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FEM ANALYSIS OF CONTAMINATE TRANSPORT IN LOAMY DESERT SOIL

Presented By,

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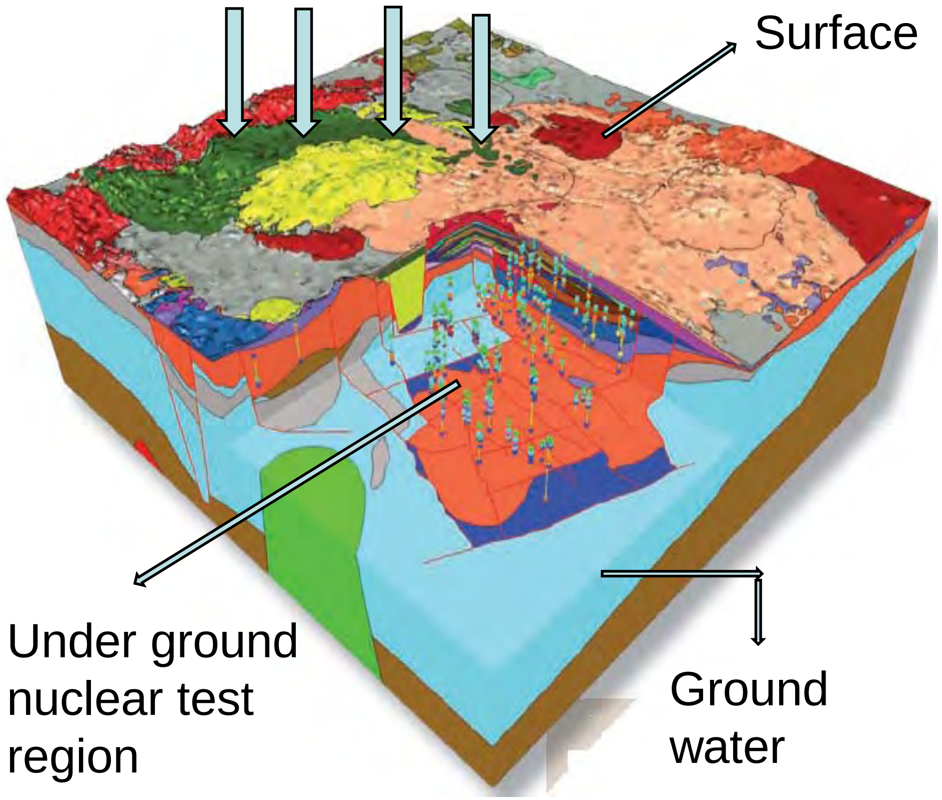
INTRODUCTION



- From 1951 to 1992, 828 underground nuclear tests were conducted at the Nevada Test Site.
- Most of these tests were conducted hundreds of feet above the groundwater table
- One third of these were near the water table
- Rain water can mobilize the radionuclide ions present in the soil and can contaminate the ground water

Figure 1: Three Dimensional representation of how water and contaminates flow through soil in Nevada test site.
Ref: www.nv.doe.gov

MODEL DISCRIPTION

- Advective Dispersion Reaction Model:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D_L\frac{\partial^2 C}{\partial^2 x} - \frac{\rho(1-\varepsilon)}{\varepsilon}\frac{\partial q}{\partial t}$$

Rate of solute change in liquid phase

Convective flux term

Solute Transport by dispersion

Rate of solute adsorption on soil phase

ρ *Density of soil, kg/cm³*

ε *Porosity of the bed*

D_L *Dispersion Coefficient, m²/min*

v *Velocity, m/min*

Equilibrium between the solid and liquid phase

$$\frac{\partial q}{\partial t} = \frac{\partial q}{\partial C}\left[\frac{\partial C}{\partial t}\right]$$

Ref: Applied contaminate transport modeling, Second edition , Chunmiao Zheng, Gordon D. Bernnett

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ADSORPTION ISOTHERM

- Langmuir Adsorption Isotherm

$$q = \frac{q_0 CK}{1 + CK}$$

q_0 Monolayer capacity, mol/kg
K Adsorption Coefficient,m^3/mol

$$\frac{\partial q}{\partial C} = \frac{q_0 K}{(1 + KC)^2}$$

First derivative of the Langmuir equation

$$\frac{\partial C}{\partial t}\left[1 + \frac{\rho(1-\varepsilon)}{\varepsilon}\frac{q_0 K}{(1+KC)^2}\right] = -v\frac{\partial C}{\partial x} + D_L \frac{\partial^2 C}{\partial^2 x}$$

Final PDE by combining equilibrium and Langmuir expression

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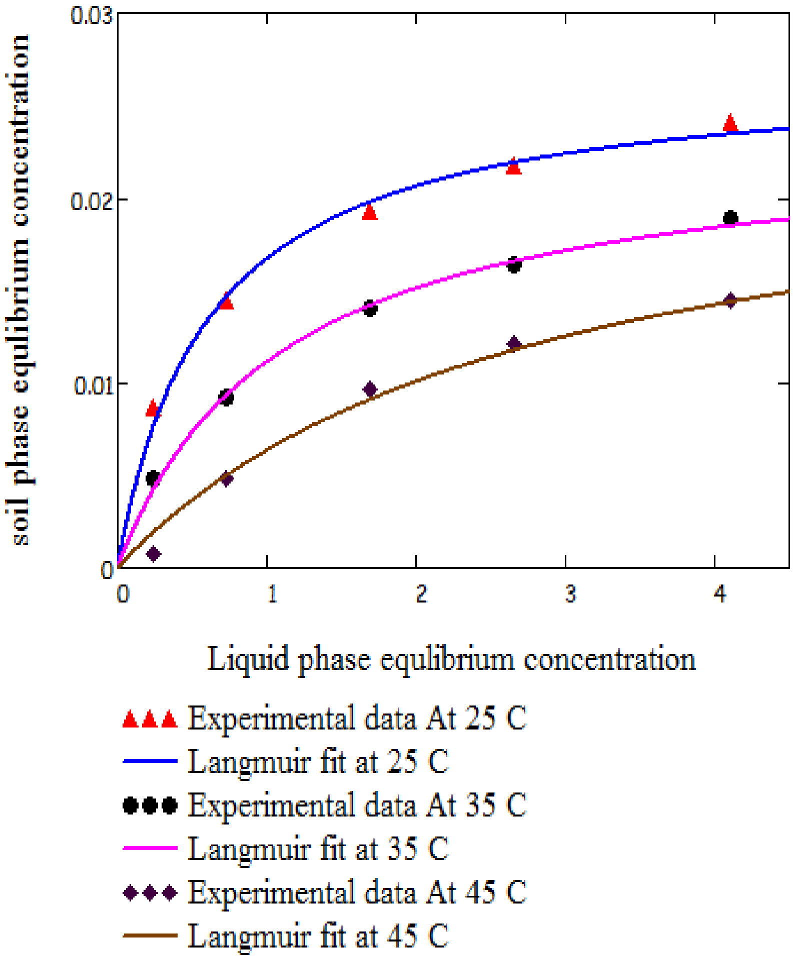
Batch Adsorption Results



T	q_0 ,mol/kg	*K* ,m^3/mol	RMSE
25^0C	0.027	1.633	0.00060
35^0C	0.023	0.906	0.00069
45^0C	0.022	0.357	0.00069

T *Temperature, ^{o}C*

q_0 *Monolayer capacity, mol/kg*

K *Adsorption Coefficient,m^3/mol*

RMSE *Root mean square error*

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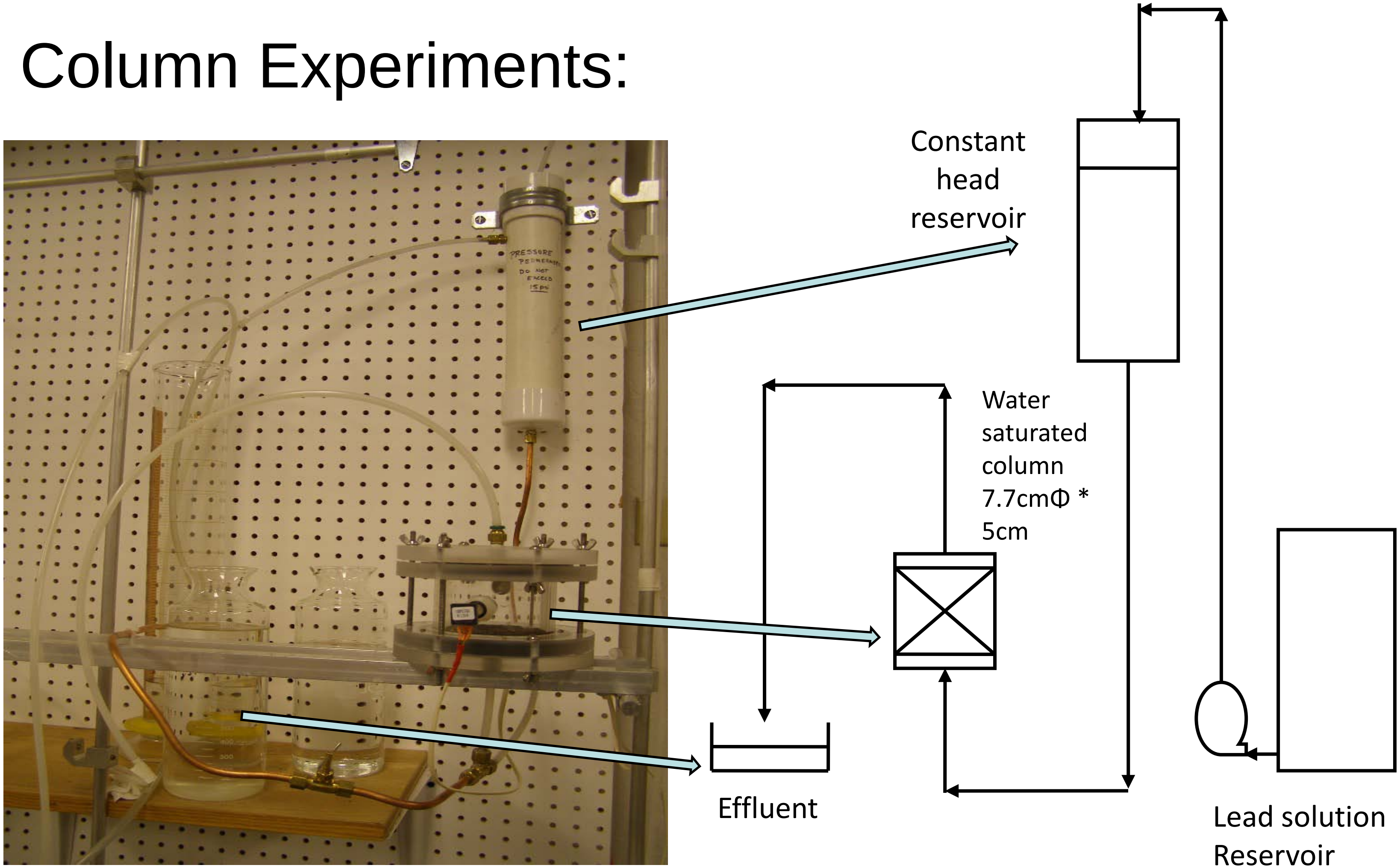
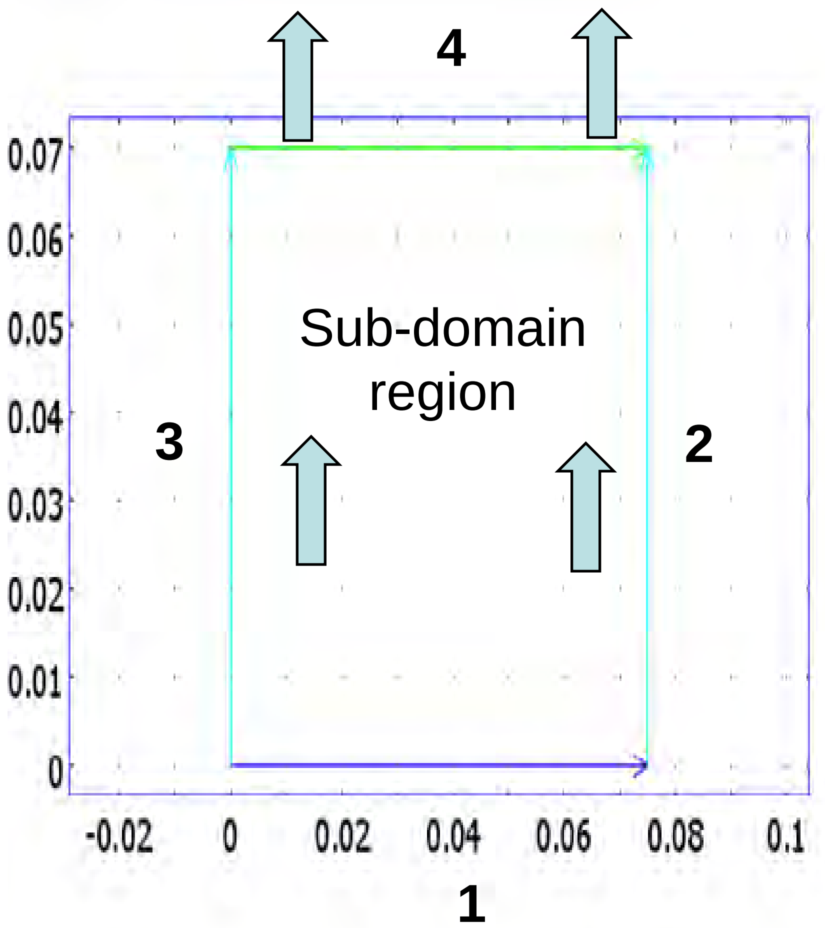
Experiments and Model Validation

Column Experiments:



Boundary and Initial Conditions



Boundaries	Boundary conditions ($t \geq 0$)
1	$C = C_0$
2	Insulation (Flux = 0) $\frac{\partial C}{\partial t} = 0$
3	Insulation (Flux = 0) $\frac{\partial C}{\partial t} = 0$
4	Convective Flux
Sub-domain region	($t=0$) $C=0$

MODEL PARAMETERS

C_0	0.314 mol/m^3
K	1.633, 0.906, 0.357 m^3/mol
ε	0.45
ρ	1500 kg/m^3
q_0	0.027, 0.023, 0.022 mol/kg
v	1.5*10^{-5} m/s
D_L	8.7*10^{-7} m^2/s
δt	$1+\frac{(1-\varepsilon)}{\varepsilon}\frac{q_0 K}{(1+KC)^2}$

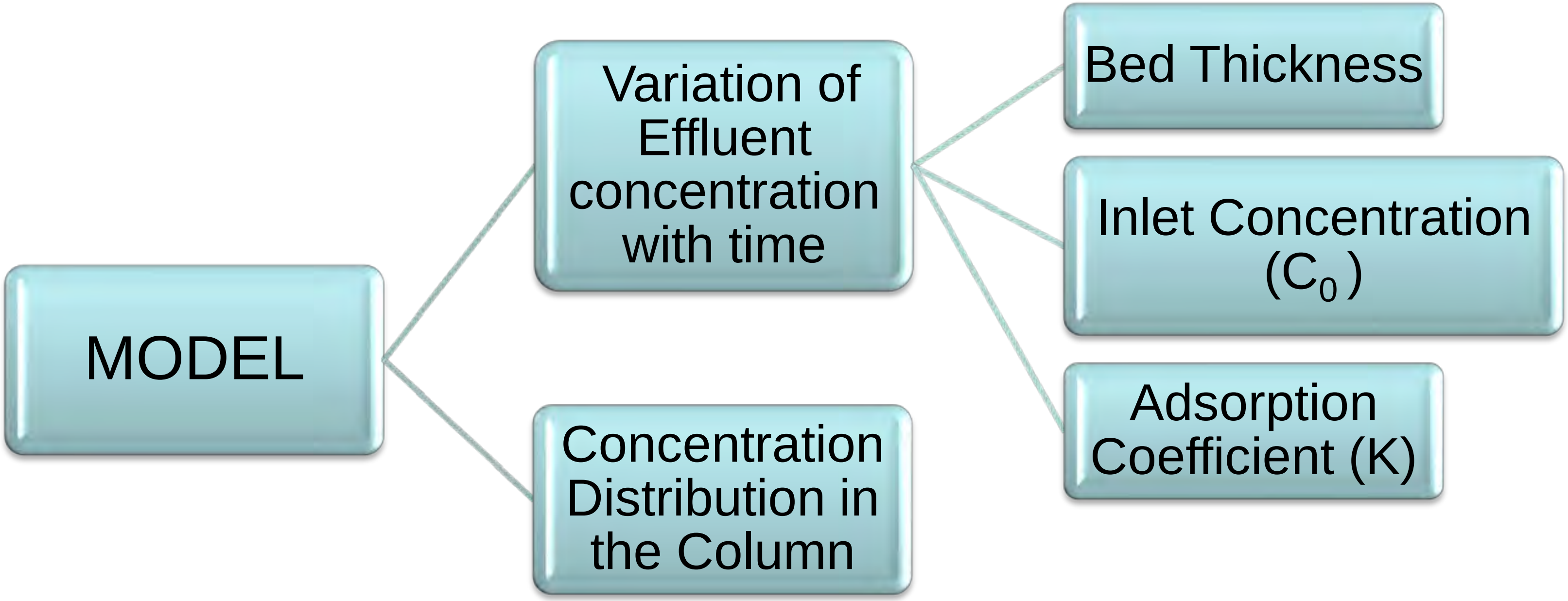
Darcy's Law to determine velocity of adsorbate solution

$$Q = \frac{KA(h_2 - h_1)}{L}$$

$$Q = Av$$

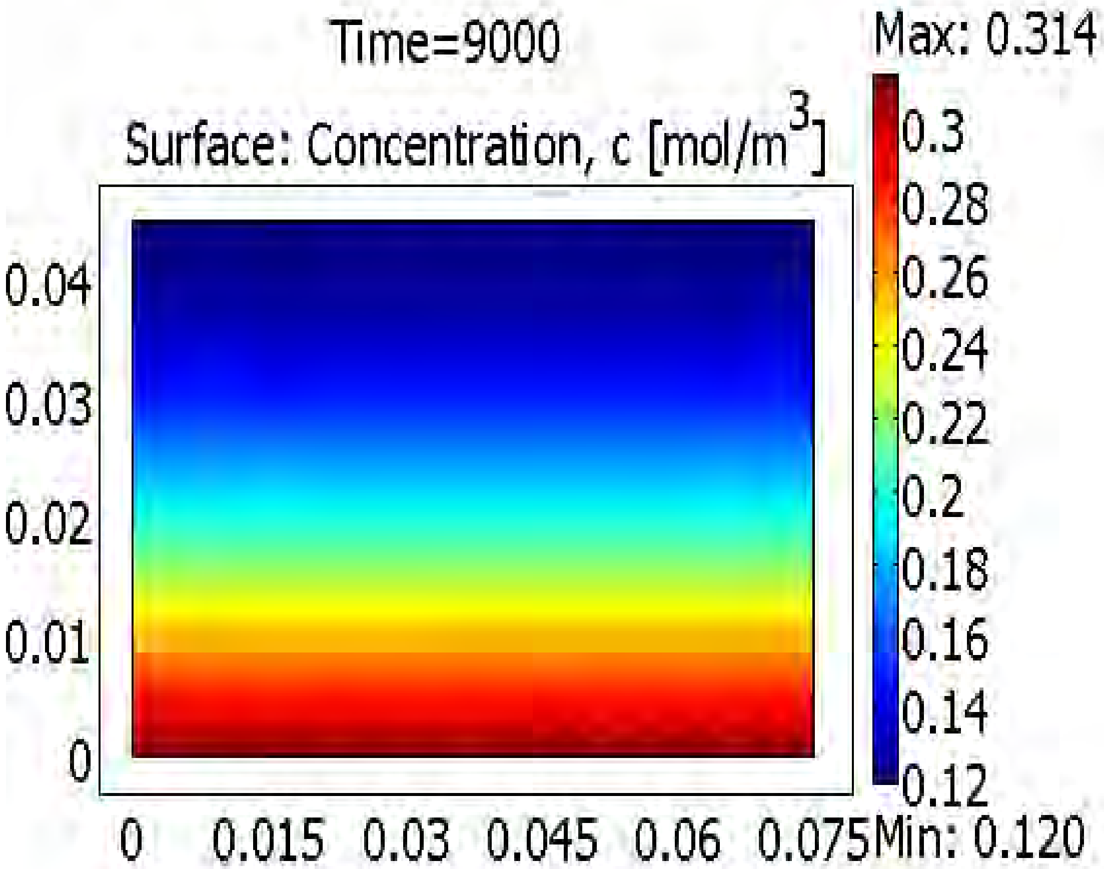
- *K Hydrodynamic conductivity, m/s*
- *A Cross sectional area,m^2*
- *L Length of the soil packing in the column ,m*
- *Q Volumetric flow rate, m^3/min*
- *v Velocity ,m/s*

Quantitative evaluation of Model



“Convection Diffusion module” in “Comsol Multiphysics 3.2” provide the best features to couple any nonlinear adsorption isotherm with the “Advective Dispersion Reaction Equation”

MODEL EVALUATION

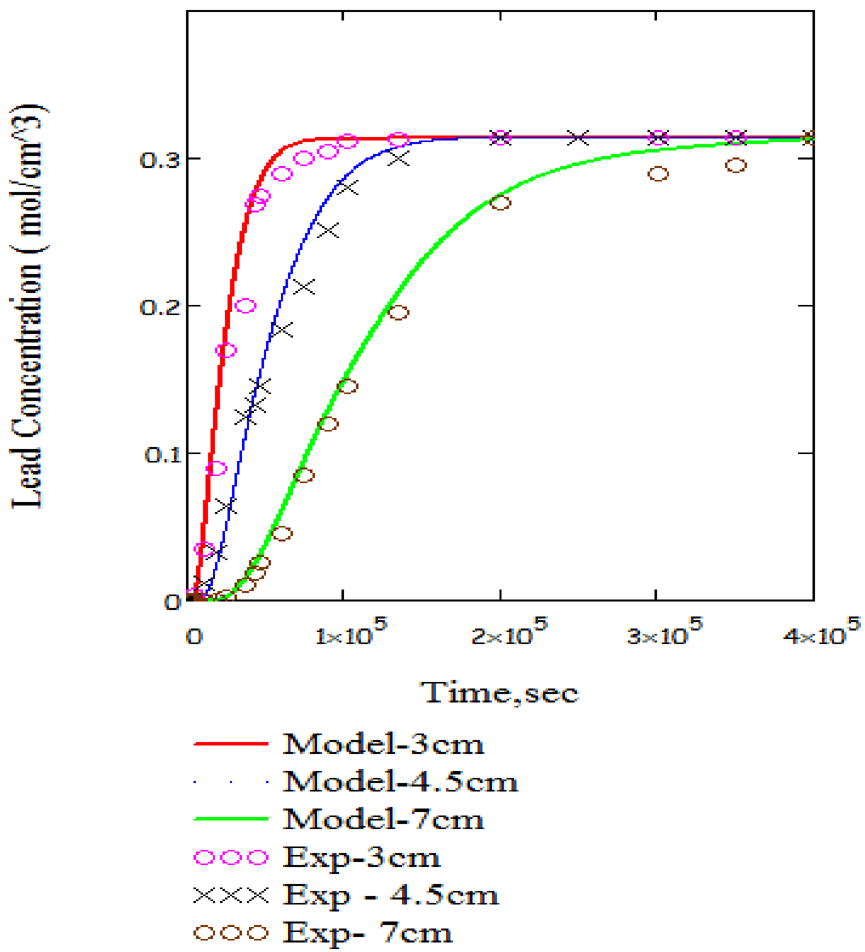


Contaminant concentration distribution in the column

Conditions:

- C_0 = 0.314 mol/m^3
- Q = 6ml/min
- *Bed thickness = 4.5 cm*
- K = 1.66 m^3/mol
- q_0 = 0.027 mol/m^3

Break through curves for different bed thickness and Experimental Validation



Bed Thickness	Saturation Time
3 .0 cm	$1.5*10^5$ sec (1day 17 hr)
4.5 cm	$2.0*10^5$ sec (2days 8hr)
7.0 cm	$5*10^5$ sec (5days 18hr)

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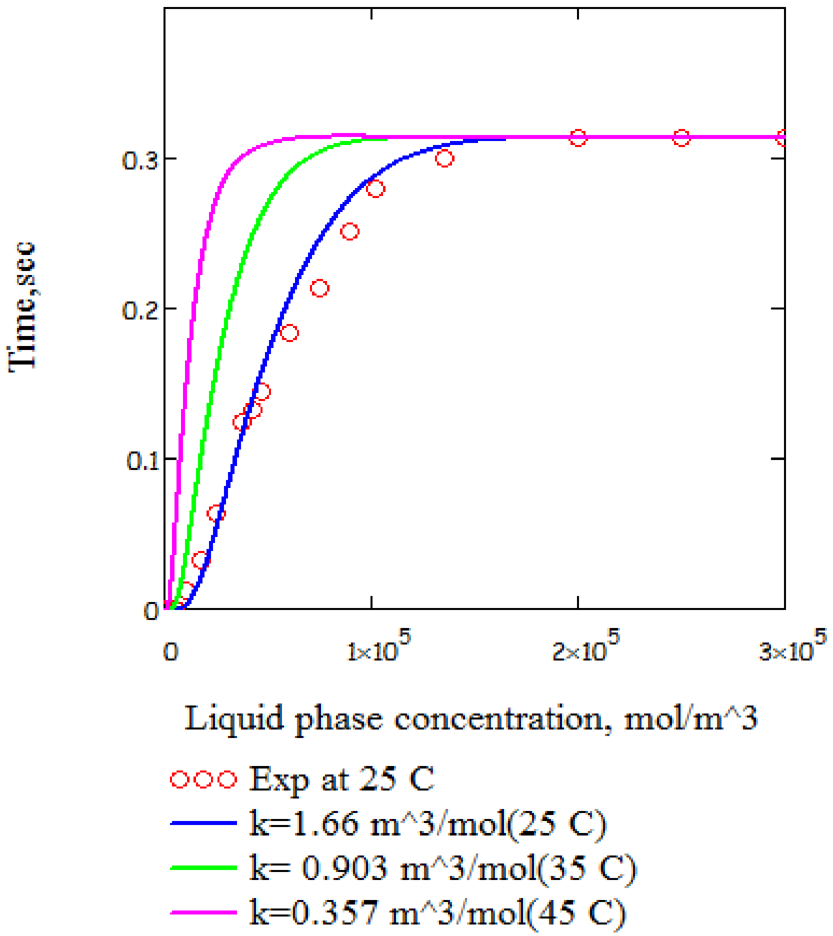
Break through curves for different values of *K*



Conditions:

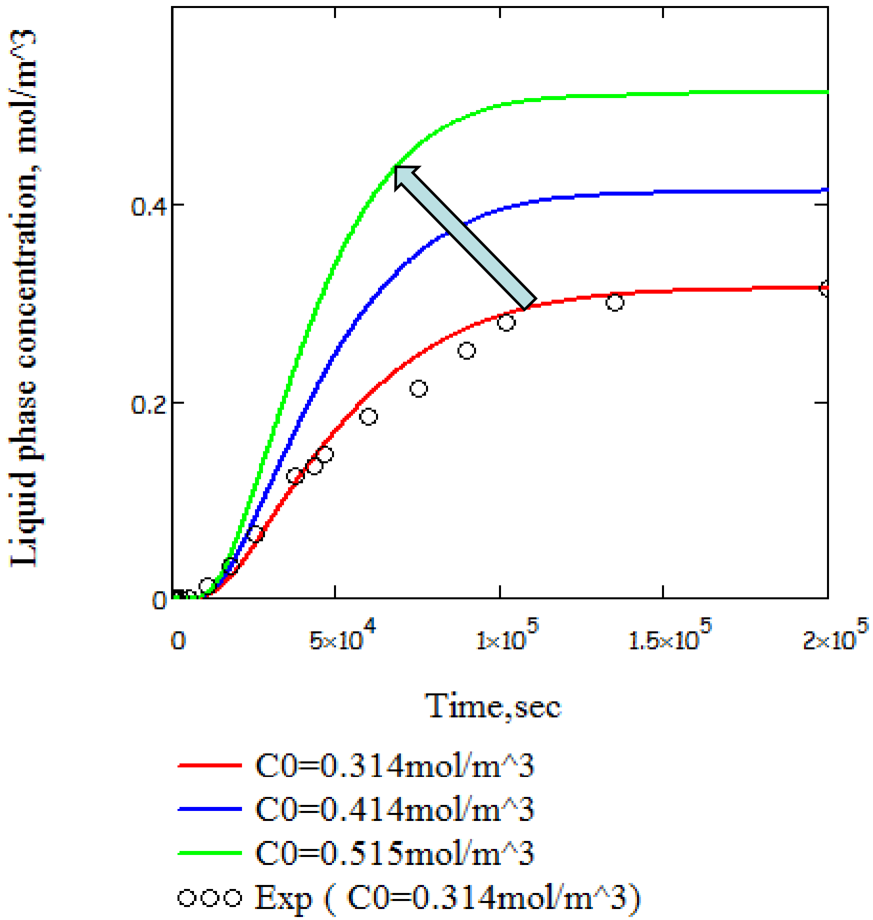
- *C_0 = 0.314 mol/m^3*
- *Q = 6ml/min*

Bed thickness = 4.5 cm

- *K values obtained from batch experiments are used to simulate the system. Model is validated for 1.66 m^3/mol.*
- *Saturation time decreases with decrease in k value.*

K m^3 /mol	Saturation Time
1.66	2*10^5 sec
0.37	0.7*10^5 sec

Break through curves for different Initial Concentrations



Conditions:

- *$K = 1.633\ m^3/mol$*
- *$q_0 = 0.027$ mol/kg*
- *Q = 6ml/min*
- *Bed thickness = 4.5 cm*

The break through curves are steeper for higher values of feed concentration

Mass transfer rate ⬆

Bed Saturation Time ⬇

Equilibrium attains faster

Conclusions and future Developments

- Advective Dispersion Reaction Equation (ADRE) coupled with Langmuir adsorption isotherm was solved using COMSOL MULTIPHYSICS -3.2
- Any Nonlinear adsorption isotherms can be readily coupled with ADRE using this model and solved by COMSOL MULTIPHYSICS -3.2
- This model can be used to predict the behavior of the system under various conditions without conducting the experiments by knowing the adsorption parameters
- Velocity variation along the length of the column was not considered, momentum equation will be coupled with ADRE to over come this limitation

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THANK YOU

QUESTIONS ?