Modeling & Simulation in Chemical Engineering

(CHE-F418)

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Problem Statements on IVP

(Applications in Chemical Engineering)

Problem Statement_IVP_Fluidized Packed Bed Catalytic Reactor

The irreversible gas phase catalytic reaction

$$A \rightarrow B$$

is to be carried out in a fluidized packed bed reactor. Material and energy balances for this reactor yield

$$\frac{dP}{d\tau} = P_e - P + H_g\left(P_p - P\right)$$

$$\frac{dT}{d\tau} = T_e - T + H_T\left(T_p - T\right) + H_W\left(T_W - T\right)$$

$$\frac{dP_p}{d\tau} = \frac{H_g}{A}\left\{P - P_p\left(1 + K\right)\right\}$$

$$\frac{dT_p}{d\tau} = \frac{H_T}{C}\left\{\left(T - T_p\right) + FKP_p\right\}$$

$$K = 6\times10^{-4}\exp\left(20.7 - \frac{1000}{T_p}\right)$$

where

T (°R) is the temperature of the reactant
P (atm) is the partial pressure of the reactant
T_p (°R) is the temperature of the reactant at the surface of the catalyst
P_p (atm) is the partial pressure of the reactant at the surface of the catalyst
K is the rate constant (dimensionless)
τ is time (dimensionless)
and the subscript e is the inlet condition

The parameters and constants used in the model equations are

$$H_g = 320,\quad T_e = 600,\quad H_T = 266.67,\quad H_W = 1.6,\quad T_W = 720,\quad F = 8000,\quad A = 0.17142,$$
$$C = 205.74,\quad P_e = 0.1$$

Solve the differential equations from $\tau = 0$ to 1500 and plot the changes of dependent variables. Initial conditions are $P(0) = 0.1$, $T(0) = 600$, $P_p = 0$, and $T_p = 761$.

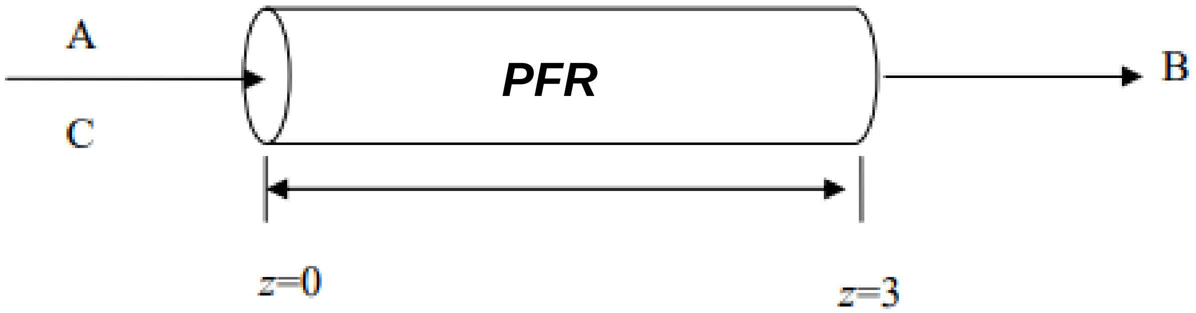
Problem Statement_IVP_Biochemical Reaction

A biological process involving the growth of a biomass from substrate can be represented as

$$\frac{dB}{dt} = \frac{kBS}{K+S}, \quad \frac{dS}{dt} = -\frac{0.75kBS}{K+S}$$

where B and S are the biomass and substrate concentrations, respectively. Solve these differential equations from $t = 0$ to 20. At $t = 0$, S and B are 5 and 0.05, respectively. The reaction kinetics are $k = 0.3$ and $K = 0.000001$.

Problem Statement_IVP_Isothermal Plug Flow Reactor



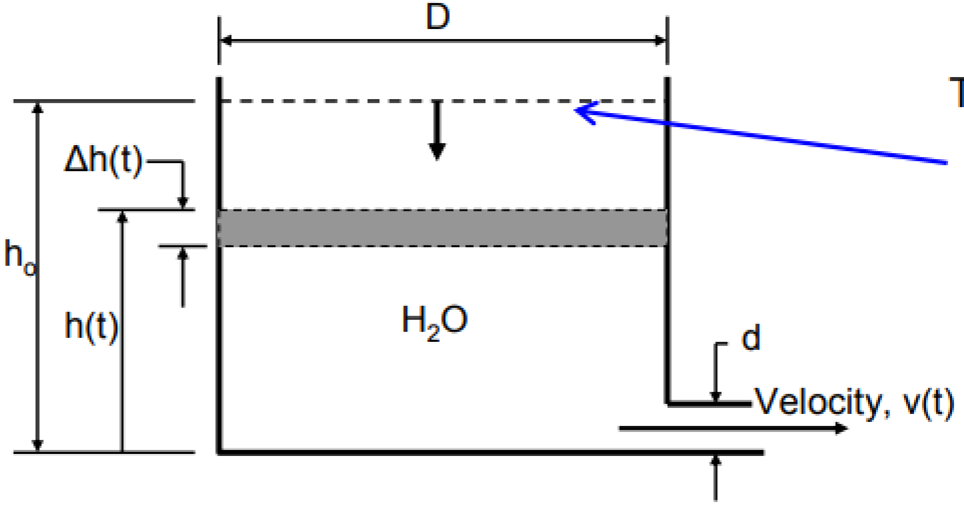
$$u\frac{dC_A}{dz} = -2kC_A^2$$
$$u\frac{dC_B}{dz} = 2kC_A^2$$
$$u\frac{dC_C}{dz} = 0$$

With the following initial values:

$$C_A(0) = 2\text{kmol/m}^3, \;\; C_B(0) = 0, \quad C_C(0) = 2\text{kmol/m}^3$$

If $u = 0.5m/s$, $k = 0.3\,m^3/kmol\,s$, and reactor length $z = 3m$. Solve the differential equations and plot the concentration of each species along the reactor length

Problem Statement_IVP_Fluid Flow



The given initial water level in the tank is h_o

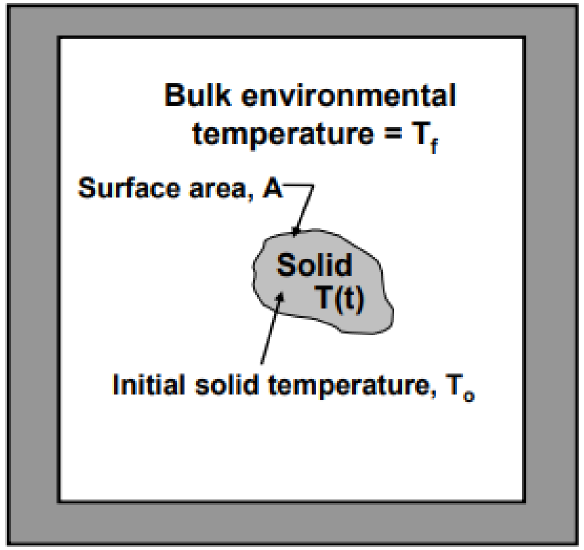
The water level keeps dropping after the tap exit is opened, and the reduction of water level is CONTINUOUS with time t

Let the water level at time t be h(t)

$$\frac{dh(t)}{dt} = -\sqrt{2g}\left(\frac{d^2}{D^2}\right)\sqrt{h(t)}$$

Tank diameter, D = 12" = 1 ft.
Drain pipe diameter, d = 1" = 1/12 ft.
Initial water level in the tank, h_o = 12" = 1 ft.
Gravitational acceleration, g = 32.2 ft/sec.

Problem Statement_IVP_Unsteady State Heat Transfer



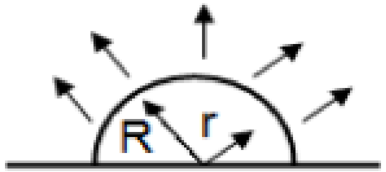
$$\frac{dT(t)}{dt} = -\alpha A\left[T(t) - T_f\right]$$

$T_o = 80^oC$, $T_f = 5^oC$, $\alpha = 0.002/m^2\text{-}s$ and $A = 0.2\ m^2$

Solve the differential equation and find out the time required to reach the steady-state conditions.

Problem Statement_IVP_Mass Transfer

A hemispherical droplet of liquid water, lying on a flat surface, evaporates by molecular diffusion through still air surrounding the droplet. The droplet initially has a radius R. As the liquid water slowly evaporates, the droplet shrinks slowly with time, but the flux of the water vapor is at a nominal steady state. The temperature of the droplet and the surrounding still air are kept constant. The air contains water vapor at an infinitely long distance from the droplet's surface.



$$N_A = -cD_{AB}\frac{dy_A}{dr} + y_A(N_A + N_B)$$

$$N_B = 0$$

$$N_A = -\frac{cD_{AB}}{(1-y_A)}\frac{dy_A}{dr}$$

Basic assumptions:

1. Steady state conditions
2. No chemical reaction
3. Constant pressure and temperature
4. One dimensional mass transfer (r direction)
5. $N_{Air} = 0$

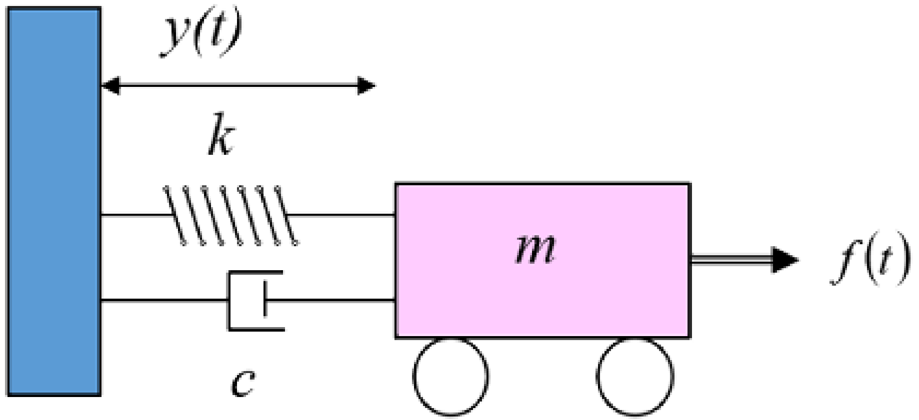
Solve the first order differential equation of IVP and find out the graphically show the variation of mole-fraction of liquid-water with r.
at r=0, $y_A(0)$= 0.8,

Data given,
c = 5 mol/m^3. D_{AB}= 10^{-2} m^2/s, N_A= 20 mol /m^2.s

Second order Differential Equation

$$\frac{d^2y}{dx^2} + P(x)\frac{dy}{dx} + Q(x)y = f(x)$$

Spring-mass-damper response theory



Sum of forces acting on suspension

$$F_m + F_d + F_k = f(t)$$

$$\frac{m}{g_c}\frac{d^2y}{dt^2} + c\frac{dy}{dt} + ky = f(t)$$

Mass acceleration

$$F_m = ma; \quad a = \frac{dv}{dt}; \quad v = \frac{dy}{dt} \quad \Rightarrow \quad a = \frac{d^2y}{dt^2}$$

$$F_m = \frac{m}{g_c}\frac{d^2y}{dt^2}$$

Damping force

$$F_d = c\frac{dy}{dt}; \quad c[=]damping\ coefficient\ \frac{lb_f}{ft/sec}$$

Spring force

$$F_k = ky; \quad k[=]spring\ constant\ \frac{lb_f}{ft}$$

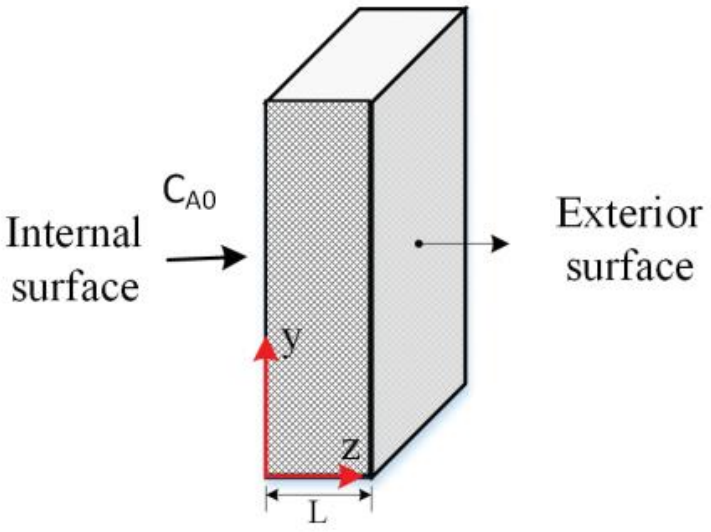
Driving bump force

$$f(t)[=]bump\ force \quad lb_f$$

Problem Statements on BVP

(Applications in Chemical Engineering)

Problem Statement: Mass Transfer with Diffusion



Diffusion with chemical reaction inside a slab catalyst

$$\overbrace{\frac{\partial C_A}{\partial t}}^{\text{accum.}} = -\left(\overbrace{v_x \frac{\partial C_A}{\partial x} + v_y \frac{\partial C_A}{\partial y} + v_z \frac{\partial C_A}{\partial z}}^{\text{Convection}}\right) + \overbrace{D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2}\right)}^{\text{Diffusion}} + \overbrace{R_A}^{\text{reaction}}$$

Assumptions:

- Steady state.
- Transportation of gas takes place by diffusion only.
- Diffusion in x and y directions are negligible.
- Diffusivity of gas in the membrane tube is constant.

B.C.1: at $z = 0,\ C_A = C_{Ao}$

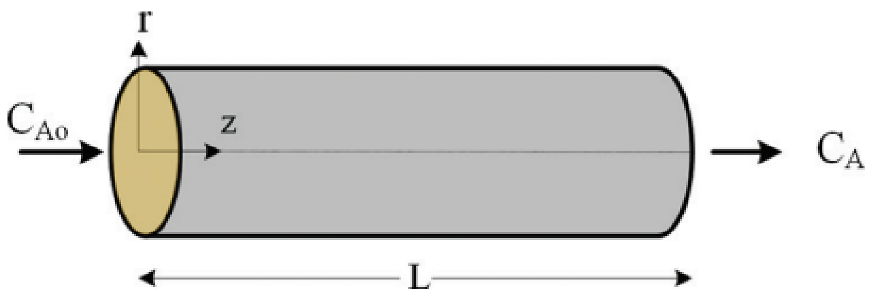
B.C.2: at $z = L,\ \frac{dC_A}{dz} = 0$

For the given assumptions and BCs, solve the diffusion-convection equation for predicting concentration, C_A

Problem Statement: PFR (Diffusion with reaction)

B.C.1: at $z = 0$, $C_A = C_{A0}$ (inlet concentration of A)

B.C.2: at $z = L$, $dC_A/dz = 0$ (convective flux at the exit of the reactor)

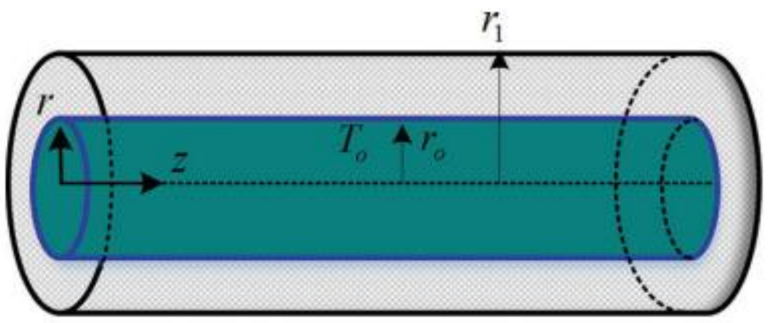


$$\frac{\partial C_A}{\partial t} = -\left(v_r \frac{\partial C_A}{\partial r} + v_\theta \frac{1}{r}\frac{\partial C_A}{\partial \theta} + v_z \frac{\partial C_A}{\partial z}\right)$$

$$+ D_A\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_A}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C_A}{\partial \theta^2} + \frac{\partial^2 C_A}{\partial z^2}\right) + R_A$$

Consider a steady-state, non-catalytic PFR reactor where the convective term is much larger than diffusive term. Solve the above mentioned mass balance equation as per given BCs for the first-order reaction and calculate C_A.

Problem Statement: Heat Diffusion in a Packed Bed Reactor



Chemical reactor with packed bed of catalyst

- Steady state
- Neglect of convective heat
- Neglect of the temperature gradients in the axial and angular direction

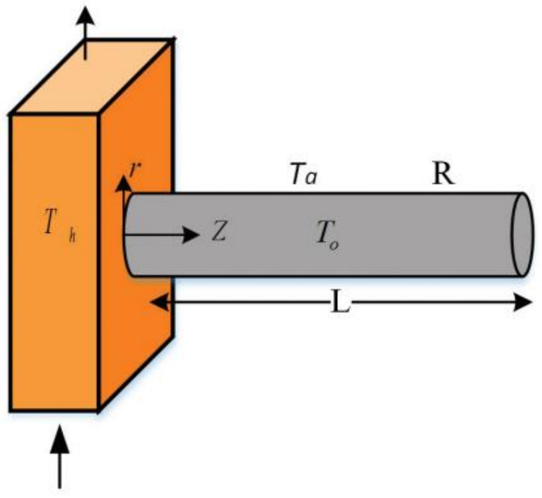
$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \left(v_r \frac{\partial T}{\partial r} + v_\theta \frac{1}{r}\frac{\partial T}{\partial \theta} + v_z \frac{\partial T}{\partial z} \right) = k \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2} \right) + \Phi_H$$

B.C.1 : $r = r_o,\ dT/dr = 0,$

B.C.2: $r = r_o,\ T = T_o.$

For a given pecked bed reactor, solve the energy balance equation as per the BCs given and predict the temperature profile across the reactor-bed.

Problem Statement: Heat Conduction Through a Fin



Assumptions:

1. Steady state condition
2. No convective heat flow
2. If the radius of the rod is very small compared to rod length so the radial temperature gradient is neglected

BC 1: at z=0, T = T_H
BC 2: at z= L, dT/dz = 0

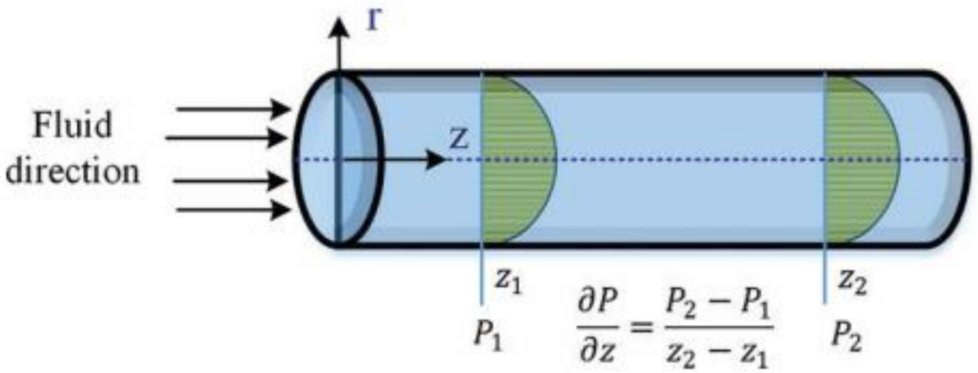
$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \left(v_r \frac{\partial T}{\partial r} + v_\theta \frac{1}{r}\frac{\partial T}{\partial \theta} + v_z \frac{\partial T}{\partial z} \right) = k \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2} \right) + \Phi_H$$

For a given extended surface (fins), solve the energy balance equation as per the given BCs and predict the temperature profile across the extended surface.

Problem Statement: Fluid Flow Through Pipe

$$\rho\frac{\partial v_z}{\partial t}+\rho\left(v_r\frac{\partial v_z}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_z}{\partial \theta}+v_z\frac{\partial v_z}{\partial z}\right)$$

$$=\mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 v_z^2}{\partial \theta^2}+\frac{\partial^2 v_z}{\partial z^2}\right)-\frac{\partial p}{\partial z}+\rho g_z$$



B.C.1: at $r=0$, $dv_z/dr=0$ (because of symmetry about the centerline)

B.C.2: at $r=R$, $v_z=0$ (the no-slip condition at the pipe surface)

For a given system where fluid is flowing through a pipe, solve the momentum balance equation (cylindrical coordinate) predict the fluid flow profile across the pipe.

* **Make suitable assumption to simplify the model equation before solving.**

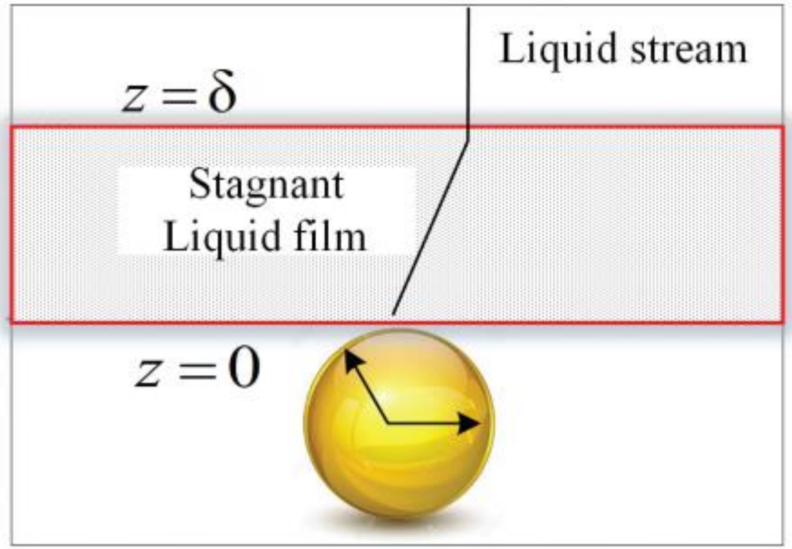
Problem Statements on BVP

(Applications in Chemical Engineering)

Modeling of Mass Transfer Systems

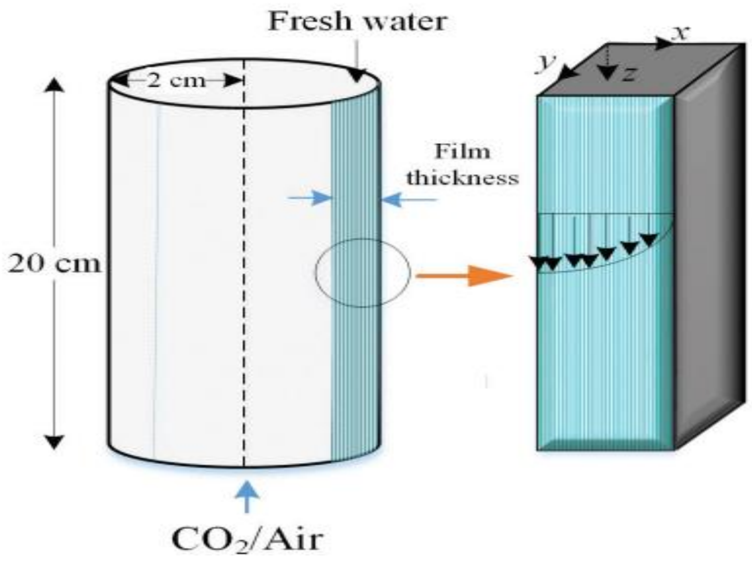
Mass Transport (Extraction)_Boundary Value Problem

Soybean oil, one of the most widely consumed cooking oils, is a vegetable oil extracted from the seeds of the soybean. Processed soybean oil is used as a base for printing inks and oil paints. In this example, a spherical soybean particle having an average diameter 2.00 mm and density $\rho = 577\,\mathrm{kg/m^3}$ is considered as a sample of an extraction process (Figure The soybean flakes contain 20% soybean oil that is to be leaked out by pure hexane solvent. The hexane solvent is flowing over the spherical particles under turbulent flow conditions. Assume a stagnant film of thickness $\delta = 0.5\,\mathrm{mm}$ around the spherical particles through which soybean oil is leached out into the bulk stream. The soybean oil density is $917\,\mathrm{kg/m^3}$, and viscosity is $\mu = 0.05$ Pa.s. The average molecular weight of soybean oil methyl esters is 292.2. The effective diffusivity is $D_{\mathrm{eff}} = 1.0 \times 10^{-11}\ \mathrm{m^2/s}$. Determine the concentration profile.



Mass Transport (Absorption)_Boundary Value Problem

Global warming is caused by the emission of greenhouse gases. Most of the emitted greenhouse gases is carbon dioxide (CO_2). In this example, carbon dioxide is being absorbed from air via a wetted wall column. The column is provided with fresh water at the top of the column, and air containing 5 mole percent CO_2 is supplied at the bottom, as described in Figure Water is flowing downward at a very low velocity of 7.96×10^{-6} m/s. The change in gas composition may be neglected due to the state of the air. The gas phase resistance to mass transfer is negligible. It is acceptable to neglect axial diffusion. Develop an expression for the carbon dioxide concentration in water.



Modeling of Heat-Transfer Systems

Heat Transport_Boundary Value Problem

A thin slab of construction insulation material is subjected to a heat source that causes volumetric heating to vary along the length of it; see Figure

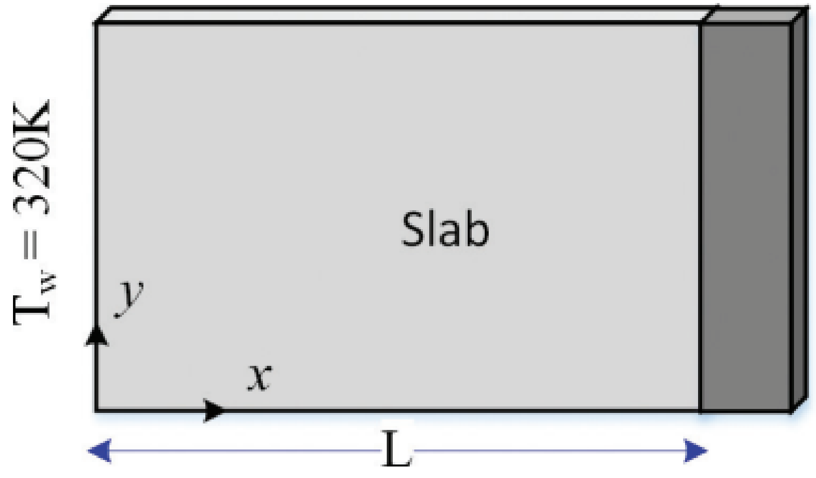
$$q = q_o\left[1 - \frac{x}{L}\right]$$

where:

q_o has a constant value of 1.8×10^5 W/m^3

slab length L is 0.06 m

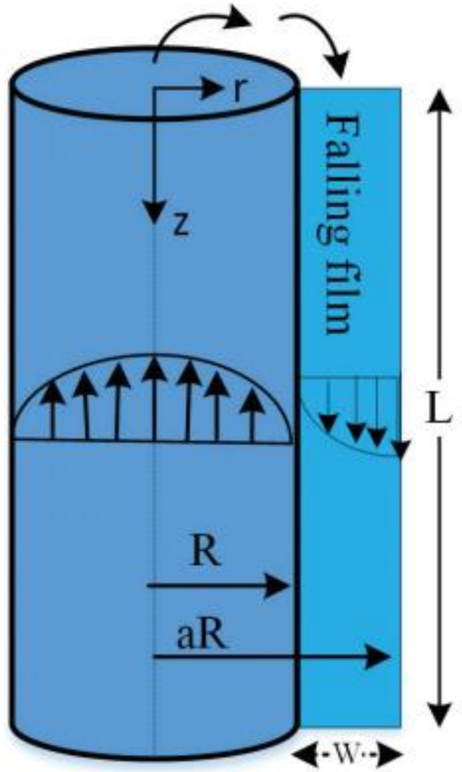
The thermal conductivity of the slab material is 0.6 W/m.K. The boundary at $x = L$ is perfectly insulated, while the surface at $x=0$ is maintained at a constant temperature of 320 K. The slab density is 1900 kg/m^3, and the specific heat capacity is 840 J/(kg . K). Develop an expression for the temperature distribution $T(x)$ in the slab. Determine an expression for the temperature profile $T(r)$, within the thin slab. What is the value of the temperate near the adiabatic wall [3]?



Modeling of Fluid-Flow Systems

Fluid Transport_Boundary Value Problem

In a gas absorption experiment, a fluid flows upward through a small circular tube and then fluid flows downward in laminar flow on the outside of the circular tube (Figure Determine the velocity distribution in the falling film, and neglect end effects. Assume the following: width, 0.1cm; height, 1cm; inlet fluid velocity, 4.35 cm/s; $R = 0.1$ cm.



There are several assumptions that can be made to shorten the problem form:

- Steady state system.
- The flow is only in z-direction.

Solving PDEs using “MATLAB & R”

1D-PDE (Diffusion-Equation) solving using "R"

Consider a one-dimensional PDE type diffusion-reaction model in a packed-bed reactor of length 10 meter. The boundary conditions for the system are given below. Use **R-solver** to predict the concentration change with time and space and also produce the concentration profile. Make100 nodes to carry out the spatial discretization.

BC:

$$\frac{\partial C}{\partial x}_{x=0} = 0$$

$$C_{x=10} = C_{ext}$$

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D \cdot \frac{\partial C}{\partial x}\right) - Q$$

The model parameters are:

```
D    <- 1    # diffusion constant
Q    <- 1    # uptake rate
Cext <- 20
```

1D-PDE (Heat-equation) solving using “MATLAB”

The temperature $u(x, t)$ in a wall of unit length can be described by the one-dimensional heat equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

The thickness of the wall is 1 m and the initial profile of the temperature in the wall at $t = 0$ sec is uniform at $T = 90^\circ$C. At time $t = 0$, the ambient temperature is suddenly changed to 15°C and

held there. If we assume that there is no convection resistance, the temperature of both sides of the wall is also held constant at 15°C. Determine the temperature distribution graphically within the wall from $t = 0$ to $t = 21{,}600$ sec. The wall property can be assumed as $\alpha = 4.8 \times 10^{-7}$ m/sec^2.