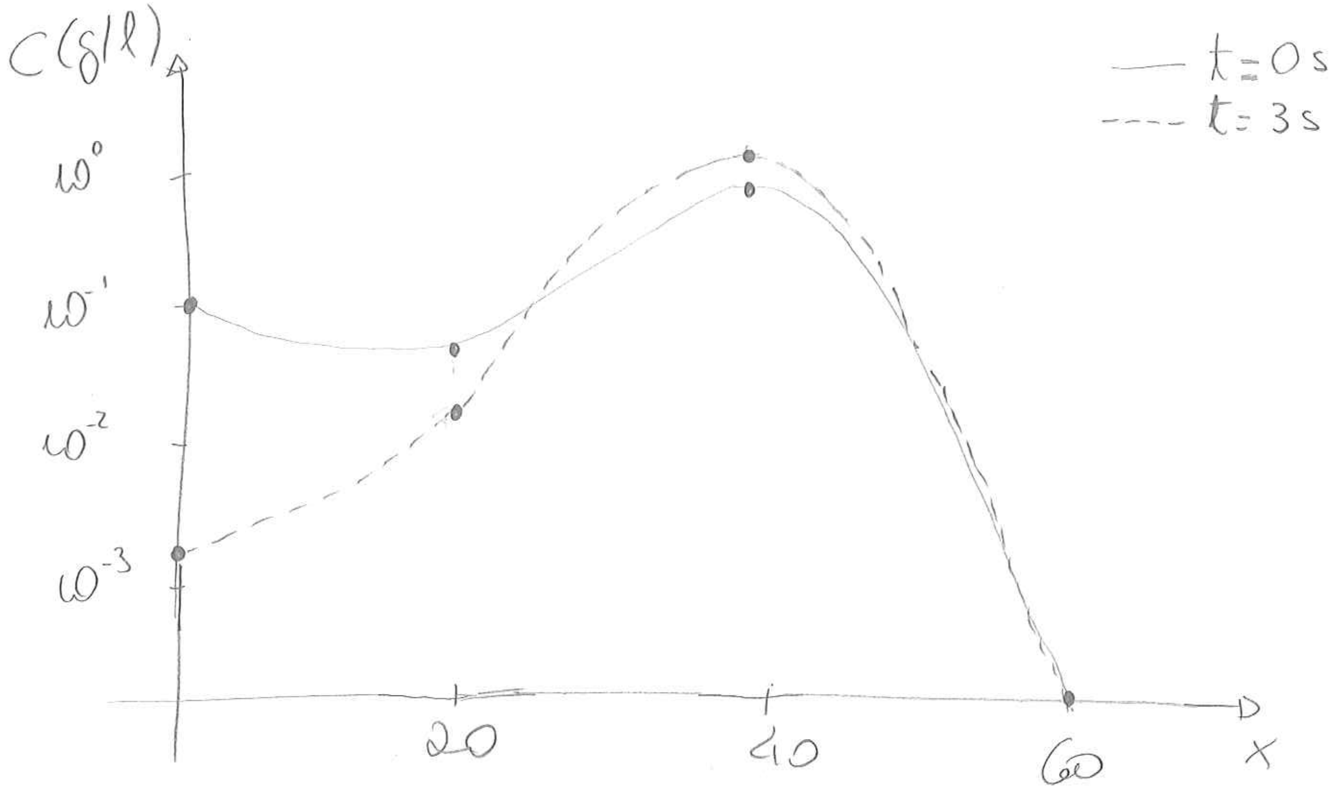
$$C_2^1 = 7.6930\times10^{-2} - \frac{0.5\times3}{20}(8.5380\times10^{-1} - 7.6930\times10^{-2})$$

$$= 1.8665\times10^{-2} \ g/l$$

$$C_3^1 = 8.5380\times10^{-1} - \frac{0.5\times3}{20}(0 - 8.5380\times10^{-1})$$

$$C_3^1 = 9.1784\times10^{-1} \ g/l$$

$$C_4^1 = 0 - \frac{0.5 \times 3}{20}(0 - 0) = 0$$



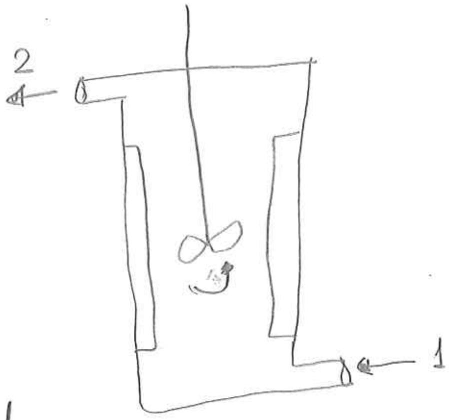
Node (i)	1	2	3	4
x_i (m)	0.0	20.0	40.0	60.0
C_i^0 (g/l)	0.1	7.6930×10^{-2}	8.5380×10^{-1}	0.0
C_i^1 (g/l)	1.7303×10^{-3}	1.8665×10^{-2}	9.1784×10^{-1}	0.0

P5:

Key-variables: $\begin{cases} \underline{v}(\underset{\sim}{x},t) \\ T(\underset{\sim}{x},t) \\ P(\underset{\sim}{x},t) \\ C_i(\underset{\sim}{x},t) \quad i \in \{1,\dots,N_c\} \end{cases}$

number of chemical components

(a) Initial assumptions:



- Fluid A (liquid) is incompressible with density ρ_A;
- Fluid B (gas) is compressible and the density $\rho_B = \rho_B(T,P)$ is obtained through an EOS;
- Fluid X (liquid) is assumed incompressible with density μ_X;
- Viscosities & thermal conductivities of all fluids are known and represented by functions, $\mu_j = \mu_j(T)$, $K_j = K_j(T)$
- Geometry of the vessel and agitators are known

and can be readily mapped;

(b) Physical formulation:

- Fluids A, B & X entered into the domain via 1 and leave at 2. Influx & outflow of total mass is constant

$$\frac{\partial}{\partial t}(m_A + m_B + m_X) = 0$$

This means the simulation is assumed to have reached steady-state regime with initial m_A^0, m_B^0, m_X^0 (or $\alpha_A^0, \alpha_B^0, \alpha_X^0$);

- Agitator is assumed to move in a prescribed rotation (angular momentum), Q_Ω (constant);

(c) Mathematical formulation:

- Conservation of mass:

$$\frac{\partial}{\partial t}(\rho_i \alpha_i) + \nabla \cdot (\rho_i \alpha_i \underset{\sim}{u_i}) = S_{cty,i} \qquad (1)$$

- Conservation of momentum:

$$\frac{\partial}{\partial t}(\rho_i \alpha_i \underset{\sim}{u_i}) + \nabla \cdot (\rho_i \alpha_i \underset{\sim}{u_i} \underset{\sim}{u_i}) = -\alpha_i \nabla p_i + \alpha_i \rho_i \underset{\sim}{g} + \nabla \underset{\approx}{\tau} + \beta(\underset{\sim}{u_i} - \underset{\sim}{u_j}) + \Gamma_i \underset{\sim}{u_i} + S_{mom,i} \qquad (2)$$

- Conservation of thermal energy:

$$\frac{\partial}{\partial t}(\rho_i \alpha_i C_{p_i} T_i) + \nabla \cdot (\rho_i \alpha_i C_{p_i} T_i \underset{\sim}{u_i}) = -p_i \nabla(\alpha_i \underset{\sim}{u_i}) + \nabla(\alpha_i K_i \nabla T_i) + \delta(T_i - T_j) + \Omega_{wi} + S_{thermal,i} \qquad (3)$$

- Conservation of species:

$$\frac{\partial}{\partial t}(\rho_i \omega_i) + \nabla(\rho_i \omega_i \underset{\sim}{u_i}) = \nabla(\rho_i D_{eff,i} \nabla \omega_i) + R_i \qquad (4)$$

where α_i is the volume fraction of species i. β, $\underset{\approx}{\tau}$, g and Γ are the interphase momentum transfer (drag) coefficient, stress tensor, gravity body force and frictional forces between surfaces and fluid i, respectively. γ, Ω, D_{eff}, ω and R are interphase heat transfer coef., wall-phase heat transfer, effective mass diffusivity, mass fraction and reaction rate, respectively. S are the source terms.

- Constitutive equations:
  - fluid densities (ρ_i): equations of state;
  - fluid viscosities (μ_i), thermal conductivities (K_i) and heat capacities (C_p): algebraic expressions
  - empirical or analytical expressions for γ and Ω (as function of Nu, Re and Pr dimensionless numbers);

- differential equations representing reactions rates (R_i);

- Initial conditions: assign specified IC:

$$\left.\begin{array}{l} T \\ p \\ \underset{\sim}{u} \\ \alpha \\ \omega \end{array}\right\} (\underset{\sim}{x}, t=0)$$

- Boundary conditions:
  - $\sum(\alpha_i \rho_i \underset{\sim}{u_i})_1 = \sum(\alpha_i \rho_i \underset{\sim}{u_i})_2$: prescribed (Dirichlet)
  - $(\alpha_i)_1$, $(\omega_i)_1$ and $(T_i)_1$: prescribed (Dirichlet)
  - No flow across the walls, baffles and agitators

$$\left(\frac{\partial \underset{\sim}{u_i}}{\partial n_i}\right)_{\omega, b, a} = 0 \qquad \text{(Robin)}$$

(d) Pre-processing:

- convert the physical geometry into computational geometry (mesh generation):

  - dimensionality (2 or 3D)
  - grid shape < triangular, quads; tets, hexs, prism., etc

- discretisation methods (depends on CFD software):
  - space (FDM, FEM, FVM, etc)
  - temporal (explicit, implicit, hybrid)

- solver options (depends on CFD software):
  - iterative methods with
  - direct methods as preconditioners.
  - tolerances.