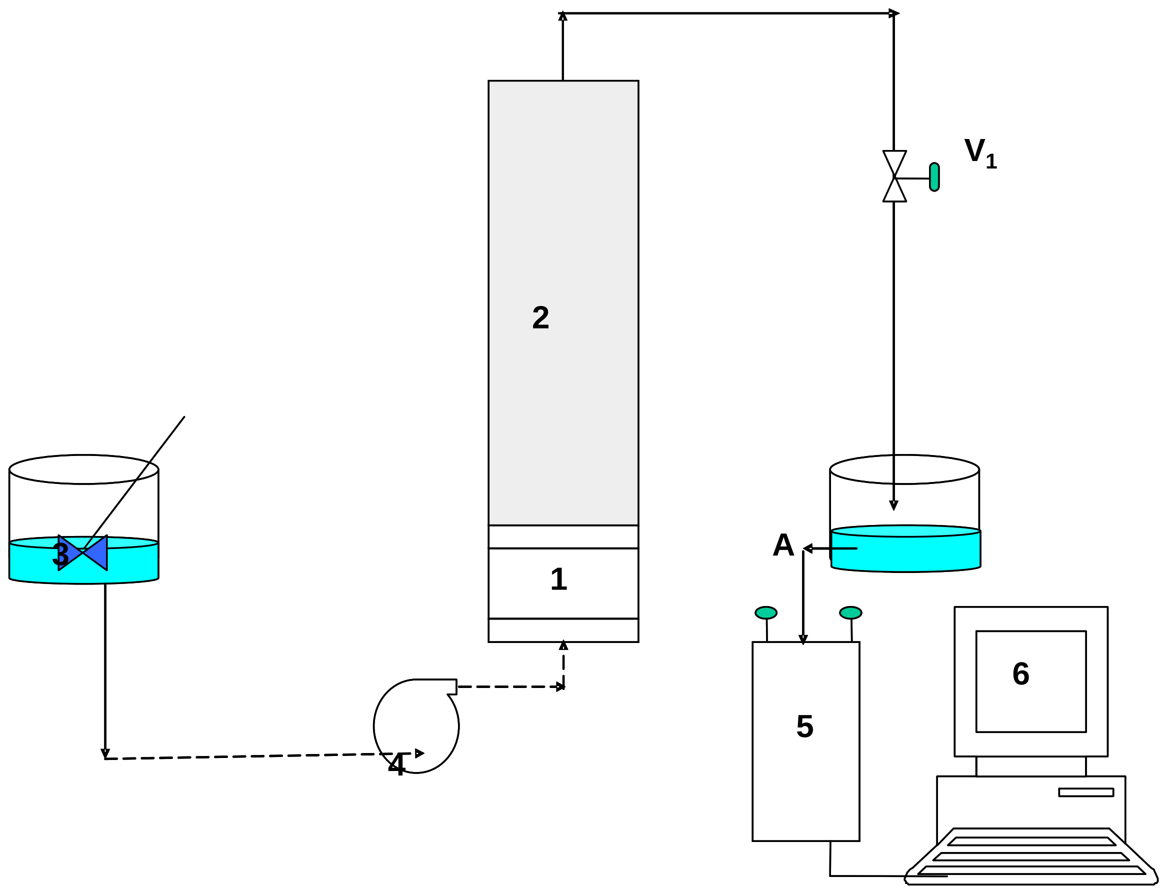
DETERMINISTIC ADSORPTION MODEL FOR WASTEWATER TREATMENT

Experimental Setup



1- Distributor section 2-Test section 3 – Feed tank 4 – Peristaltic pump 5 – Conductivity meter 6 – Computer. A is sampling port for measuring TDS

Model Assumptions

- Flow is One-dimensional in the vertical direction and uniform across the cross sectional area
- The equilibrium adsorption relation is represented by modified BET adsorption isotherm.
- The bed is fully saturated with liquid.(i.e. all interparticle voids are filled with liquid)
- There is no mass transfer resistance on the liquid side.

MODELING AND SIMULATION

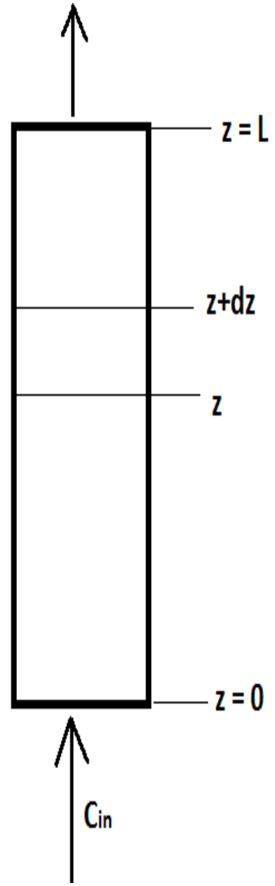
One dimensional solute transport equation :

Accumulation = input- output + generation

$$\left(\varepsilon C|_{t+\Delta t}\,.A.\Delta Z\right)-\left(\varepsilon C|_{t}\,.A.\Delta Z\right)=\ \varepsilon.A.\Delta t\left(-D.\frac{\partial C}{\partial Z}\Big|_{Z}+uC|_{Z}\right)-\left(\varepsilon.A.\Delta t\left(-D.\frac{\partial C}{\partial Z}\Big|_{Z+\Delta Z}+\right.\right.$$

$$\left.\left.uC|_{Z+\Delta Z}\right)\right)-(1-\varepsilon)\rho\frac{\partial q}{\partial t}A.\Delta Z.\Delta t$$

$$\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial Z^2}-u\frac{\partial C}{\partial Z}-\frac{(1-\varepsilon)\rho}{\varepsilon}.\frac{\partial q}{\partial t}. \quad \textbf{...(1)}$$



BET isotherm : for liquid phase Bio-Reactor adsorption

$$q = q_m \frac{k_s\, C[1 - (N+1)(k_l C)^N + N(k_l C)^{N+1}]}{(1 - k_l C)[(1 + \left(\frac{k_s}{k_l} - 1\right) k_l C - \frac{k_s}{k_l}(k_l C)^{N+1}]} \quad \textbf{...(2)}$$

When N→∞ , $$q = q_m \frac{k_s C}{(1 - k_l C)(1 - k_l C + k_s C)} \quad \textbf{...(3)}$$

When N = 1, $$q = q_m \frac{k_s C}{1 + k_s C} \quad \textbf{...(4)}$$

Where,

N is no. of layers

q_m- monolayer adsorption capacity, mg/g

C- is the equilibrium liquid phase concentration, mg/L

Modeling and simulation

- Solving the one dimensional transport equation with adsorption isotherm equation we will lead to the expression in this form,

$$\frac{\partial C}{\partial t} = D\,\frac{\dfrac{\partial^2 C}{\partial z^2} - u\,\dfrac{\partial C}{\partial z}}{g(C)} \qquad \textbf{...(5)}$$

Where g(C) is a function of concentration and it will be different for different situations**.**

Modeling and simulation

Using Eqs (1) and (2)

$$g(C) = 1 + \frac{(1-\varepsilon)\rho q_m k_s}{\varepsilon . B^2}\left[B\{1-(N+1)^2(k_l . C)^N + N(N+2)(k_l C)^{N+1}\}\right.$$

$$\left. - A\left\{k_s - 2k_l - k_s(k_l C)^N(N+1) - 2k_s k_l C + 2k_l^2 C + (N+2)k_s(k_l C)^{N+1}\right\}\right]$$

here, $A = C[1-(N+1)(k_l C)^N + N(k_l C)^{N+1}]$

$$B = (1-k_l C)\left[\left(1 + \left(\frac{k_s}{k_l} - 1\right)k_l C - \frac{k_s}{k_l}(k_l C)^{N+1}\right]\right.$$

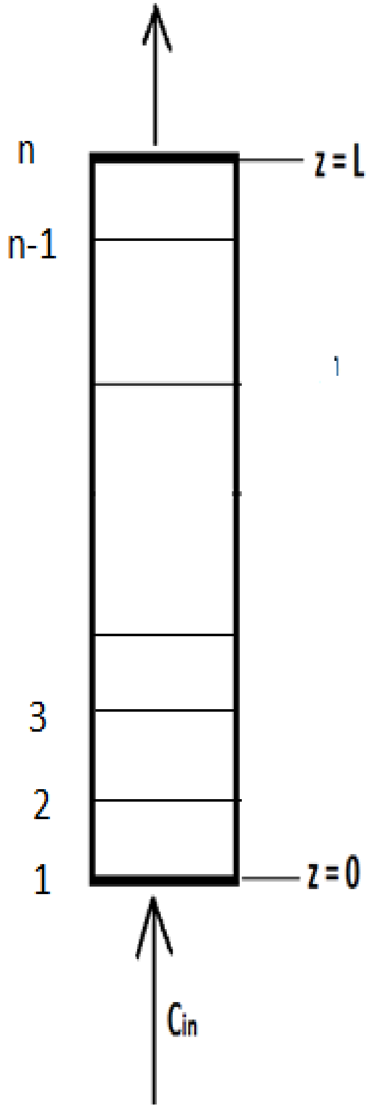
Using Eqs (1) and (3)

$$g(c) = 1 + \frac{(1-\varepsilon)}{\varepsilon}\rho q_m k_s \frac{[1 - k_l^2 C^2 + k_l k_s C^2]}{[(1-k_l C)(1-k_l C + k_s C)]^2}$$

Using Eqs (1) and (4)

$$g(c) = 1 + \frac{(1-\varepsilon)}{\varepsilon}\frac{\rho q_m k_s}{(1+k_s C)^2}$$

- To solve Eqs 5 finite difference scheme was used.
- The concentration in the bed is discretized in the spatial direction. For that bed is divided into n-1 grids (n grid points).
- The grid points are numbered from 1 to n as we vary Z from 0 (entrance) to L (exit).
- The evaluation of the concentration with time in each node is modeled through ordinary differential equations.



For i th grid point, eq. 5 can be written as

$$\frac{\partial C_i}{\partial t} = D\,\frac{\dfrac{\partial^2 C_i}{\partial Z^2} - u\dfrac{\partial C_i}{\partial Z}}{g(C_i)} \qquad \textbf{...(6)}$$

By Central difference approximation of $\frac{\partial C}{\partial Z}$ at node 'i' is,

$$\left.\frac{\partial C}{\partial Z}\right|_i = \frac{C_{i+1} - C_{i-1}}{2\Delta Z} \qquad \textbf{...(7)}$$

By Central difference approximation of $\frac{\partial^2 C}{\partial Z^2}$ at node 'i' is,

$$\left.\frac{\partial^2 C}{\partial Z^2}\right|_i = \frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta Z^2} \qquad \textbf{...(8)}$$

Modeling and simulation

Using central difference scheme for the derivatives we obtain,

$$\frac{dC_i}{dt} = \frac{D\left({C_{i+1} - 2C_i + C_{i-1}}/{\Delta Z^2}\right) - u\left({C_{i+1} - C_{i-1}}/{2\Delta Z}\right)}{g(C_i)} \qquad \textbf{...(9)}$$

for i = 1,

$$\frac{dC_1}{dt} = \frac{D\left({C_2 - 2C_1 + C_0}/{\Delta Z^2}\right) - u\left({C_2 - C_0}/{2\Delta Z}\right)}{g(C_1)} \qquad \textbf{...(10)}$$

Similarly for i = n,

$$\frac{dC_n}{dt} = \frac{D\left({C_{n+1} - 2C_n + C_{n-1}}/{\Delta Z^2}\right) - u\left({C_{n+1} - C_{n-1}}/{2\Delta Z}\right)}{g(C_n)} \qquad \textbf{...(11)}$$

Initial and boundary conditions

- Initial condition is: C (t=0) =0; for 0<z<L

  Closed Danckwerts Boundary condition
- Boundary conditions are

At z=0 (entry)

$$\boxed{uC_{in} = -D\frac{\partial C}{\partial z} + uC}$$

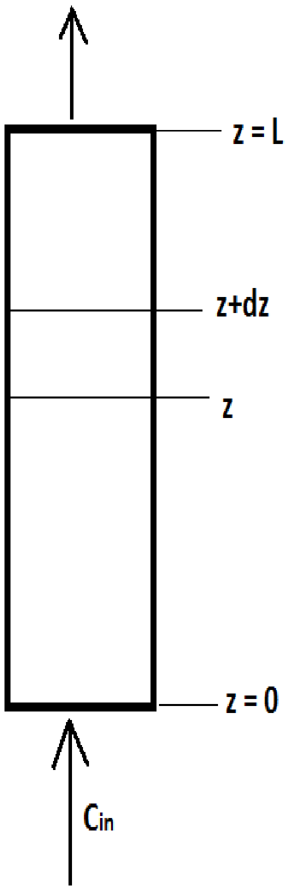
At z = L (exit)

$$uC(L^+) = uC(L^-) - D\frac{\partial C(L^-)}{\partial z}$$

imposing continuity of concentration at the exit of the bed we obtain

$$D\frac{\partial C(L^-)}{\partial Z} = 0$$

$$uC(L^+) = uC(L^-)$$



Using central difference scheme for boundary condition at the inlet and the outlet of the tower

$$C_0 = C_2 - \frac{2u\Delta Z}{D}(C_1 - C_{in})$$

$$C_{n+1} = C_{n-1}, \qquad \text{At node n}$$

Thus Eq. (11) will be reduced to

$$\frac{dC_n}{dt} = \frac{\left({2D}/{\Delta Z^2}\right)(C_{n-1} - C_n)}{g(C_n)}$$

These n differential Equations are subjected to n initial condition. The concentration evolution with time was obtained using MATLAB

Initial and boundary conditions: recycle mode

Initial and boundary conditions

- Initial conditions:

  C (t=0) =0; for 0<z<L and $C_{tank} = C_{feed}$

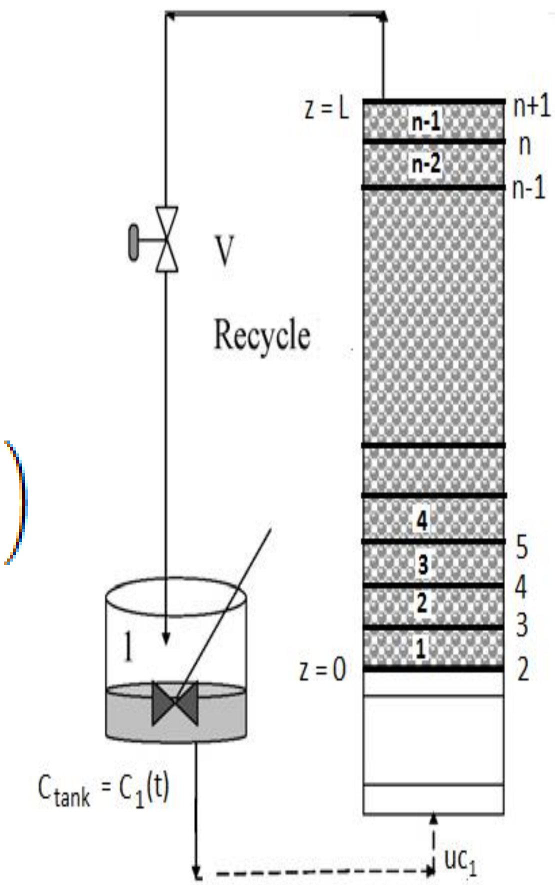
- Boundary conditions :

At z=0 (at node 2 i.e. inlet)

$$uC_{tank} = \left(-D.\frac{\partial C}{\partial Z}\bigg|_2 + uC|_2 \right)$$

At z = L (exit)

$$uC(L^+) = -D\frac{\partial C(L^-)}{\partial Z} + uC(L^-)$$



$$D\frac{\partial C(L^-)}{\partial Z} = 0 \qquad uC(L^+) = uC(L^-)$$

Modeling and simulation: Recycle mode

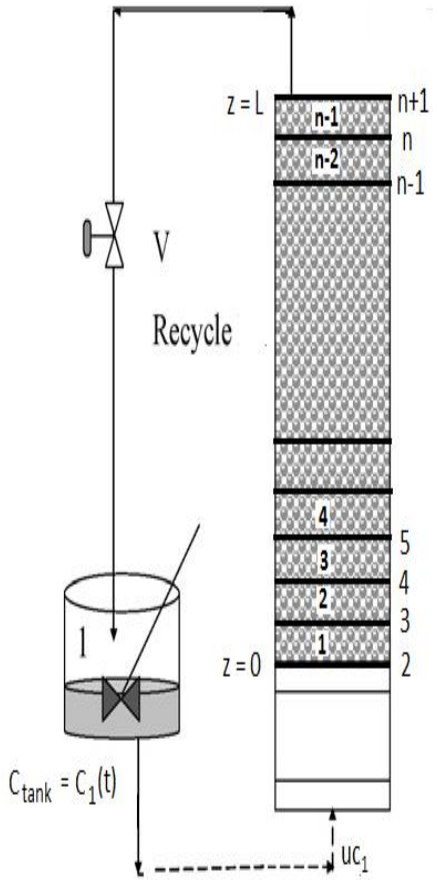
For tank Accumulation = Input - Output

$$V\frac{dC_{tank}}{dt} = v[C(L) - C_{tank}]$$

$$\frac{dC_{tank}}{dt} = \frac{v}{V}[C(L) - C_{tank}]$$

$$\frac{dC_1}{dt} = A_1[C(L) - C_1] \qquad A_1 = \frac{v}{V}$$

$$\frac{dC_1}{dt} = A_1[C_{n+1} - C_1] \qquad C_{tank} = C_1$$



Modeling and simulation: Recycle mode

BET isotherm

$$q = q_m \frac{k_s C[1 - (N+1)(k_l C)^N + N(k_l C)^{N+1}]}{(1 - k_l C)[(1 + \left(\frac{k_s}{k_l} - 1\right) k_l C - \frac{k_s}{k_l}(k_l C)^{N+1}]}$$

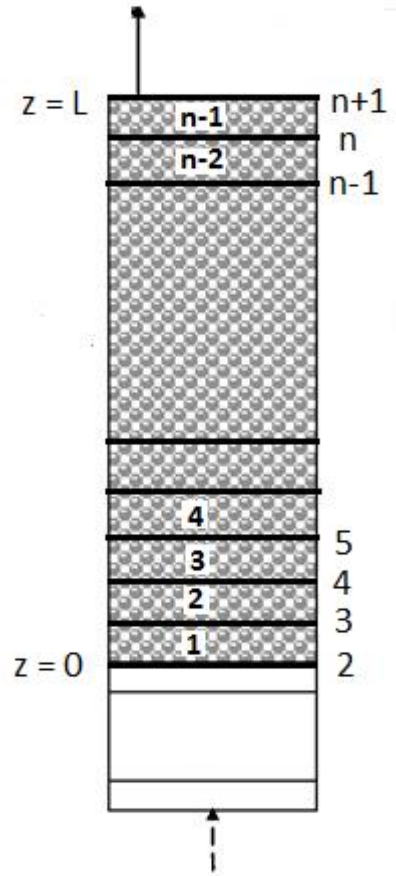
For N$\longrightarrow$ $q = q_m \dfrac{k_s C}{(1 - k_l C)(1 - k_l C + k_s C)}$

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial Z^2} - u \frac{\partial C}{\partial Z} - \frac{(1-\varepsilon)\rho}{\varepsilon} . \frac{\partial q}{\partial t} .$$

One dimension solute transport equation

The concentration in the bed is discritized in the spatial direction.

$$\frac{\partial C}{\partial t} = D\,\frac{\frac{\partial^2 C}{\partial z^2} - u\,\frac{\partial C}{\partial z}}{g(C)}$$



Where g(C) is a function of concentratio

For that bed is divided into n-1 grids using n grid points (from 2 to n+1).

In packed bed At i^th node

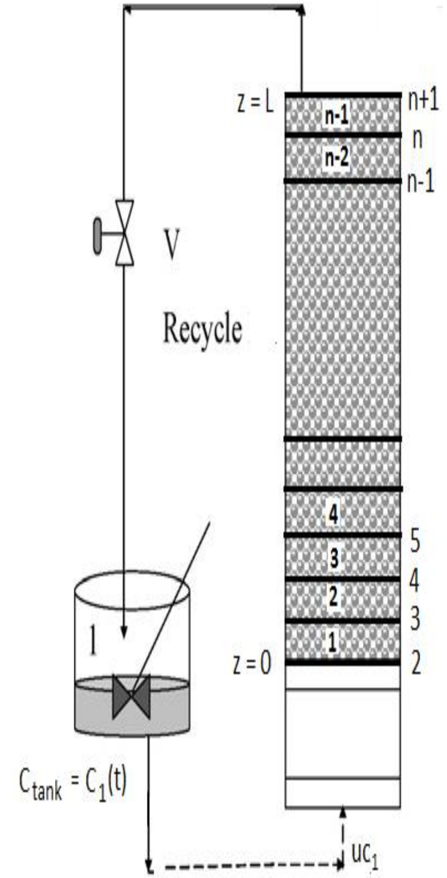
$$\frac{dC_i}{dt} = \frac{D\left(C_{i+1} - 2C_i + C_{i-1}/_{\Delta Z^2}\right) - u\left(C_{i+1} - C_{i-1}/_{2\Delta Z}\right)}{g(C_i)}$$

At node 2

$$\frac{dC_2}{dt} = \frac{D\left(C_3 - 2C_2 + C_1'/_{\Delta Z^2}\right) - u\left(C_3 - C_1'/_{2\Delta Z}\right)}{g(C_2)}$$

$$uC_{tank} = \left(-D.\frac{\partial C}{\partial Z}\bigg|_2 + uC|_2\right)$$

$$uC_{tank} = \left(-D.\frac{\partial C}{\partial Z}\bigg|_2 + uC|_2\right) \longrightarrow C_1' = C_3 - \frac{2u\Delta Z}{D}(C_2 - C_1)$$



From node 3 to n

$$\frac{dC_i}{dt} = \frac{D\left(C_{i+1} - 2C_i + C_{i-1}/_{\Delta Z^2}\right) - u\left(C_{i+1} - C_{i-1}/_{2\Delta Z}\right)}{g(C_i)}$$

At node n+1 (exit)

$$\frac{dC_{n+1}}{dt} = \frac{D\left(C_{n+2} - 2C_{n+1} + C_n/_{\Delta Z^2}\right) - u\left(C_{n+2} - C_n/_{2\Delta Z}\right)}{g(C_{n+1})}$$

$$uC(L^+) = -D\frac{\partial C(L^-)}{\partial Z} + uC(L^-) \qquad D\frac{\partial C(L^-)}{\partial Z} = 0$$

$$uC(L^+) = uC(L^-) \longrightarrow C_{n+2} = C_n$$

$$\frac{dC_{n+1}}{dt} = \frac{\left(2D/_{\Delta Z^2}\right)(C_n - C_{n+1})}{g(C_{n+1})}$$

So we get n+1 ODEs subjected to n+1 initial conditions

which can be solved using MATLAB.