Applied Groundwater Flow and Contaminant Transport Modeling

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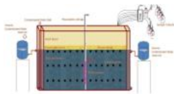
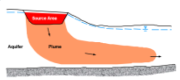
Groundwater Salinity Issues and Management Solutions, February 17th -19th, 2021

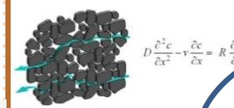
Areas of Research Interest

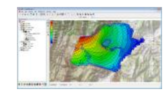
Practical
(field & Lab)
Experiments



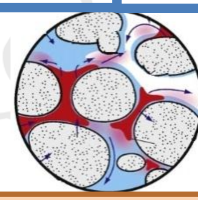


Subsurface water flow & Contaminant transport





Numerical
(1/2/3 D)
Modeling



Remediation Techniques
(Engineered bioremediation, Phytoremediation, Wetlands, PRBs etc.)

Density Dependent Flow
(CO_2 sequestration , Salt water intrusion, Multiphase flow)

Vadose zone hydrology
(Plant-Soil-Atmospheric Interactions, solute transport)

Subsurface flow and contaminant transport

- Assessment of water/contaminant movement in subsurface plays a important role in managing soil-water resources.
- GW laboratory is developed for conducting experiments and numerical modeling related to flow/transport through variably saturated zones.
- Multi-D experimental setups (microcosms, column, lysimeters, 2/3-D tank) are developed for investigating subsurface processes under varying BCs.
- Computing tools MODFLOW, HYDRUS 2/3D, STOMP, COMSOL are used for numerical modeling.
- Research problems related to fate and transport of heavy metals, hydrocarbons, salt and nitrates in subsurface are particularly addressed using this facility
- This facility is also used in imparting hands-on training to students of institute and other participants visiting to us during training courses.

Problems with Groundwater

- ➢ Groundwater overdraft / mining
- ➢ Subsidence
- ➢ Waterlogging
- ➢ Seawater intrusion
- ➢ Groundwater pollution

Groundwater Pollutants

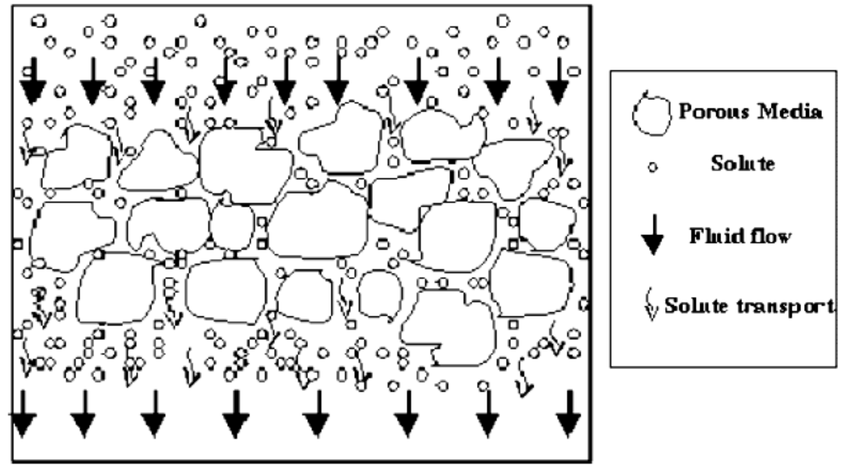
- Volatile Organic Compounds
- Heavy Metals
- Pathogens
- Nitrates and Pesticides
- Salts
- Emerging Pollutants
- Oxygen demanding wastes

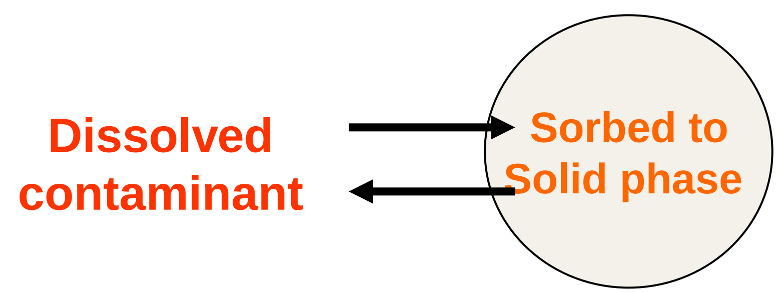
Point and diffuse (non-point) sources,
Miscible and immiscible (NAPLs),
Volatile and Non-volatile,
Conservative and Reactive,
Naturally occurring* and *anthropogenic contaminants

Mass Transport Vs Mass Transfer

1. Mass Transport
    1. Advection
    2. Dispersion
    3. Diffusion
2. Mass Transfer
    1. (De)sorption
    2. Absorption
    2. Dissolution
    3. Volatilization
    4. Decay

Contaminant migration through soil





(De)sorption in porous media

Contaminant Transport

$$J = J_{adv} + J_{dis} + J_{diff}$$

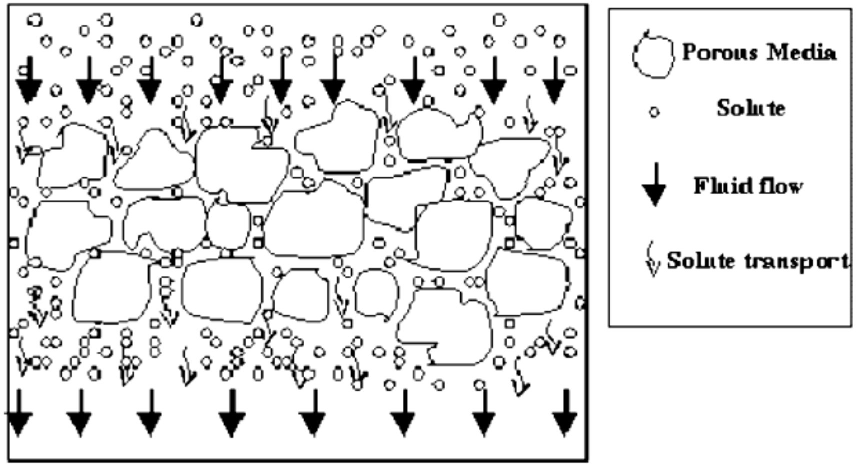
Advective Flux

$$J_{adv} = q\,C = v\theta C$$

Diffusive Flux

$$J_{diff} = -\tau D_0 \theta \frac{\partial C}{\partial z}$$

Dispersive Flux



Contaminant migration through soil

$$J_{dis} = -D_m \theta \frac{\partial C}{\partial z}$$ where $$D_m = \alpha_L v = \alpha_L q/\theta$$

$$J = J_{adv} + J_{dis} + J_{diff} = q\,C - D\theta \frac{\partial C}{\partial z}$$ where $$D = \tau D_0 + \alpha_L q/\theta$$

Contaminant Transport in Unsaturated Zone

With Sink term

$$J = qC - D\theta\frac{\partial C}{\partial z}$$

Advection-dispersion equation

$$\frac{\partial C}{\partial t} + \frac{\partial(\rho_s S^d)}{\partial t} = -\frac{\partial J}{\partial z} - S_C$$

$$\frac{\partial(\rho_s S^d)}{\partial t} + \frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial z}\left[D\theta\frac{\partial C}{\partial z} - qC\right] - S_C$$

$S_C = 0$

Without Sink

$$\frac{\partial(\rho_s S^d)}{\partial t} + \frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial z}\left[D\theta\frac{\partial C}{\partial z} - qC\right]$$

C = Contaminant concentration in the soil [ML-3]

S^d = Contaminant adsorbed to the soil [MM^{-1}]

D = Hydrodynamic dispersion coefficient [M^2S^{-1}]

ρ = Bulk density of soil [ML^{-3}]

S_c = uptake term [$ML^{-3}S^{-1}$].

Adsorption Isotherms

In some cases, the assumption of linearity may not hold.

Therefore, a nonlinear relationship between s and C must be proposed. There are two well-known forms: **Langmuir** and **Freundlich**.

Freundlich Isotherm

For cases that there is no limitation of sites (no limit of the solute amount sorbed on the soild), Freundlich adsorption isotherm applies:

$$S = K\,C^{m}$$

K = Freundlich constant

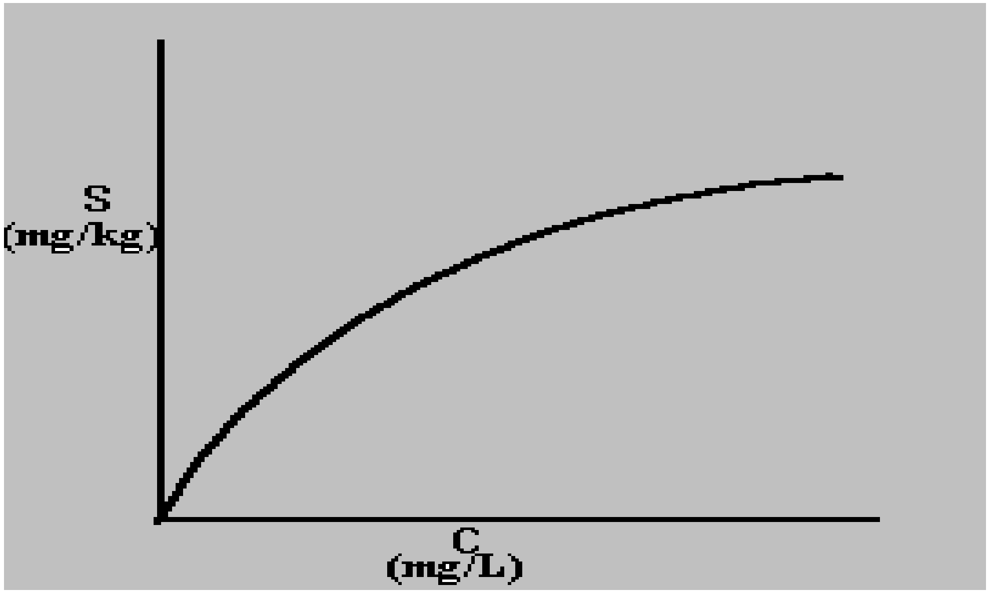
m = fitting parameter

Langmuir Isotherm

Freundlich isptherm doest not limit the solute amount sorbed on the soil matrix (sorbent)

Langmuir sorption isotherm is developed with concept that a sorbent contains a finite number of reactive sites. The Langmuir isotherm by given by:

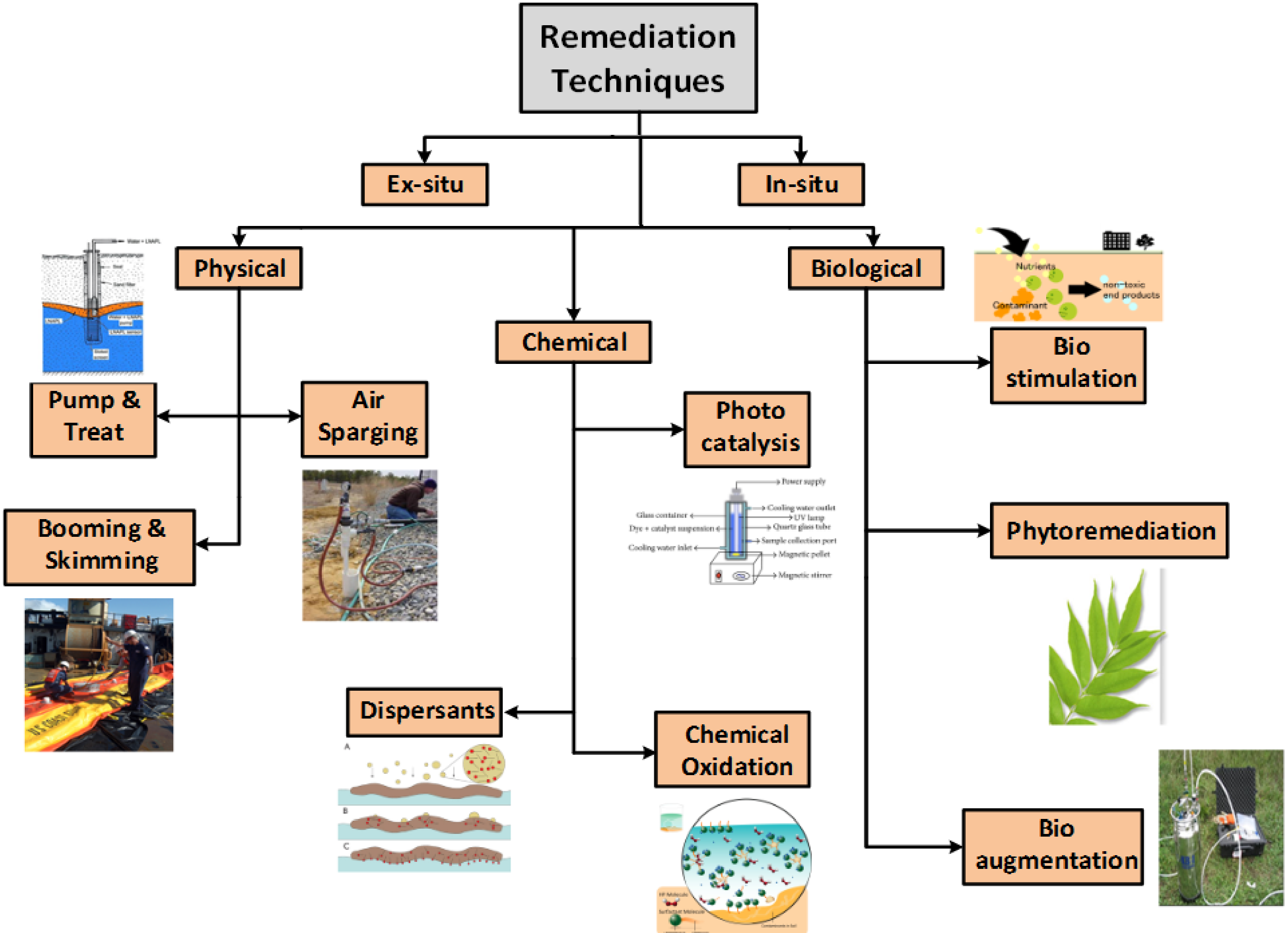
$$s = \frac{K_L S_{\max} C}{1 + K_L C}$$



$$if \quad K_L C << 1 \rightarrow \quad S = S_{\max} K_L C = K_D C$$

$$if \quad K_L C >> 1 \rightarrow \quad S = S_{\max}$$

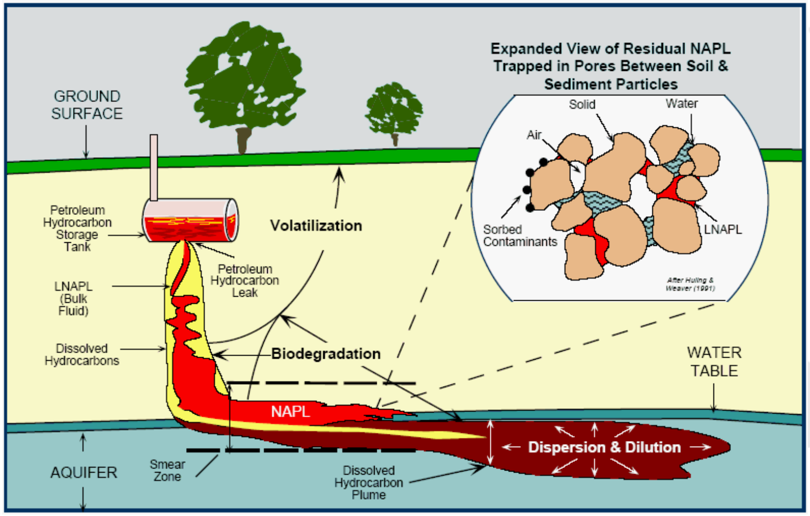
Treatment Methods: Engineered Biological methods

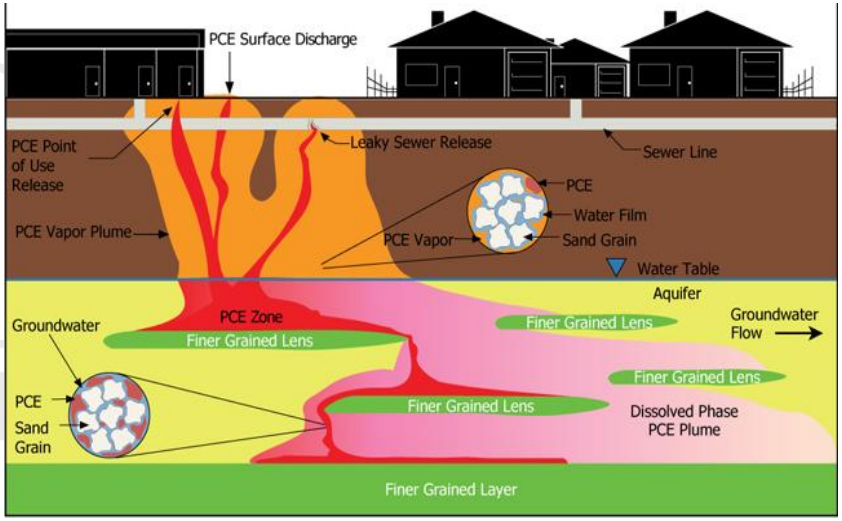


NAPL polluted soil-water

- LNAPLs are Hydrocarbon Oils
- NAPL -> Non-Aqueous Phase Liquid
- Non-Aqueous -> NAPL and water do not mix
- Light and Dense NAPL (LNAPL & DNAPL)

WHAT HAPPENS WHEN NAPL IS RELEASED?





Examples of LNAPL: Mono-aromatic hydrocarbons, BTEX

DNAPL: PCE, TCE, other chlorinated solvents

Engineered Bioremediation

Bio-remediation is a grouping of technologies that use microbiota to degrade/transform contaminants located in soil-water systems to less/non toxic by-products

Microbiota: are the microorganisms comprising of: bacteria, fungi, yeast

Enhanced bioremediation

Bio-stimulation	Bio-augmentation	Plant Enhanced
Supplemental nutrients/electron acceptors for indigenous micro biota • speed up the natural degradation process	• certain natural microbial strains or a genetically engineered variant introduced to treat contaminated soil water systems	Plants can actively promote microbial activity in rhizosphere, accelerate biodegradation of contaminated soil and water in several ways

Assessment of engineered bioremediation techniques

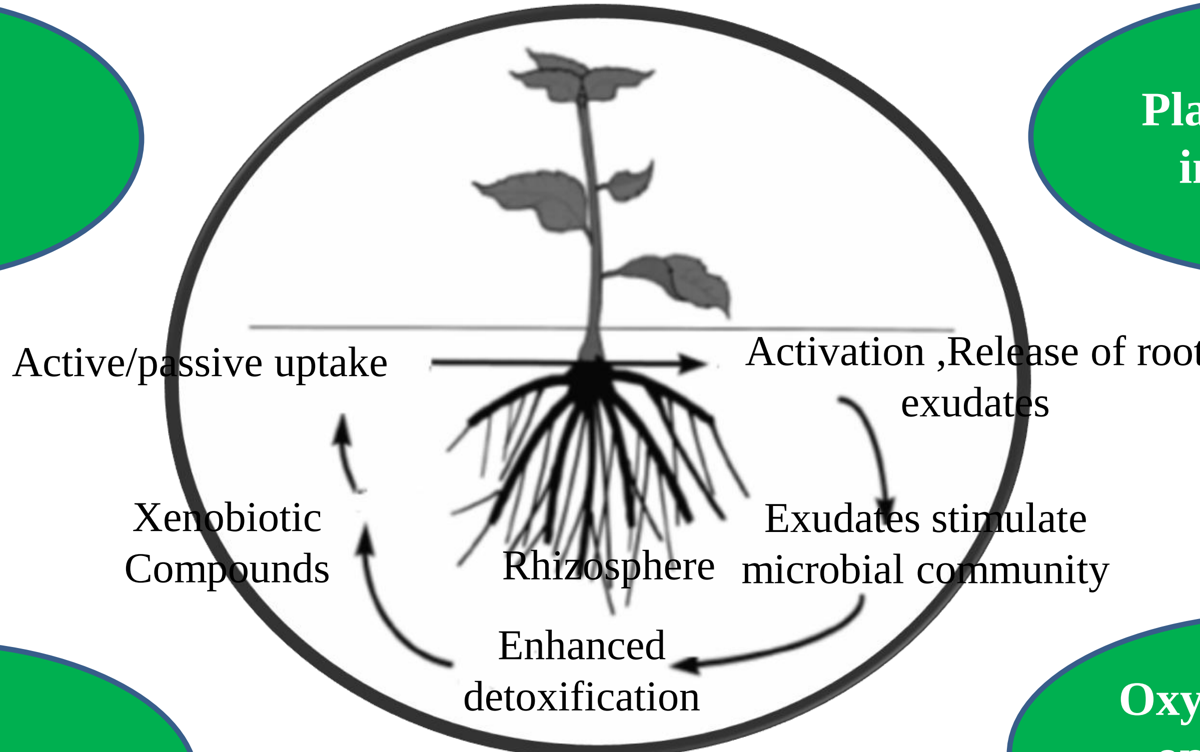
- Role of site specific environmental factors on bioremediation
- Integrated impact of environmental factors on fate and transport of NAPLs

Role of Plants

Nutrients bioavailability

Root Exudates

Plant microbial interactions



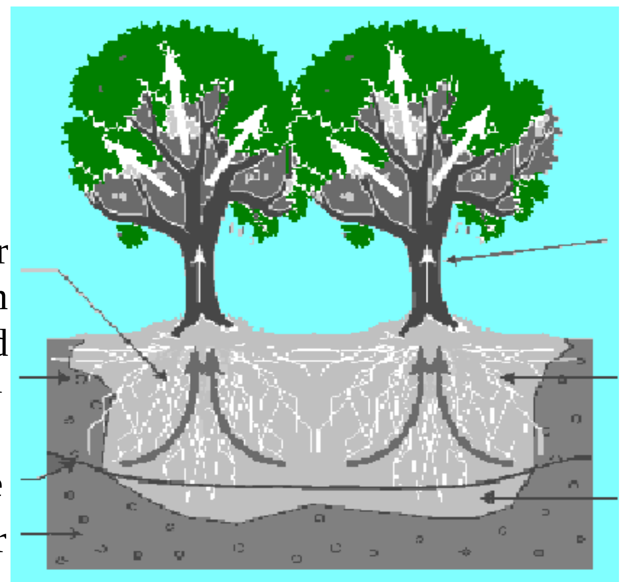
Direct uptake

Oxygen transfer, optimum soil temperature

Phytoremediation Mechanisms

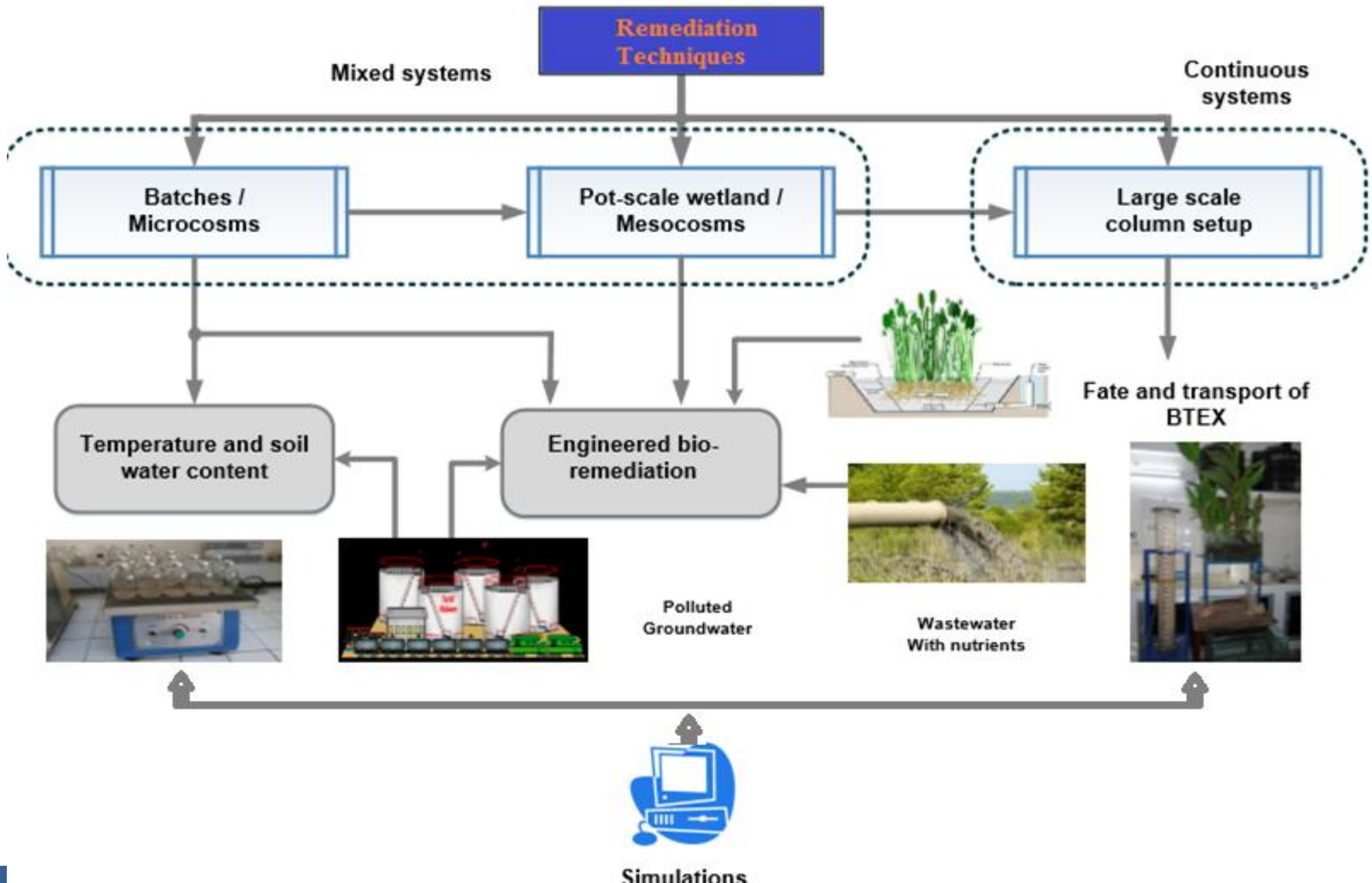
Bioremediation → enhanced → Phytoremediation

Phytoremediation →
- Phytoextraction
- Rhizofiltration
- Phytostabilization
- Phytodegradation
- Rhizodegradation
- Phytovolatilization

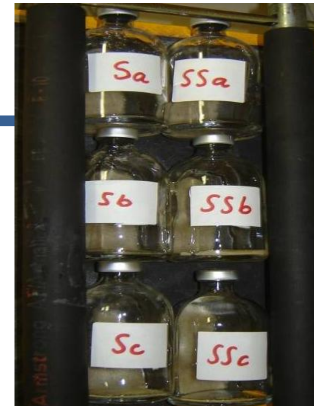


Research Framework

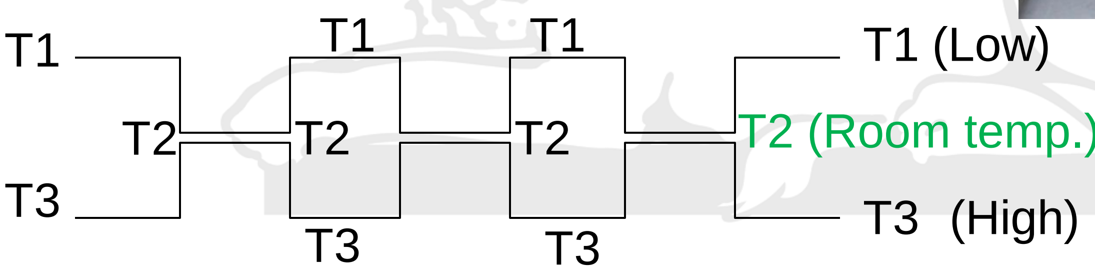
Yadav, B. K. and Hassanizadeh, S. M (2011) "An Overview of Biodegradation of LNAPL-polluted Regions in (Semi)-arid Environment" Water, Air, & Soil Pollution, 220 (1-4), 225-239



Temperature & Bioremediation



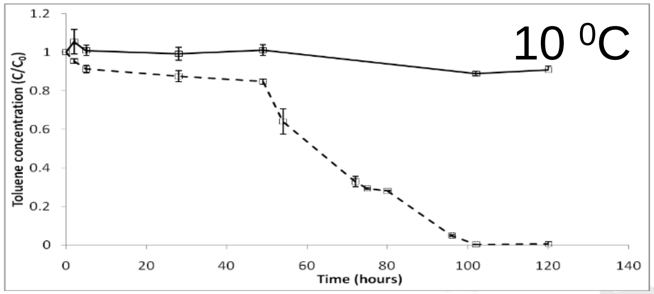
- Completely mixed soil-water
- Contaminated groundwater
- No limitation of water
- Constant temperatures (T1, T2 and T3 C)
- Varying temperature

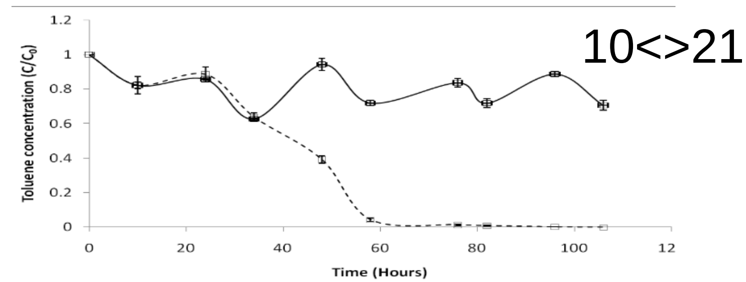


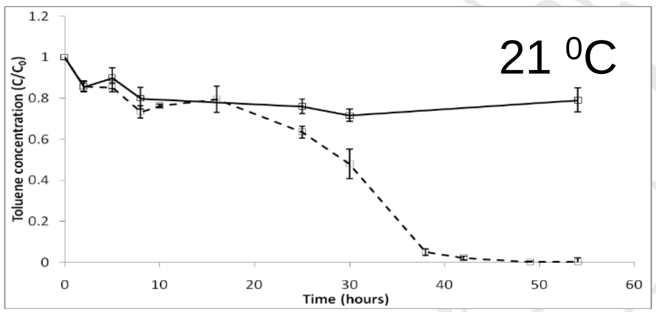
Winter Scenario

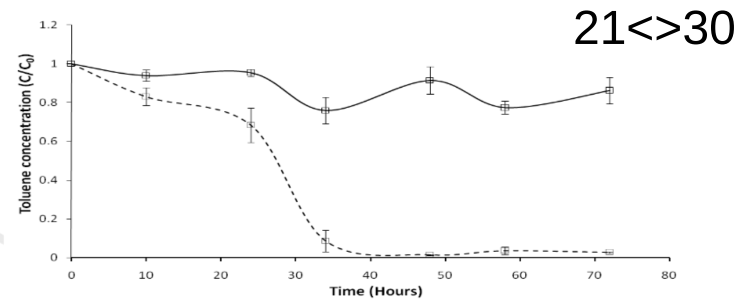
Summer Scenario

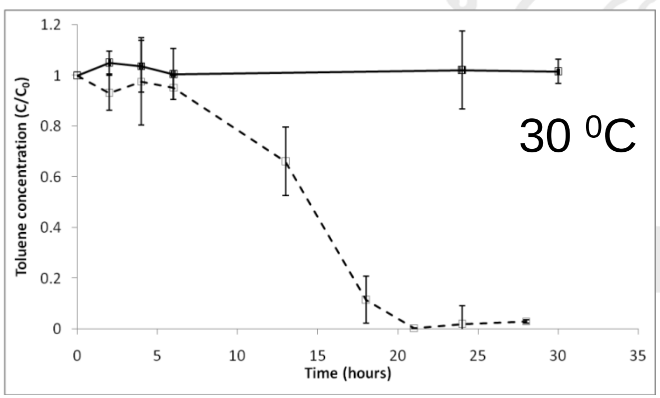
Impact of Temperature Fluctuations

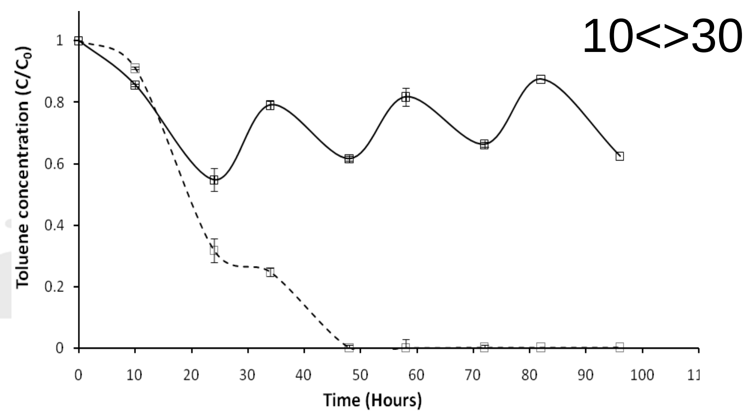










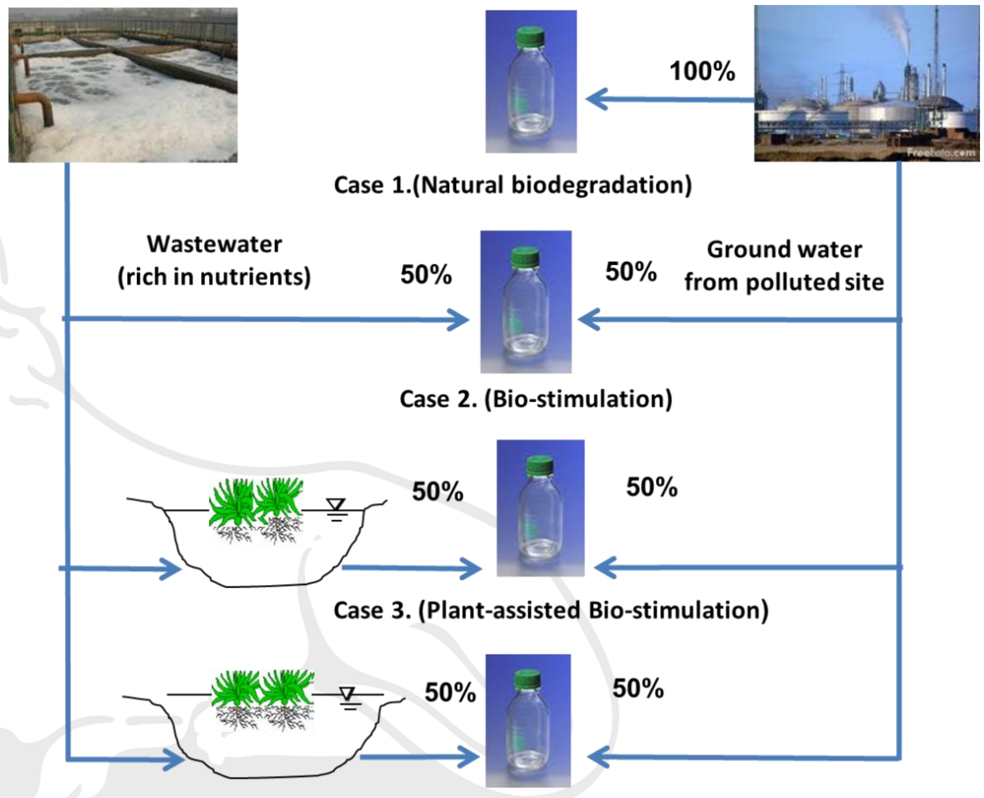


Yadav, B.K., Shrestha, S.R. & Hassanizadeh, S.M., (2012). Biodegradation of toluene under seasonal and diurnal fluctuations of soil-water temperature. Water, Air, and Soil Pollution, 223(7), pp.3579–3588.


James Thomason Building

Assessment of Engineered Bioremediation for a field site

Case 1: Natural bioremediation; Case 2: Biostimulation, Case 3: Plant assisted biostimulation; Case 4: Bioaugmentation+biostimulation



- The rate of degradation of LNAPL is found as follows:

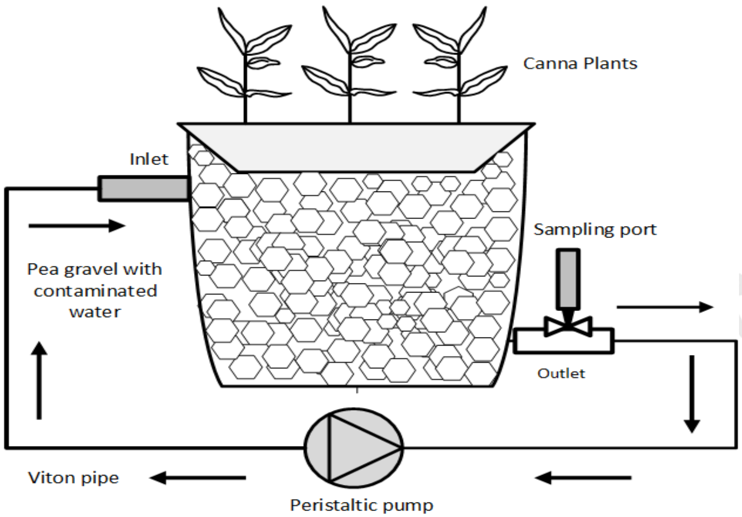
  Natural degradation≃ bio-stimulation

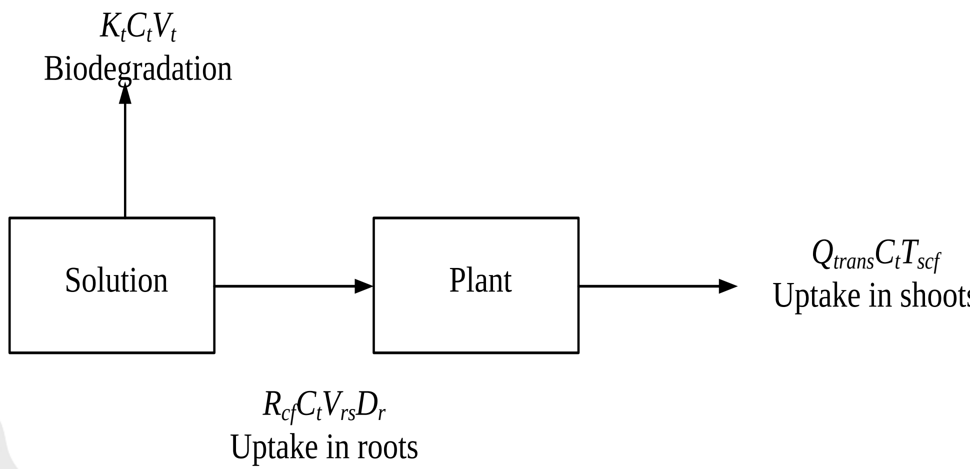
  < plant-assisted bio-stimulation

  << combination of bio-augmentation and bio-stimulation.

Yadav, B.K., Ansari, F.A. & Basu, S., (2014). Remediation of LNAPL Contaminated Groundwater Using Plant-Assisted Bio-stimulation and Bio-augmentation Methods. Water Air Soil Pollut , 225:1793

Enhanced Bioremediation: Plant Uptake



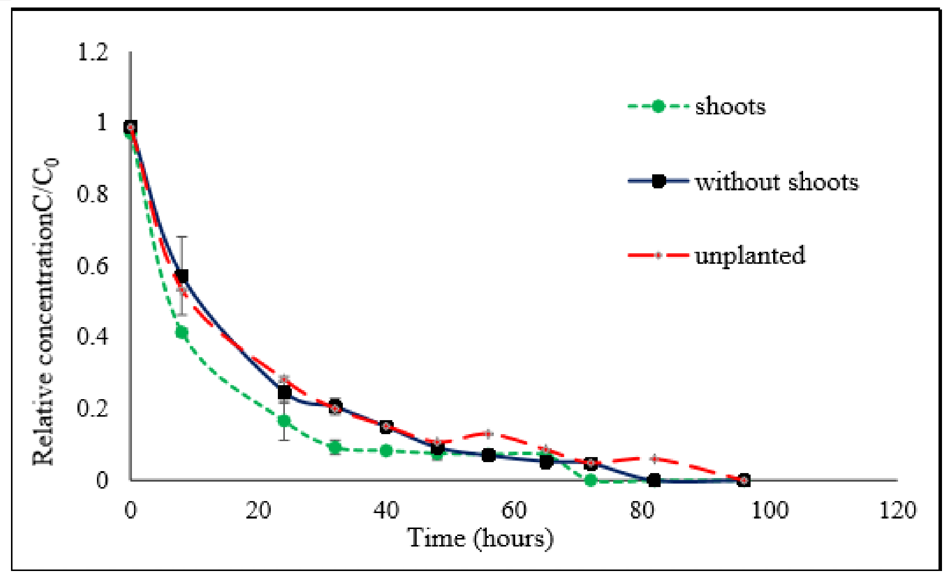


Wetland without shoot

$$V_t \frac{\partial C_t}{\partial t} = -K_t C_t V_t - R_{cf} C_t V_{rs} D_r$$

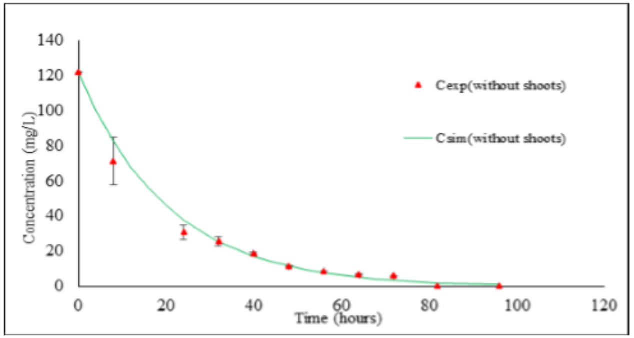
Wetland with shoot

$$V_t \frac{\partial C_t}{\partial t} = -K_t C_t V_t - R_{cf} C_t V_{rs} D_r - Q_{trans} C_t T_{scf}$$

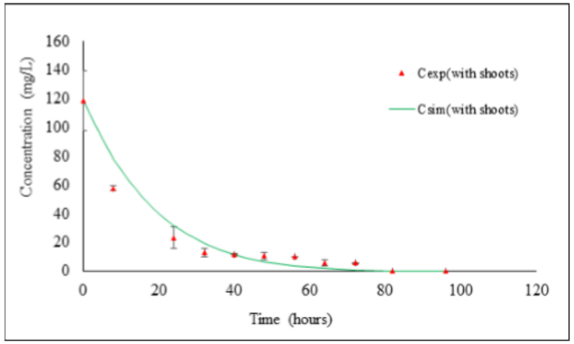


Enhanced Bioremediation : Plant Uptake

A

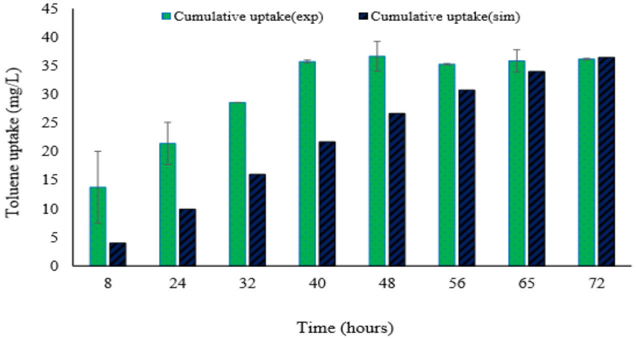


B

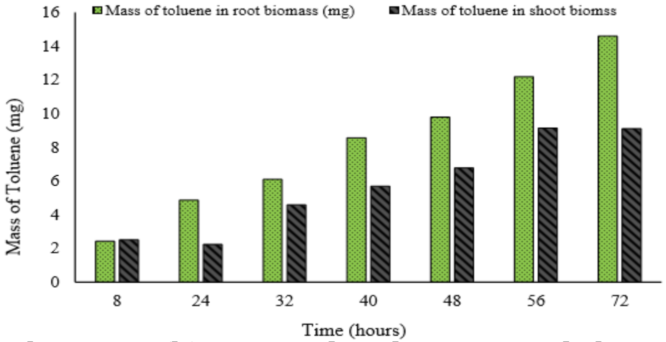


Simulated and experimental comparison for wetland (a)without and (b) with shoot biomass

A



B

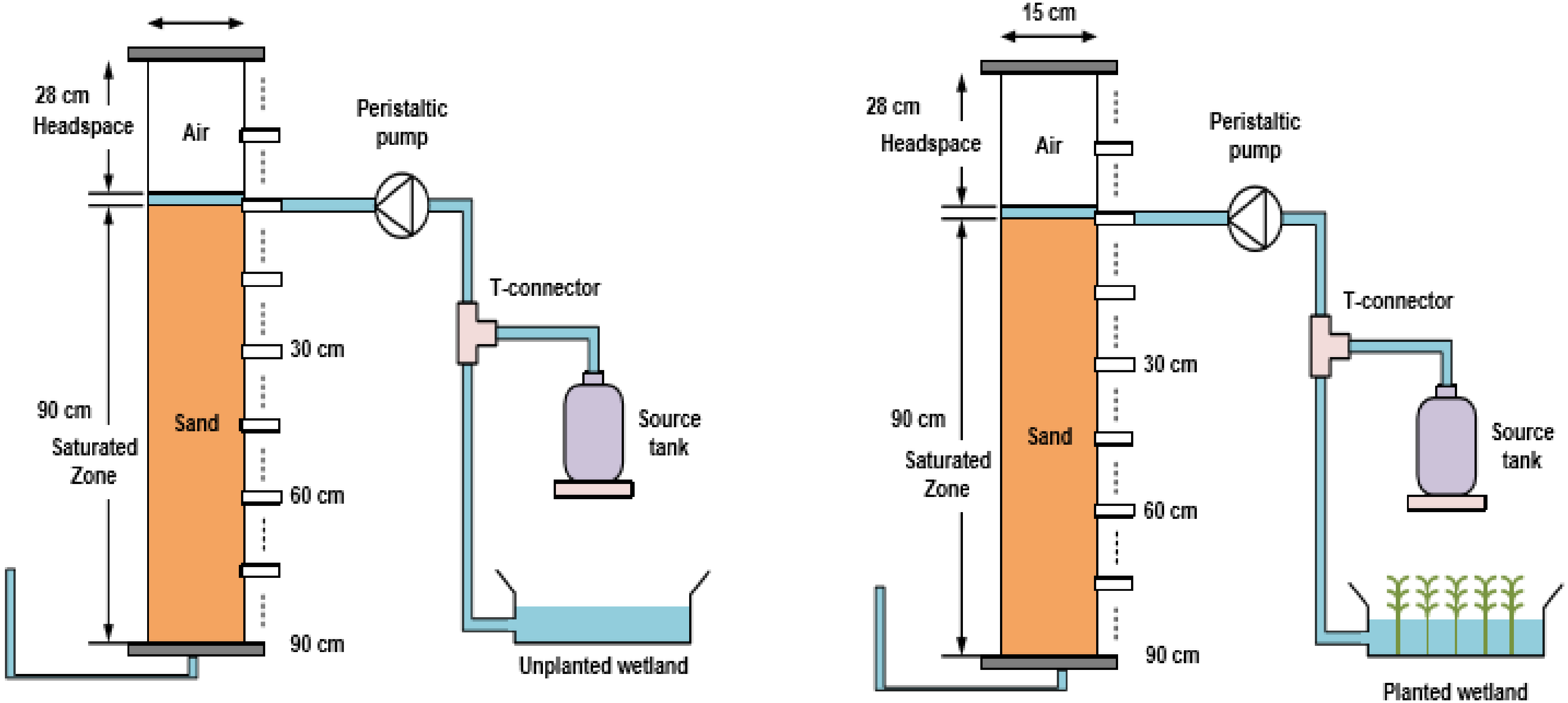


(a) Comparison of simulated and experimental uptake of toluene by shoot biomass (b) accumulated in root and shoot biomass with time.

- The removal time of toluene was reduced significantly, 25 %, in presence of plants as compared to the unplanted gravel bed.

Basu, S, **Yadav. B. K.,** and Mathur, S. (2015) "Enhanced Bioremediation of BTEX Contaminated Groundwater in Pot-Scale Wetlands". Environmental Science and Pollution Research, 22(24), 20041-20049

Enhanced Bioremediation in column set-up integrated with wetlands



Schematic diagram of the column set-up integrated with wetlands (a) without and (b) with plants of *Canna generalis* for investigating toluene fate and transport in vadose zone.

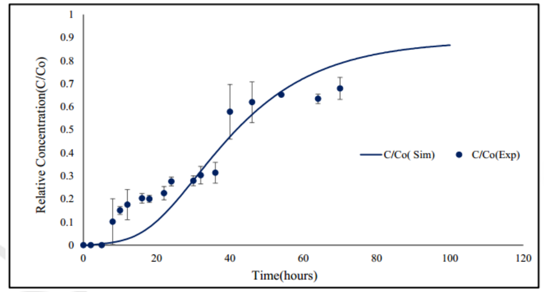
Enhanced Bioremediation in column set-up integrated with wetlands

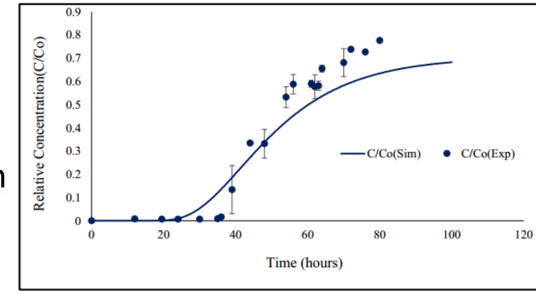
- Comparison of experimental and simulated BTCs for unplanted and planted system

- Plants have enhanced the bioremediation by a factor of 2.5 as compared to the unplanted case

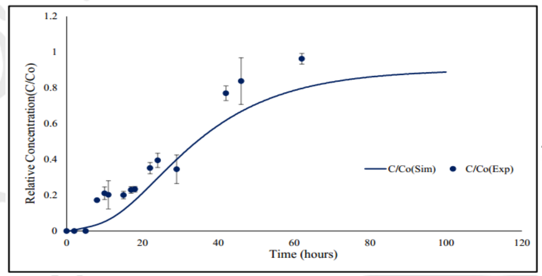
Basu S., **Yadav B.K.**, Mathur S., 2015. Fate and Transport of Dissolved BTEX in Soil Column Setup Integrated with a Treatment Wetland" Journal of Contaminant Hydrology –In review

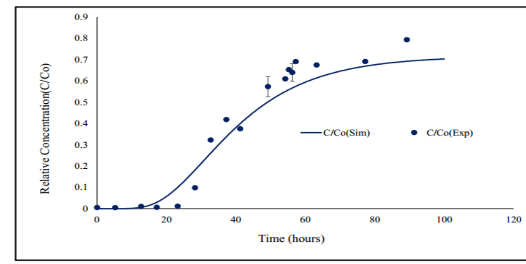
Unplanted | Planted



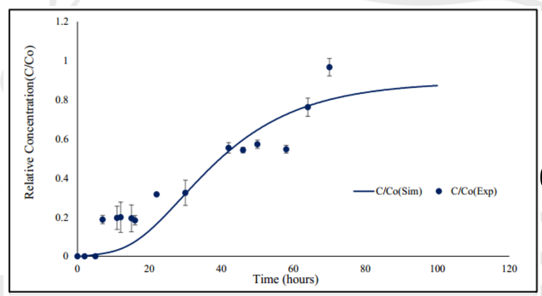


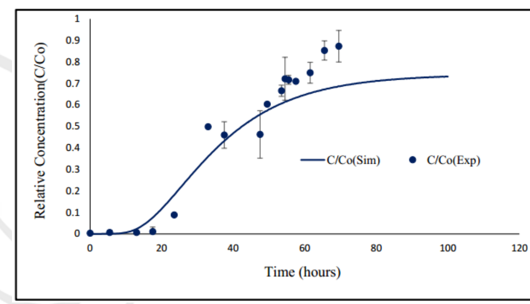
85 cm



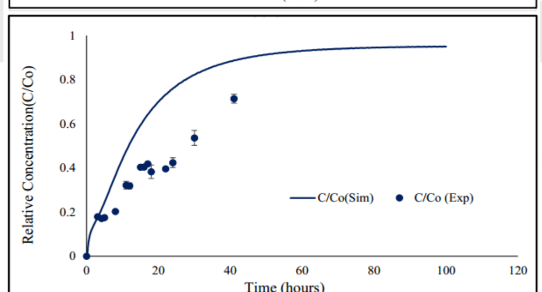


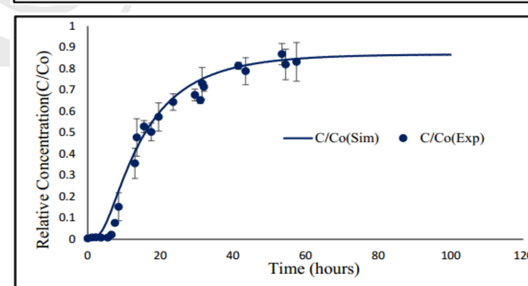
75 cm





65 cm



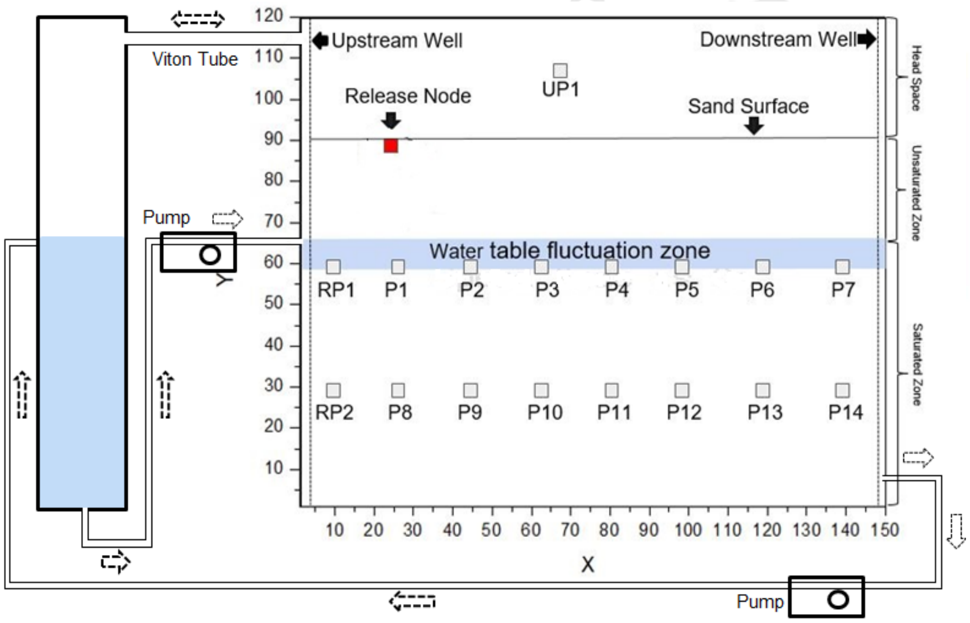


55 cm

Groundwater Variations and Biodegradation

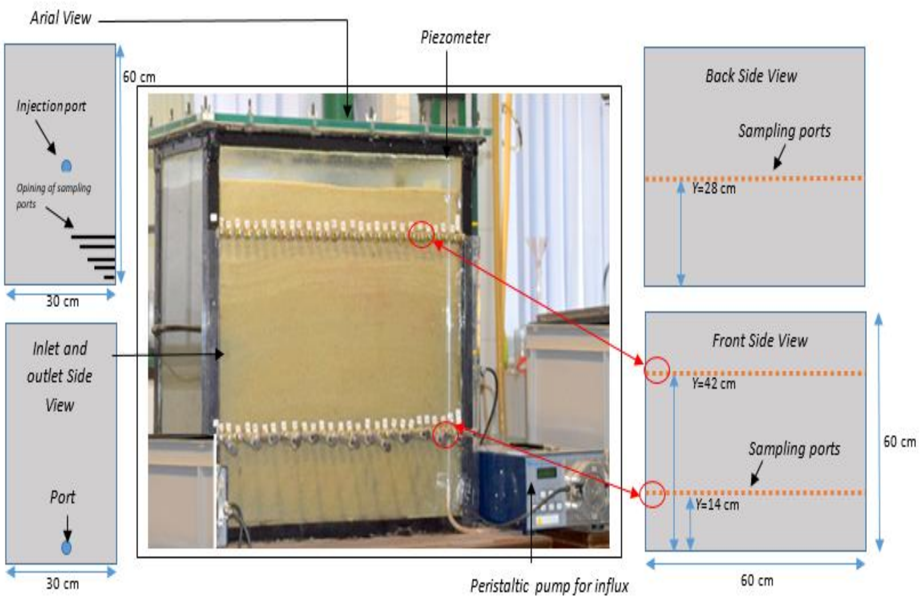
Roles of groundwater variations (water table dynamics and flow velocity) on spatial and temporal biodegradation and transport of LNAPL are investigated using three dimensional practical and simulation experiments.

2D tank



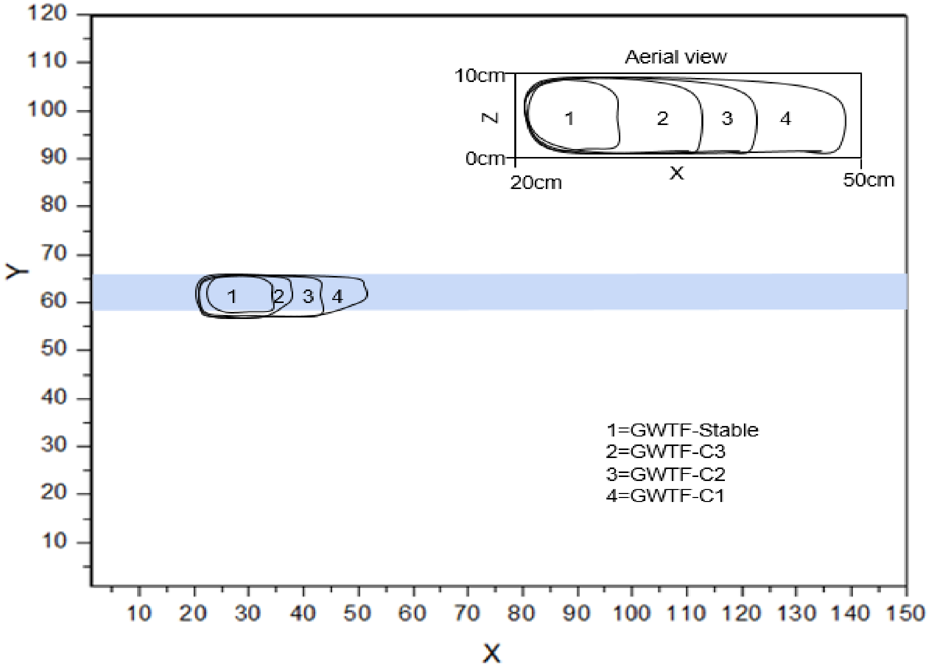
2D sand tank setup used to investigate fate and transport of LNAPL in subsurface under dynamic groundwater table

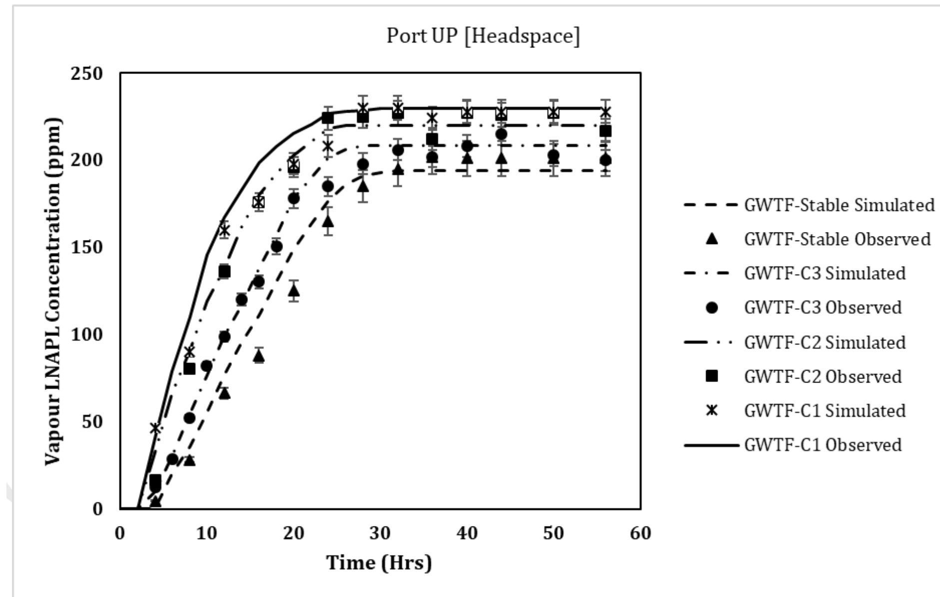
3D tank



3D sand tank used to investigate the role of groundwater flow variation on fate and transport of LNAPL pollutants in subsurface

LNAPL pool spreading under varying GW table





- **GW table fluctuation enlarge pure phase LNAPL in smear zone, and accelerates dissolution rate**
- **Microbial growth was found to be increasing as plume moves away from the LNAPL pool**
- **A high biodegradation rate was observed in regions having concentration ranges from 140-160 ppm.**

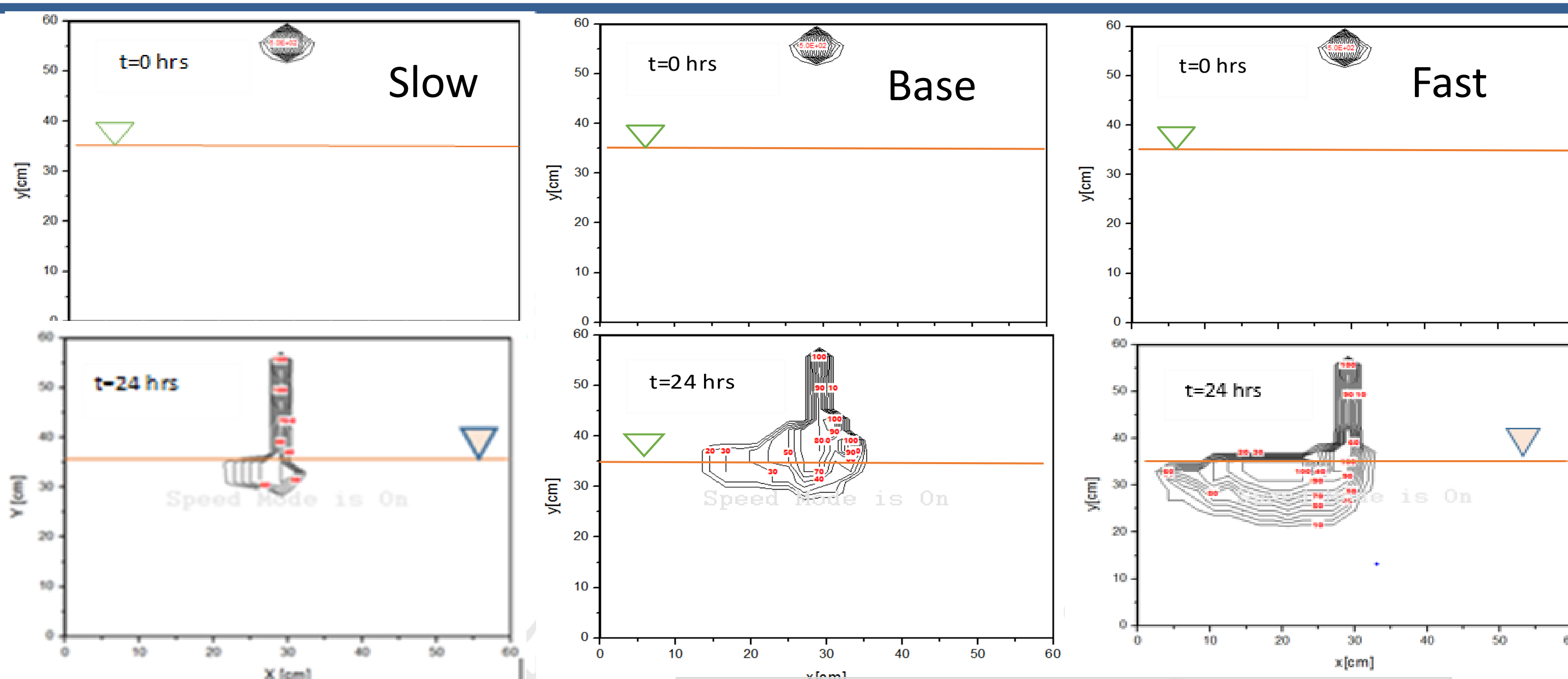
Gupta, P.K. and **Yadav*, B. K.** (2020) "Three-dimensional Laboratory Experiments on Fate and Transport of Light NAPL under Varying Groundwater Flow Conditions". ASCE *Journal of Environmental Engineering*, 146(4), 04020010

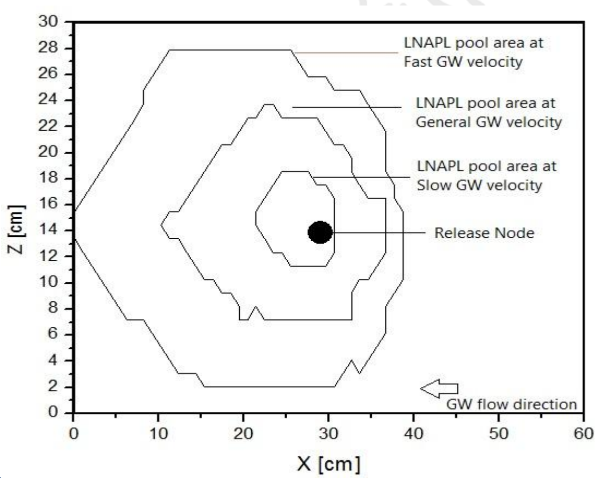
Gupta P.K., Yadav, B., **Yadav* B. K.,** (2019) "Assessment of LNAPL in Subsurface under Fluctuating Groundwater Table using 2D Sand Tank Experiments". **ASCE** *Journal of Environmental Engineering*, 145 (9), 04019048.

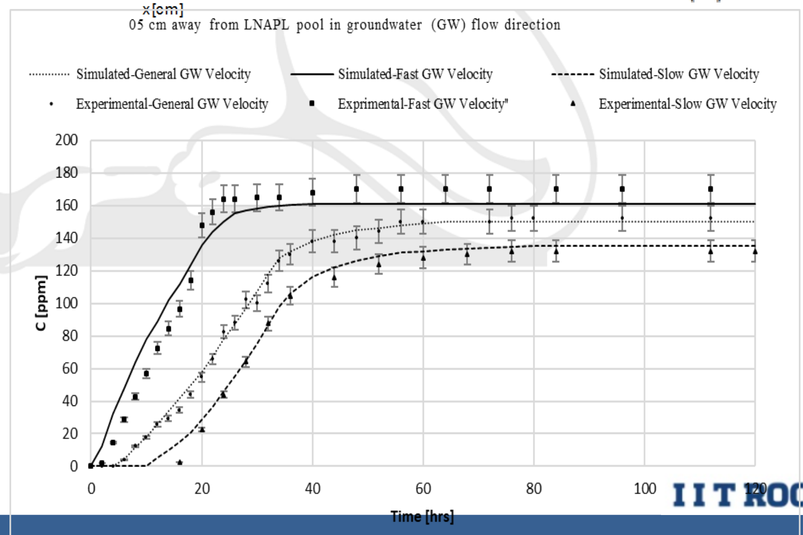
LNAPL pool spreading under varying GW velocity

0 hr.

24 hr.

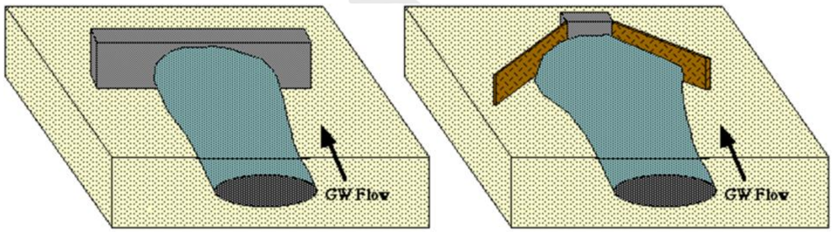


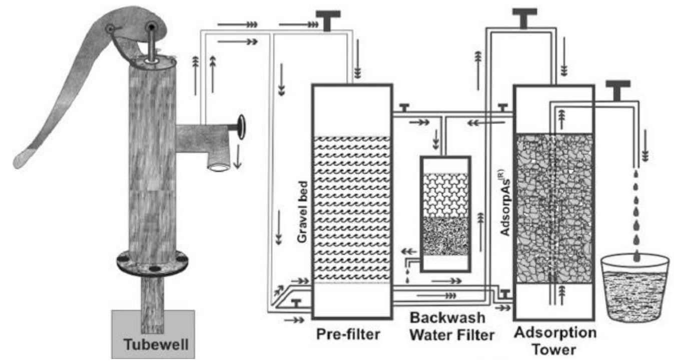




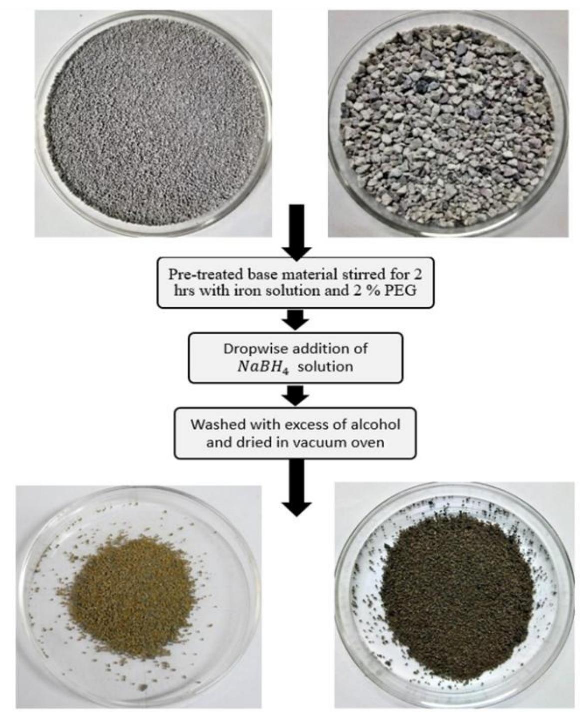
Remediation gelogenic polluted GW with PRBs

- Polluted groundwater is treated using adsorption based Ex-situ treatment techniques
- Use of permeable reactive barriers (PRBs) seems a promising way for in-situ remediation of arsenic/fluoride contaminated groundwater.



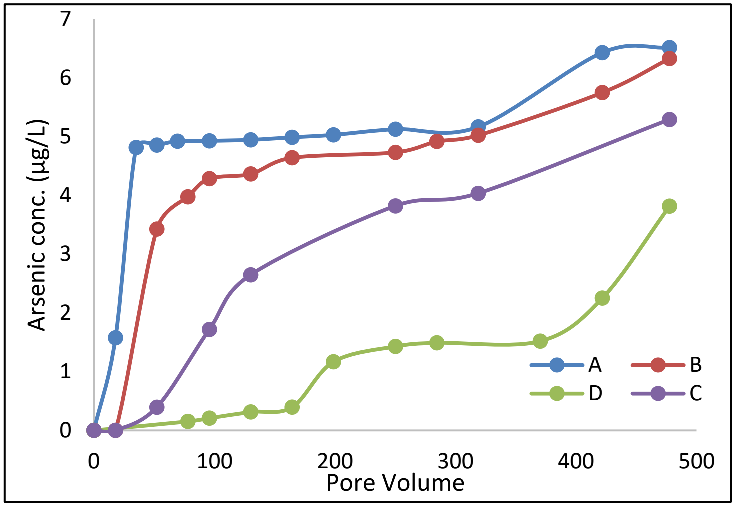


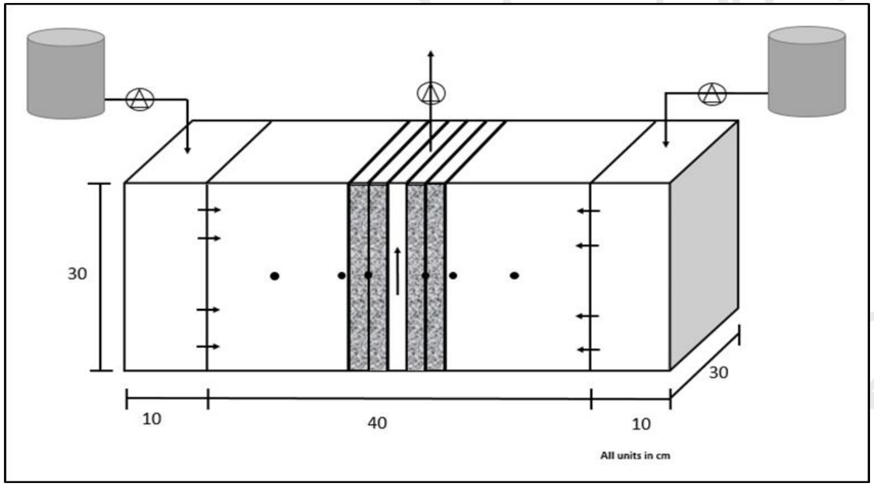
- However, designing and installation of PRBs are challenging tasks particularly when pollutant source/path is not known.
- Also application of adsorbents in field is limited due to formation of aggregates, which reduces the hydraulic conductivity and their reactivity.
- zero valent iron nanoparticles loaded pumice and zeolite composites and iron oxide maghemite loaded pumice, P-maghemite, are developed (liquid-phase reduction and chemical co-precipitation methods) for As(III) and As(V) removal.
- A series of experiments (batch, column & tank) were conducted to study the removal of As using the developed adsorbent



Experimental findings

- Adsorption kinetics were investigated using the batch experiments at various conditions
- Column experiments were then conducted to assess the feasibility of developed composites as the reactive material in PRBs for in-situ As remediation
- Well-integrated PRB was investigated using tank setup having 2cm thick reaction chambers at the centre.





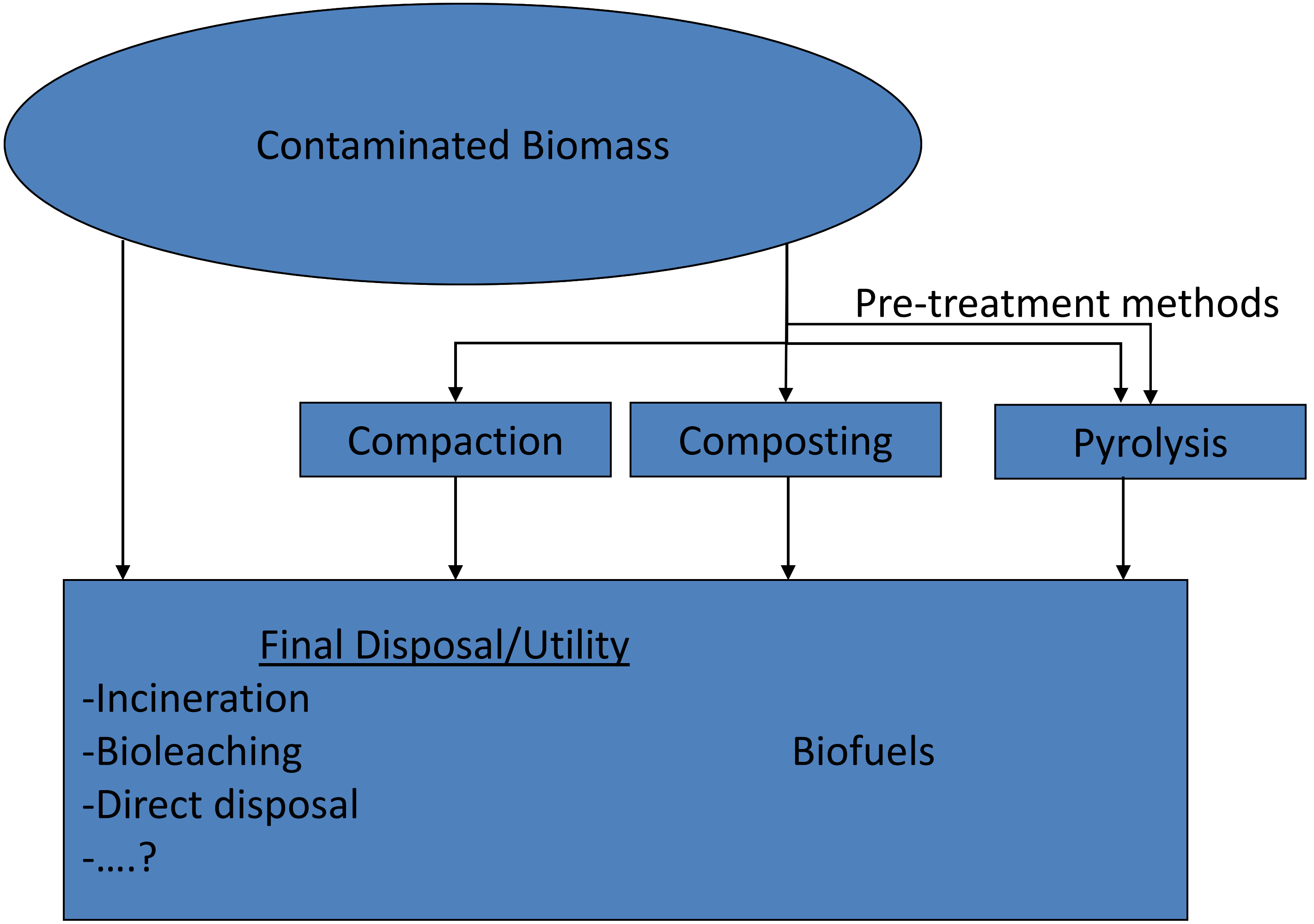
Element	Average conc. outlet (µg/L)	Average conc. Input (µg/L)	% Removal
As	2.215	652	99.66
Zn	58.45	208	67.48
Mg	3076.8	24710	73.54
Ca	8148.42	102460	92.14
Fe	496.37	6020	91.85
K	863.2	5920	88.84
Mn	113.2	1300	90.88
Na	8110.2	25500	68.57

Ranjan, S, **Yadav*, B. K.**, and Joshi, H (2020) Development of nZVI-Pumice/Zeolite Composites for Effective Removal of Arsenic (III) from Aqueous Solution, ASCE's Journal of Hazardous, Toxic, and Radioactive Waste, 24 (3), 04020014

Example of a small-scale wetland use in research

Example of a Field-scale phytoremediation research

Methods of Contaminated Biomass Disposal/Utilization



Thanks…