



INDIAN INSTITUTE OF TECHNOLOGY ROORKEE



Linked Simulation Optimization Modeling for Management of Polluted Land Sites

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Water Resources Development and Management (WRD&M)





Outline of the Presentation



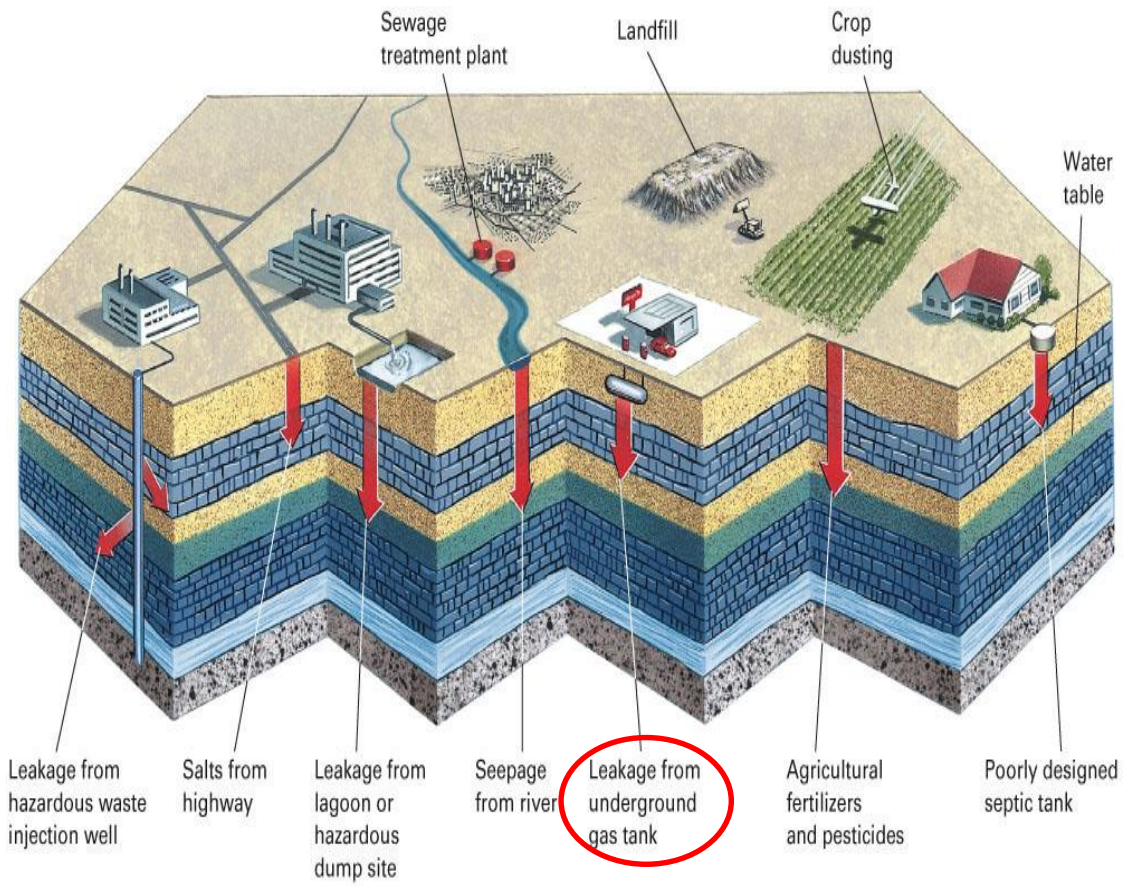
- Design of a optimal in-situ- bioremediation system for sites contaminated with BTEX compound
- Consideration of well clogging during cost optimization
- Groundwater table fluctuation and its impact on biodegradation
- Impact of soil moisture and temperature on system design cost



Groundwater Contamination and Remediation



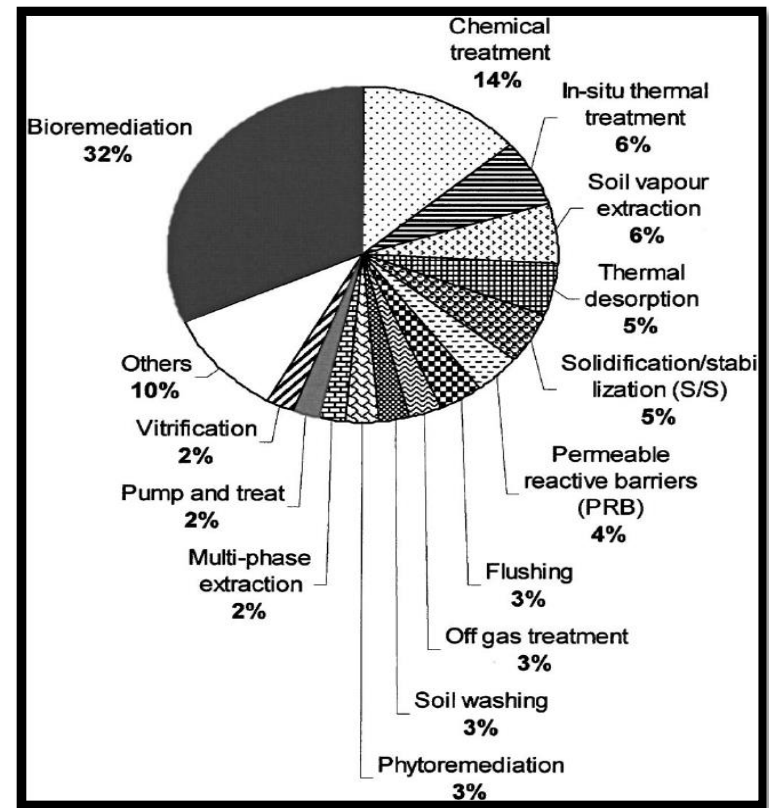
➤ Contaminants enter groundwater through variety of sources



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Guntur district=100,000 liters



Different technologies adopted for remediation (Source: Satinder K. Brar, 2006)

1 liter of petroleum can contaminate 10⁶ litre of groundwater



What is Bioremediation??



- Using subsurface microorganisms to transform petroleum hydrocarbons into harmless byproducts, such as carbon dioxide and water
- Techniques or types of bioremediation:
 - A component of Natural Attenuation (Not fast enough, Not complete enough – 16 % of 40 ppm degraded in 5 years (Shieh & Peralta 2005))
 - Enhanced Bioremediation- stimulate/enhance microbial growth



Lack of proper condition to survive & growth

Addition of electron acceptors/adequate nutrients

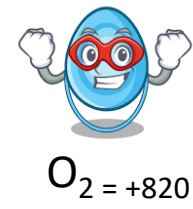
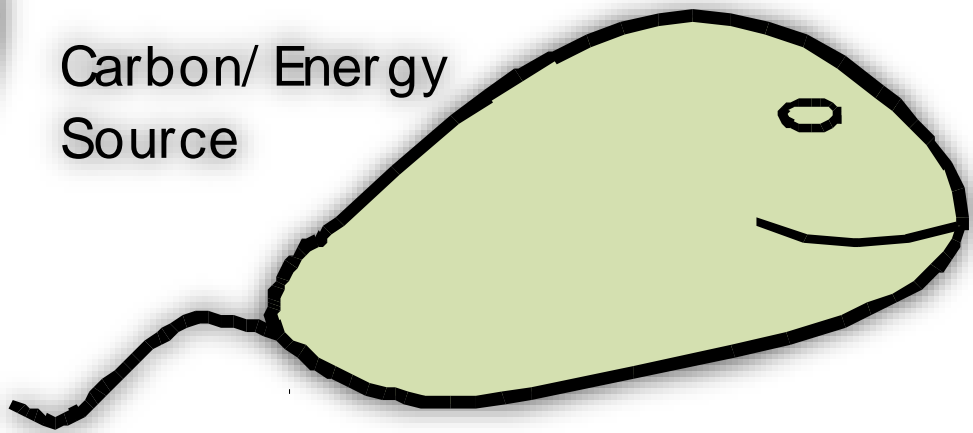


Requirements of Enhanced Bioremediation



Electron Acceptor
(O_2 , NO_3^- , SO_4^{2-} , et c.)

Carbon/ Energy
Source



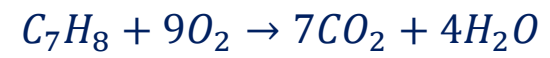
Environmental
Conditions

Nutrients (N, P)

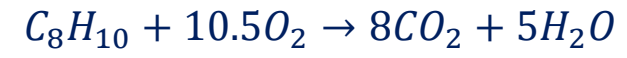
Reaction for Benzene



Reaction for Toluene

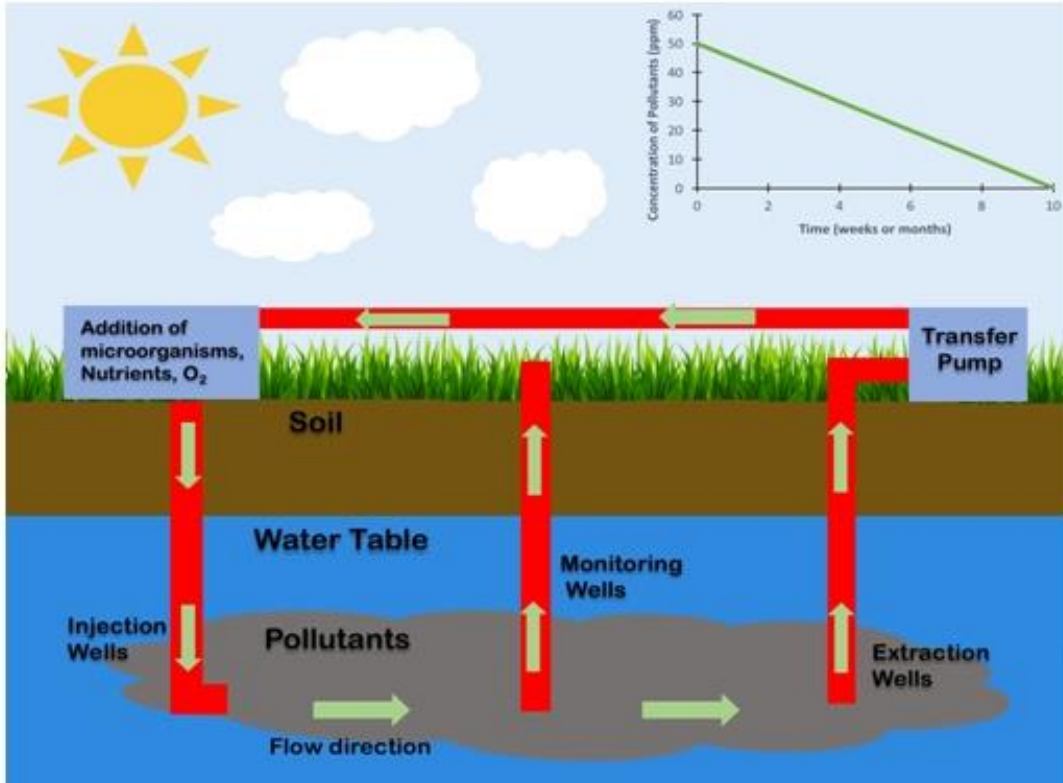


Reaction for Ethylbenzene and Xylene



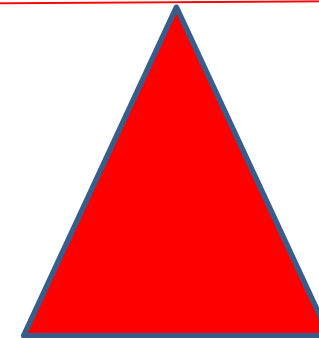


Bioremediation system design issues



- What is ideal location and number of wells (Injection/extraction /monitoring)
- What are the optimum pumping rates?
- What would be the system/ operational cost?

Toxicological Risk Ecosystem Impact

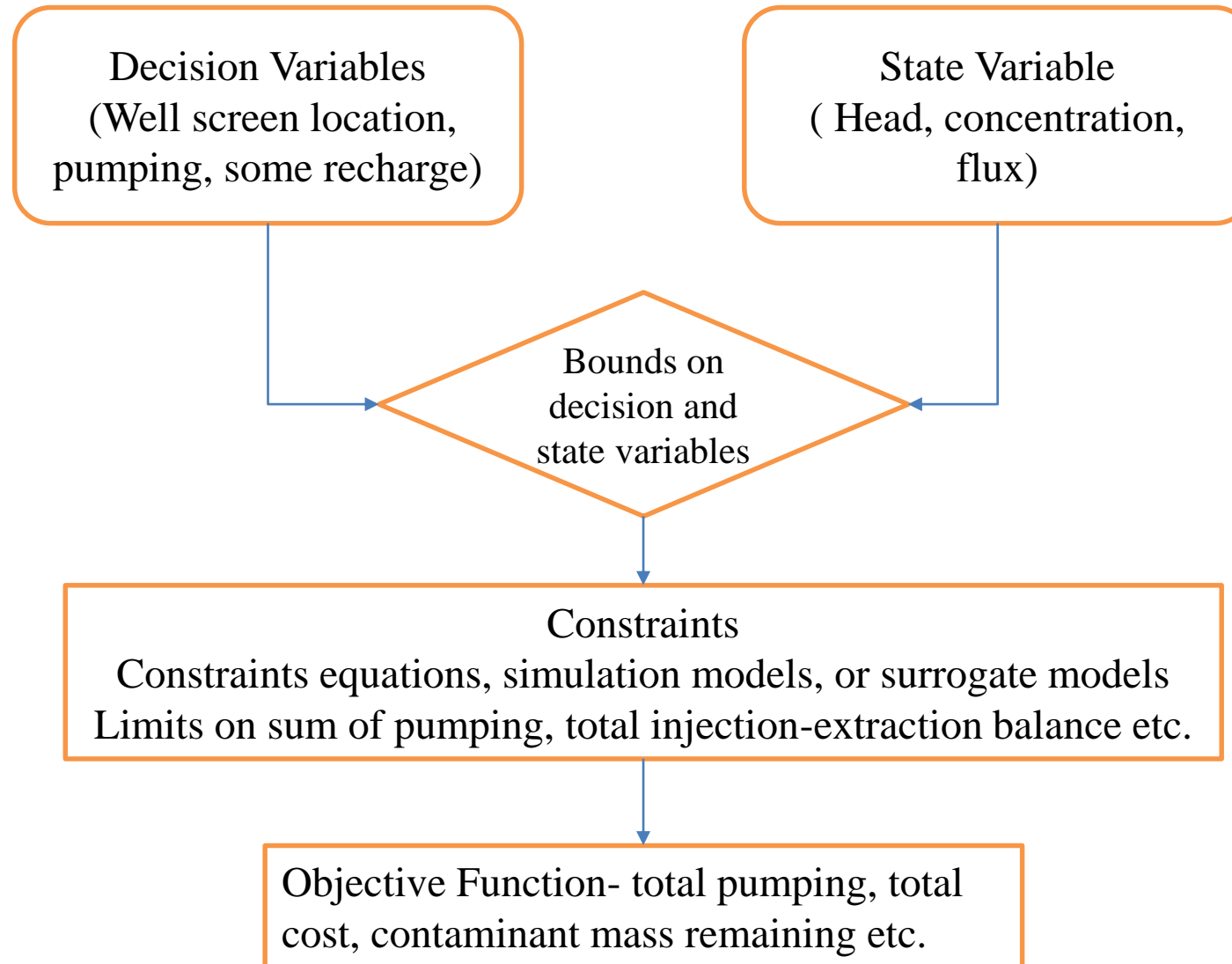


How do we weigh it?

- **Goal**-to provide water for human activities- other species and prerequisite ecosystem- Extended to consider laws, regulations, needs, costs, and benefits



Optimization component in Groundwater System Design





Simulation of in-situ Groundwater System



Technique

Summary/recommendations

Physically based models- BIOPLUME III, MODEFLOW, HYDRUS, SEAWAT

- Captures the process completely and used as a physical simulator
- Requires many parameters
- Time consuming when requires multiple recalling in case of optimization
- Problem of source code

Data based models- ANN, SVM, ELM

- Very few parameters requires to develop them
 - Simulation is very quick and can be used in simulation-optimization as code is available
 - Requires large number of data to be trained effectively
-



- Simulate- aerobic and anaerobic biodegradation with advection, dispersion, sorption.

$$\frac{\partial(bC_s)}{\partial t} = \frac{1}{R_s} \left[\frac{\partial}{\partial x_j} \left(bD_{ij} \frac{\partial C_s}{\partial x_j} \right) - \frac{\partial(bC_s v_i)}{\partial x_i} \right] - \frac{qC'_s}{\theta}$$

$$\frac{\partial(bC_o)}{\partial t} = \left[\frac{\partial}{\partial x_j} \left(bD_{ij} \frac{\partial C_o}{\partial x_j} \right) - \frac{\partial(bC_o v_i)}{\partial x_i} \right] - \frac{qC'_o}{\theta}$$

- Instantaneous reaction kinetics (Borden and Bedient, 1986).

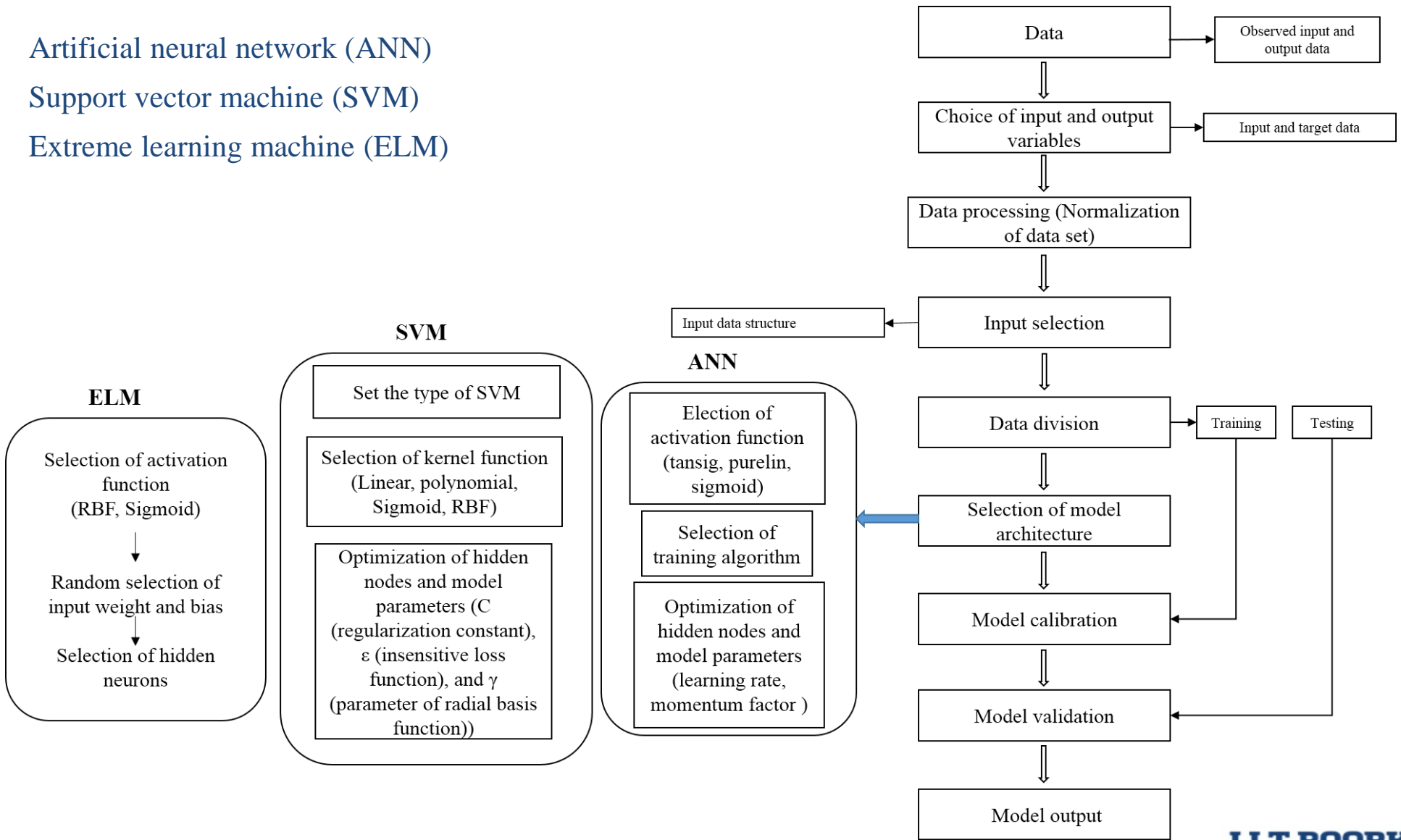
1. How long will the plume extend if no engineered/source controls are implemented?
2. How long will the plume persist until natural attenuation processes completely dissipate the contaminants?
3. How long will the plume extend or persist if some engineered controls or source reduction measures are undertaken (for example contamination removal)?



Types of data based models

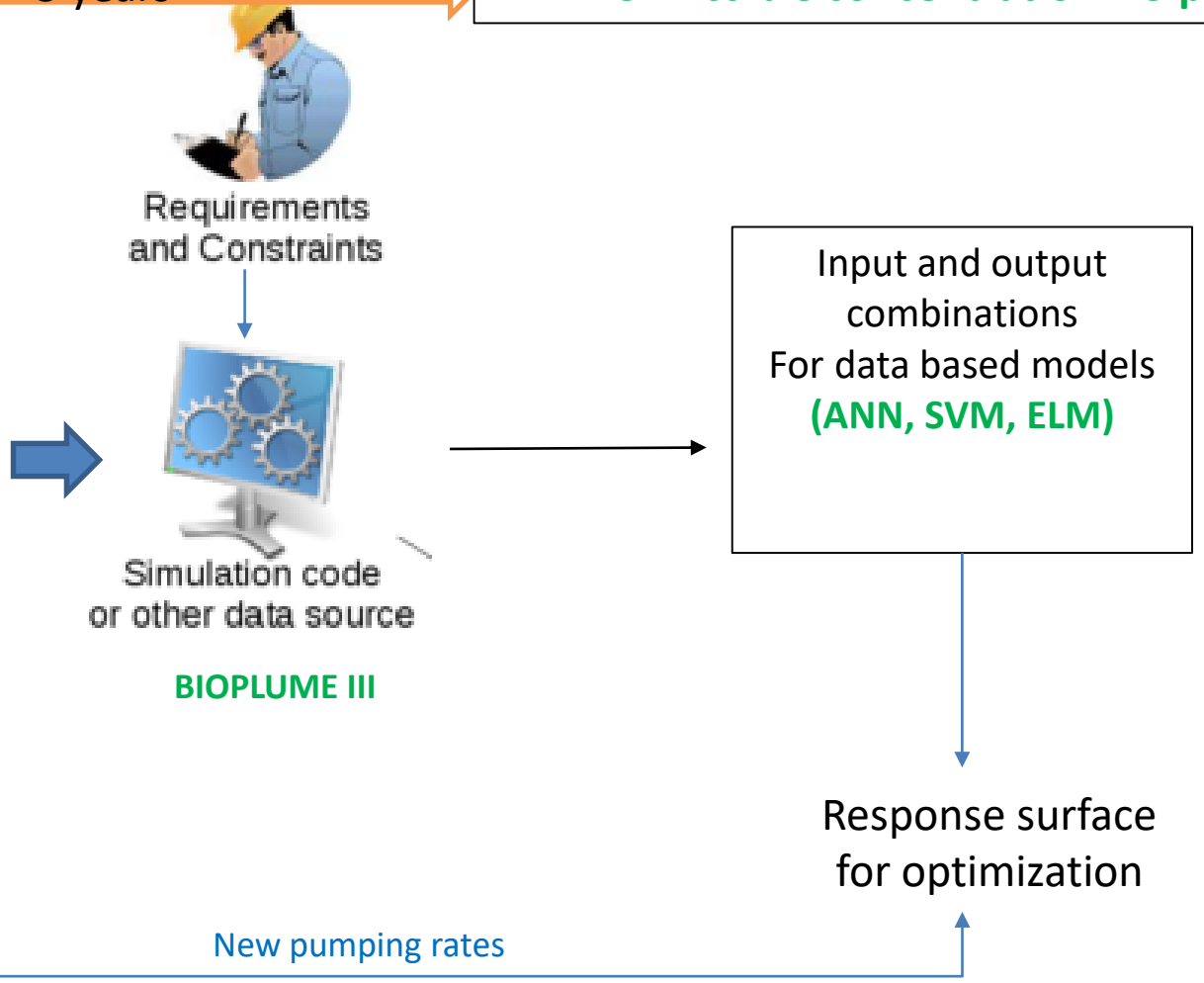
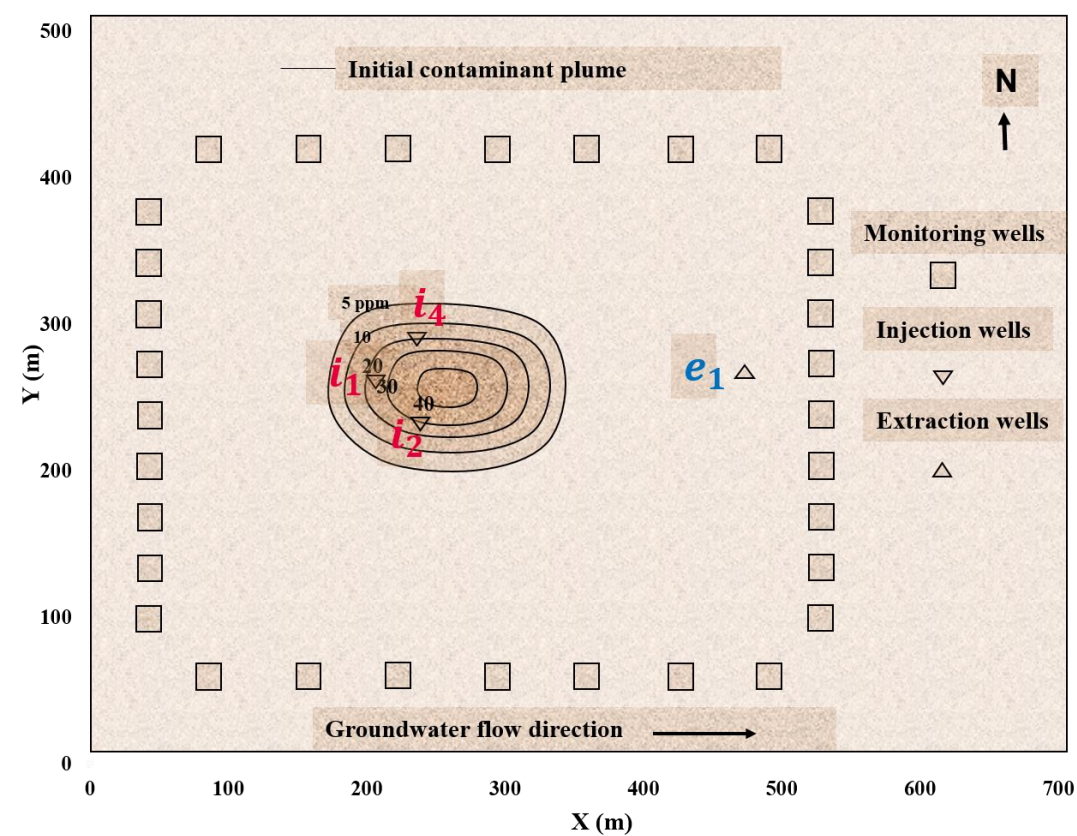


- Artificial neural network (ANN)
- Support vector machine (SVM)
- Extreme learning machine (ELM)





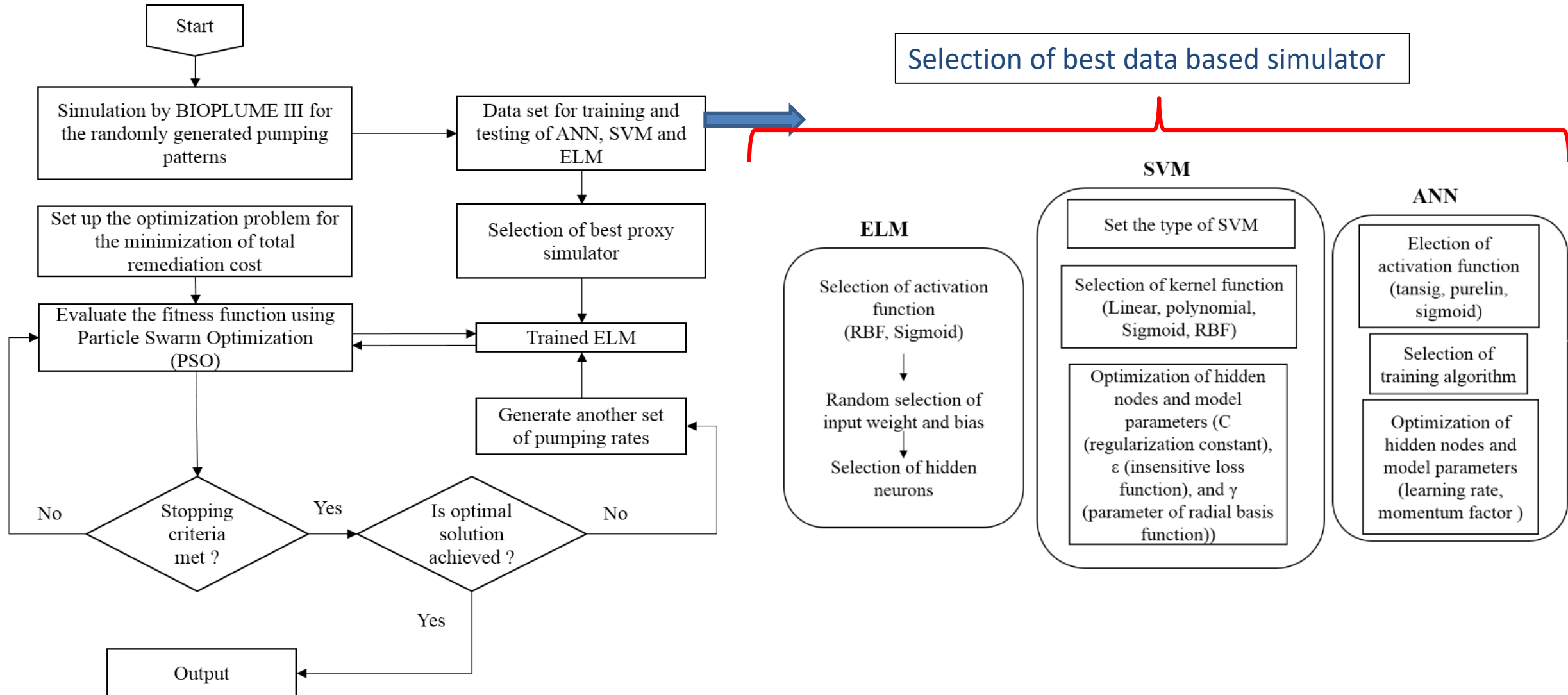
Remediation system design using Simulation-optimization approach



Yadav, B., Ch, S., Mathur, S., & Adamowski, J. (2016). Estimation of in-situ bioremediation system cost using a hybrid Extreme Learning Machine (ELM)-particle swarm optimization approach. *Journal of Hydrology*, 543, 373-385.



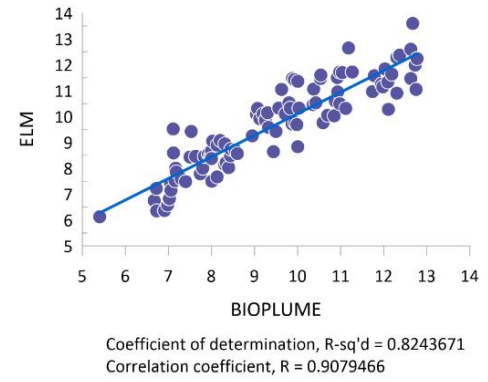
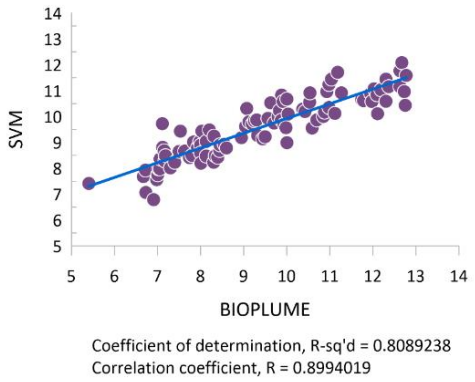
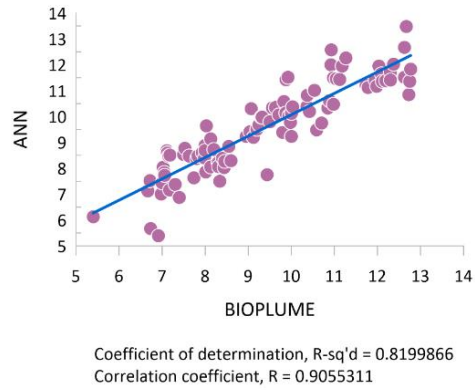
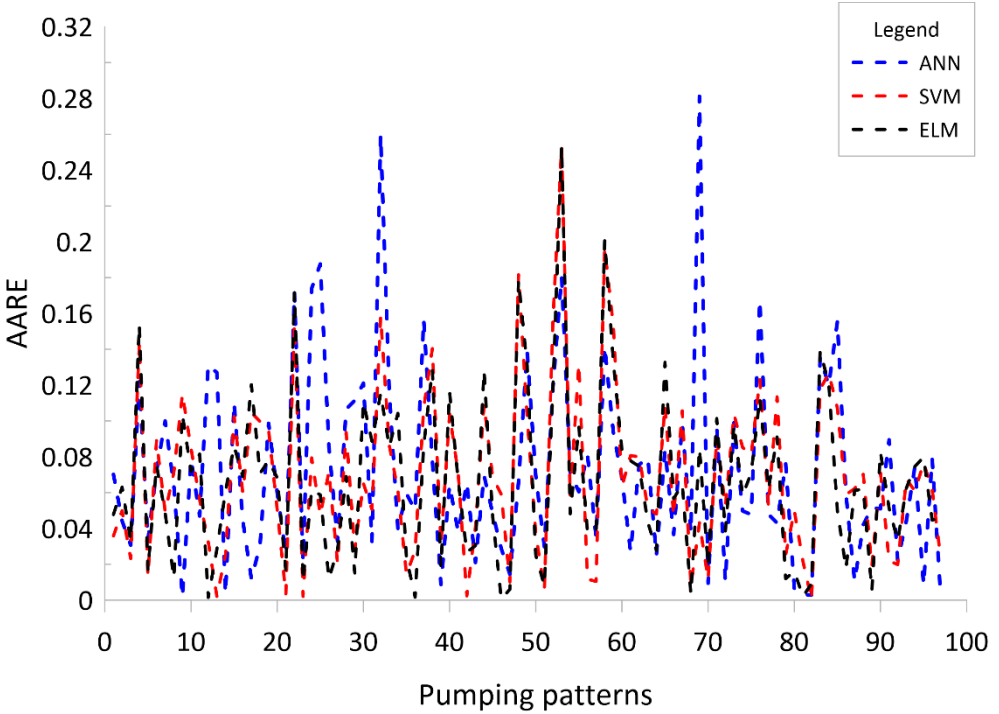
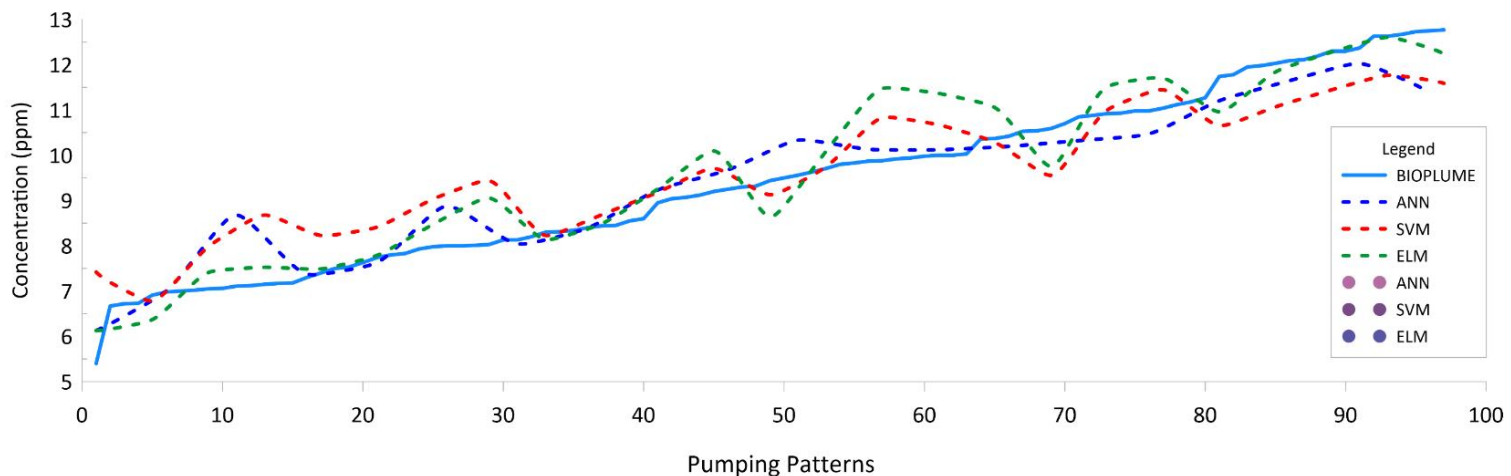
Simulation-optimization approach with data based simulator



Yadav, B., Ch, S., Mathur, S., & Adamowski, J. (2016). Estimation of in-situ bioremediation system cost using a hybrid Extreme Learning Machine (ELM)-particle swarm optimization approach. *Journal of Hydrology*, 543, 373-385.



Comparison of ANN, SVM and ELM for the simulation of maximum allowable Concentration



Yadav, B., Ch, S., Mathur, S., & Adamowski, J. (2016). Estimation of in-situ bioremediation system cost using a hybrid Extreme Learning Machine (ELM)-particle swarm optimization approach. *Journal of Hydrology*, 543, 373-385.



Minimize the design and operational cost



Cost Coefficient	Numerical Value
Discount rate	0.05
Injection cost, which include oxygen, nutrient and pumping operation	4,755 (\$ per lps-yr)
extraction cost, it include treatment and pumping operation	15,850 (\$ per lps-yr)
well installation cost	12,000 (\$ per well)
injection facility cost	$D_{1.26 \text{ lps}} = \$ 20,000$
treatment facility capital cost	$E_{1.26 \text{ lps}} = \$ 30,000$

$$\begin{aligned} \text{Minimize } F = & \sum_{k=1}^T \left(\frac{1}{(1+i_r)^k} \right) \sum_{x=1}^{Nw} C^q(x)q(x, k) + \sum_{x=1}^{Nw} C^{IP}(x)IP(x) \\ & + \text{Max} \left\{ D \left(\sum_{x=1}^{Nw^i} q(x, k) \right) \right\}_{k=1}^T \\ & + \text{Max} \left\{ E \left(\sum_{x=1}^{Nw^e} q(x, k) \right) \right\}_{k=1}^T \end{aligned}$$

Simulation-
Optimization
approach
ELM-PSO

Contaminant concentration

$$0 \leq C_s^T(j_0) \leq C_{max}(j_0) \quad \forall j_0 \in \Phi$$

$$0 \leq C_s^k(j_0) \leq C_{max}(j_0) \quad k = 1, \dots, T \quad \forall j_0 \in \Psi$$

Hydraulic heads

$$h^k(j_0) \leq h^{max}(j_0) \quad k = 1, \dots, T \quad \forall j_0 \in \Phi$$

$$h^{min}(j_0) \leq h^k(j_0) \quad k = 1, \dots, T \quad \forall j_0 \in \Phi$$

Extraction rate and injection rate

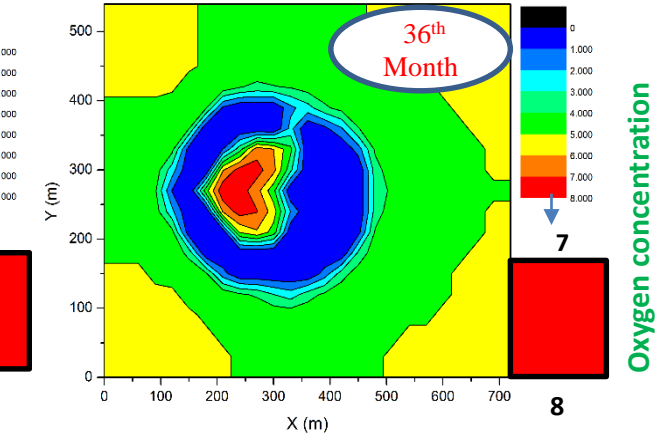
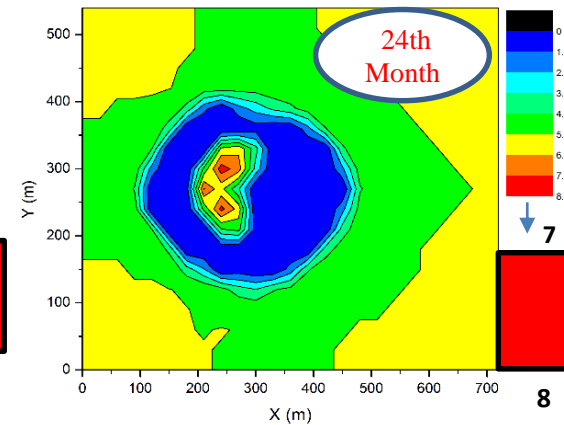
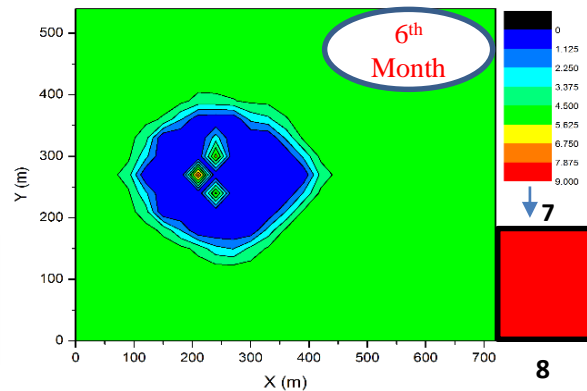
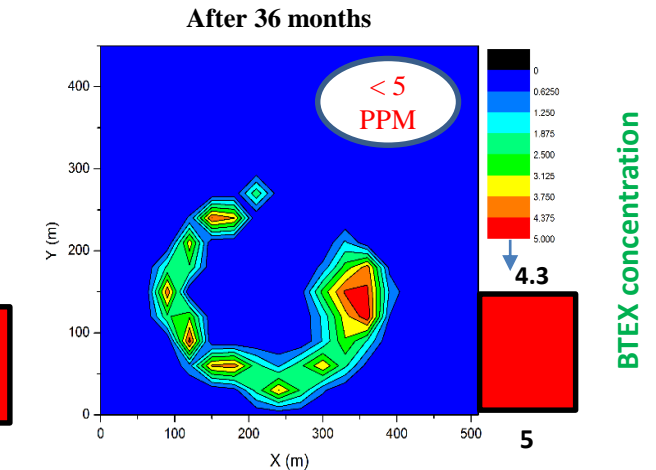
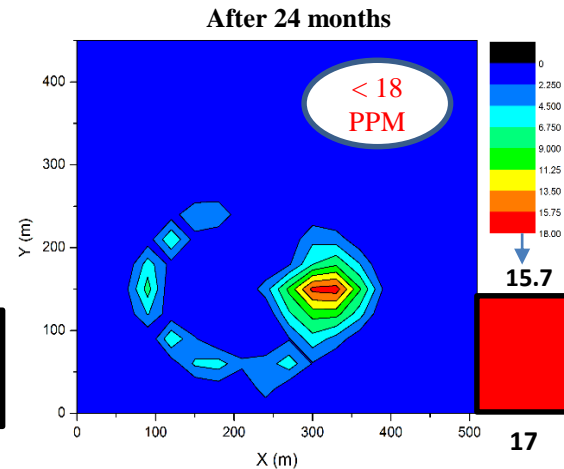
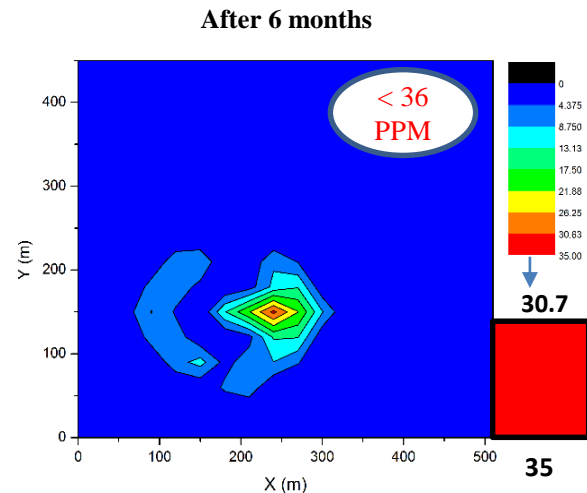
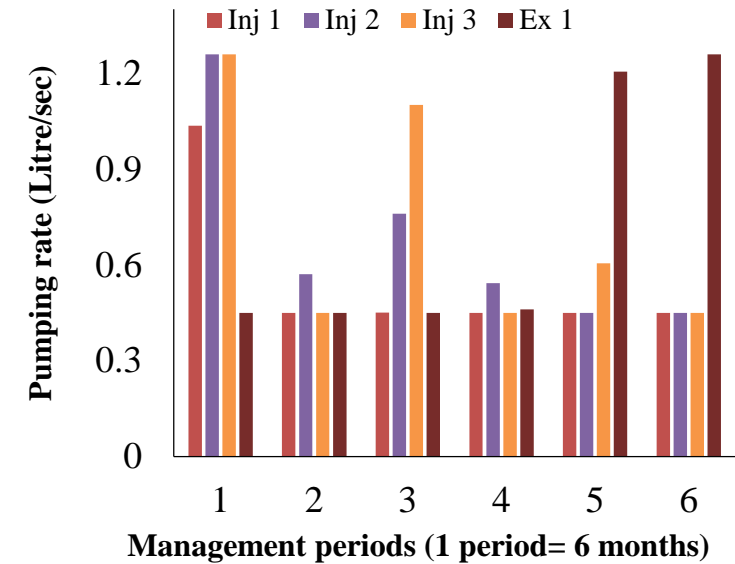
$$0 \leq q_{ex}^k \leq q_{ex}^{max^k} \quad k = 1, \dots, T$$

$$0 \leq q_{ix}^k \leq q_{ix}^{max^k} \quad k = 1, \dots, T$$

Yadav, B., Ch, S., Mathur, S., & Adamowski, J. (2016). Estimation of in-situ bioremediation system cost using a hybrid Extreme Learning Machine (ELM)-particle swarm optimization approach. *Journal of Hydrology*, 543, 373-385.



Optimized pumping rates, BTEX-Oxygen concentration and cost for remediation



Simulation-Optimization algorithm

ELM-PSO

Pumping strategy

Time varying

Number of wells

i_1, i_2, i_4, e_1

Total cost (\$)

158,229

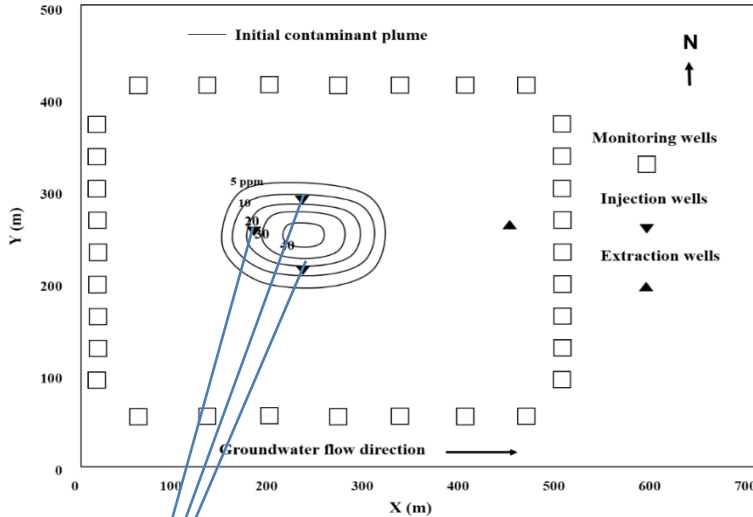
Yadav, B., Ch, S., Mathur, S., & Adamowski, J. (2016). Estimation of in-situ bioremediation system cost using a hybrid Extreme Learning Machine (ELM)-particle swarm optimization approach. *Journal of Hydrology*, 543, 373-385.



Consideration of well clogging in remediation cost estimation

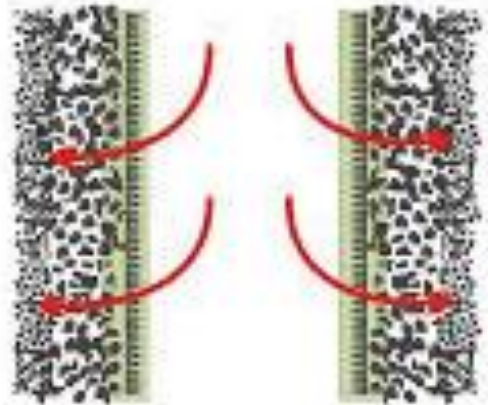


Consideration of Well clogging

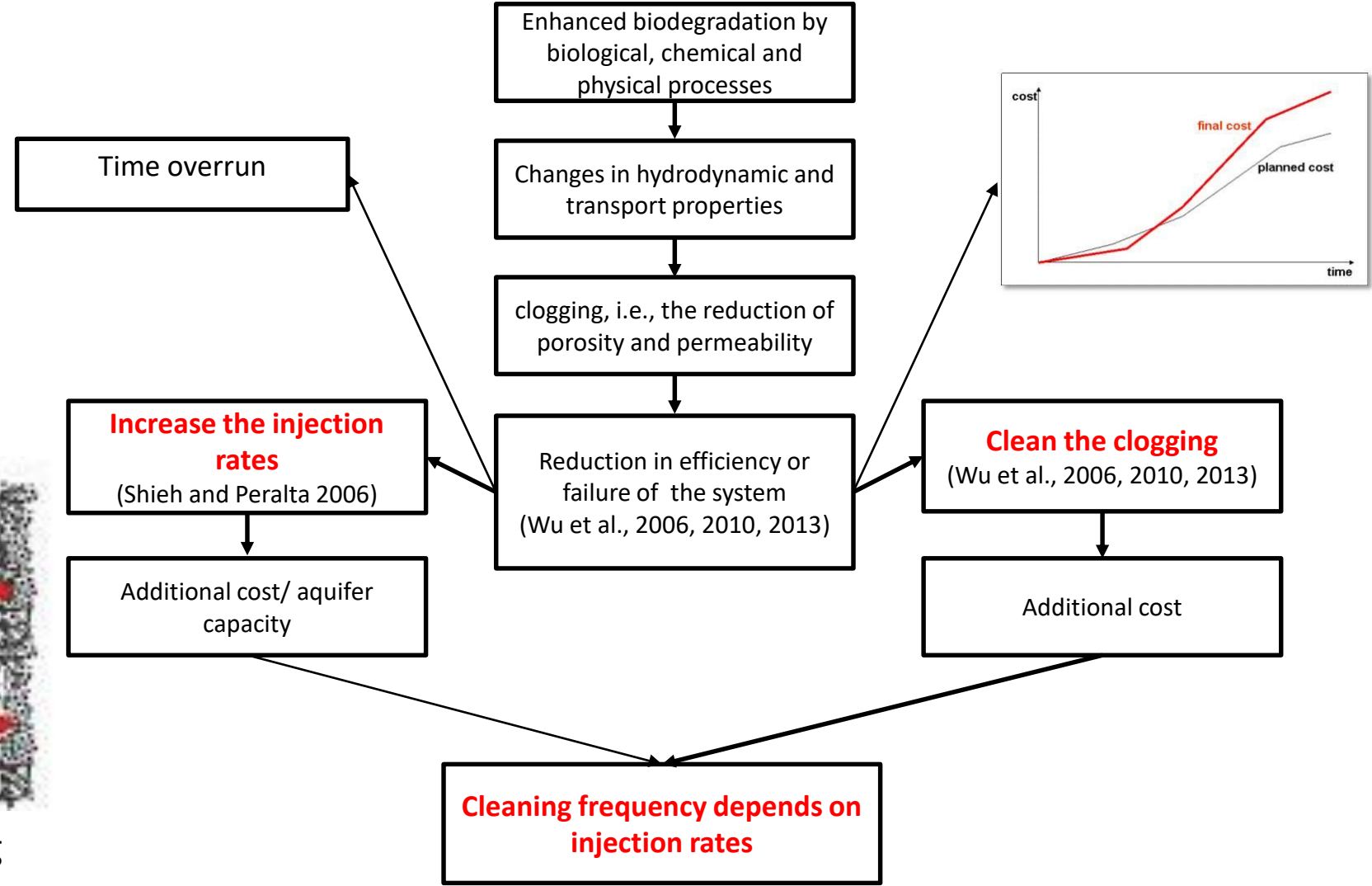


Three injection wells

Consideration of Well clogging



Biological clogging

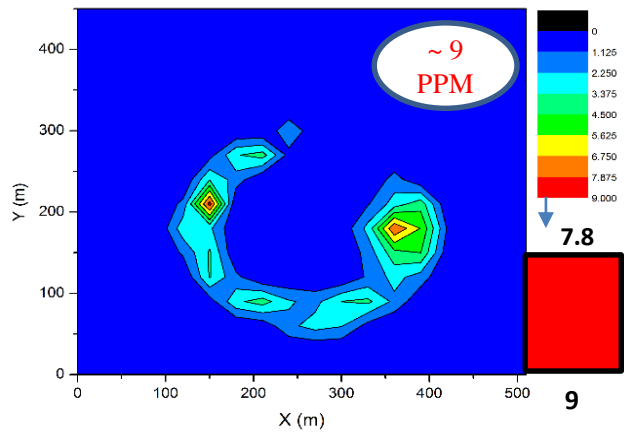


Yadav, B., Mathur, S., & Yadav, B. K. (2018). Simulation-Optimization Approach for the Consideration of Well Clogging during Cost Estimation of In Situ Bioremediation System. *Journal of Hydrologic Engineering*, 23(3), 04018001.

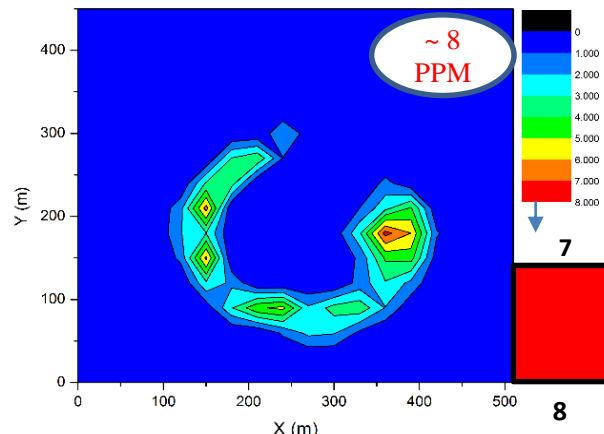
Optimal system design with well clogging assumed to the extreme case



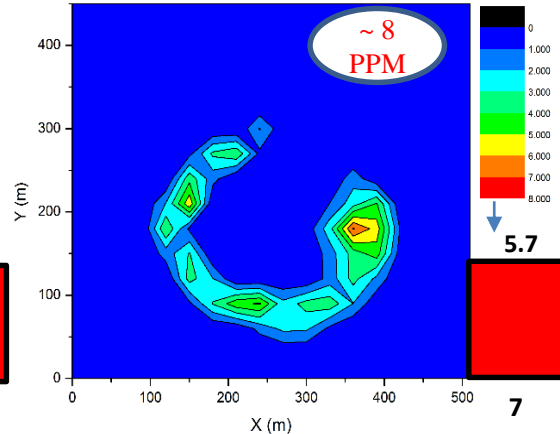
BTEX concentrations



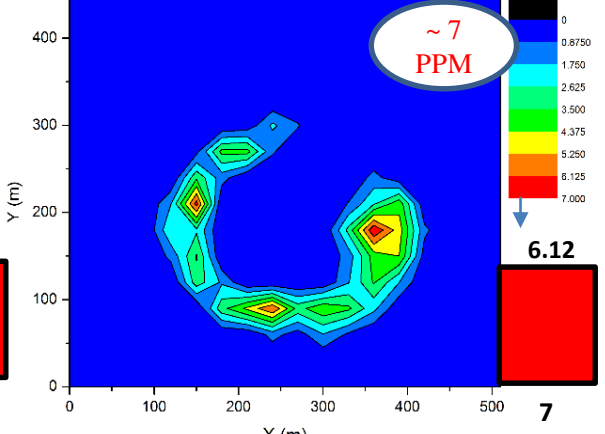
Well 1 fails after 24 months



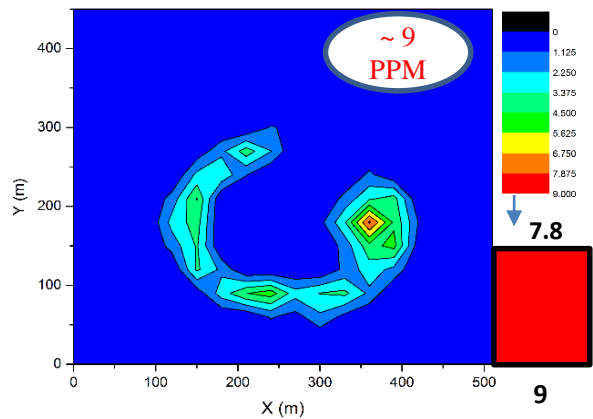
Well 1 fails after 30 months



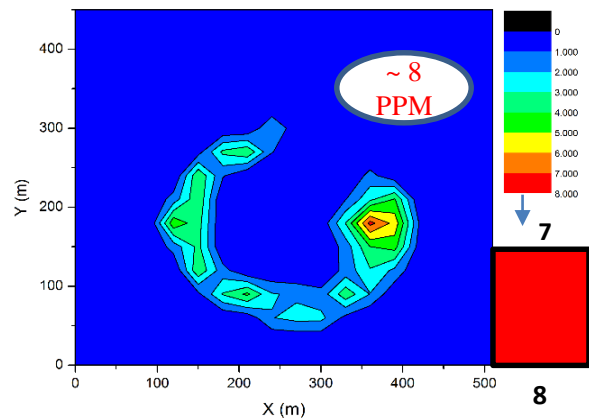
Well 3 fails after 24 months



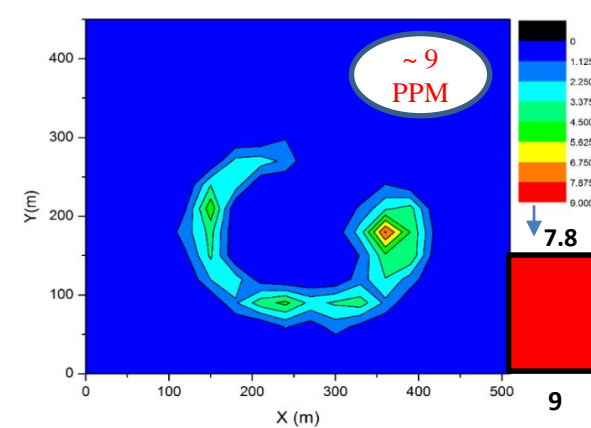
Well 3 fails after 30 months



Well 2 fails after 24 months



Well 2 fails after 30 months



All three wells fails after 30 months

Yadav, B., Mathur, S., & Yadav, B. K. (2018). Simulation-Optimization Approach for the Consideration of Well Clogging during Cost Estimation of In Situ Bioremediation System. *Journal of Hydrologic Engineering*, 23(3), 04018001.



The objective function- if increase of injection rates is the option

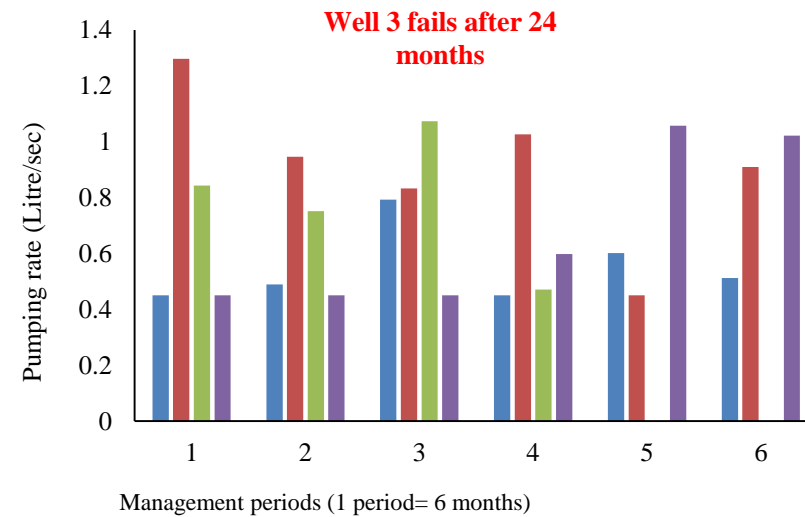
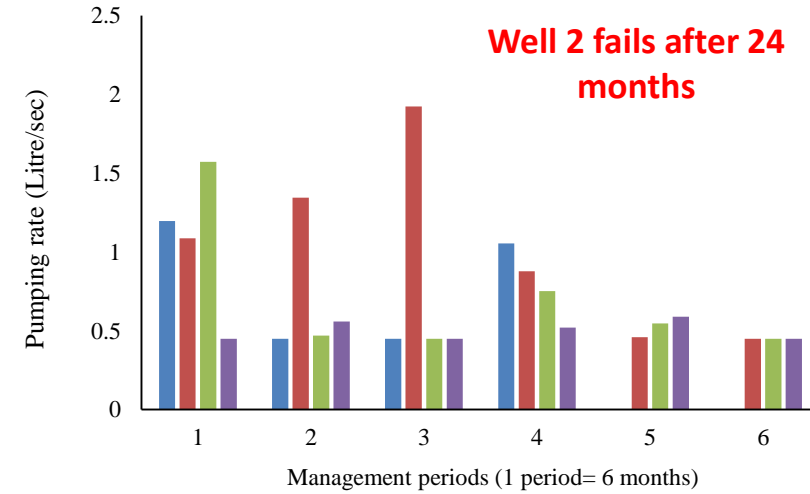
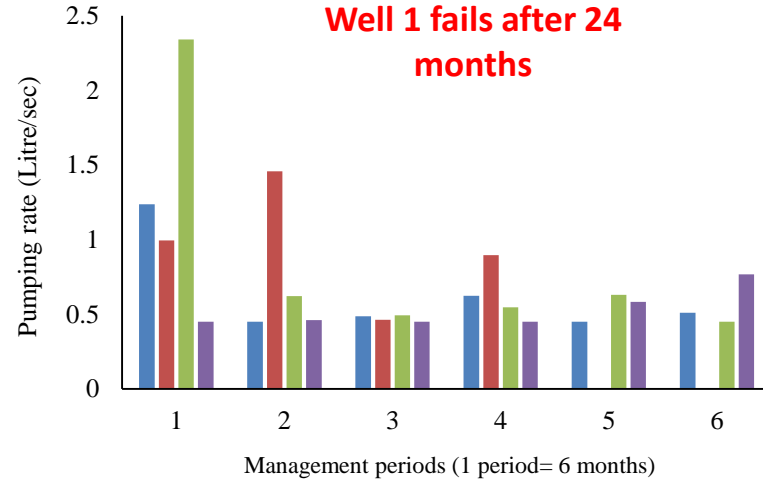


$$\begin{aligned} \text{Minimize } Z = & \sum_{k=1}^T \left(\frac{1}{(1+i_r)^k} \right) \sum_{x=1}^{Nw} C^q(x)q(x, k) + \sum_{x=1}^{Nw} C^{IP}(x)IP(x) + \text{Max} \left\{ D \left(\sum_{x=1}^{Nw^i} q(x, k) \right) \right\}_{k=1}^T \\ & + \text{Max} \left\{ E \left(\sum_{x=1}^{Nw^e} q(x, k) \right) \right\}_{k=1}^T \end{aligned}$$

Constraints relaxed- $0 \leq q_{ix}^k \quad k = 1, \dots, T$



If increase of injection rates is the option



Maximum injection/extraction rate is >1.26 Litre/Sec



The objective function- if cleaning is the option



$$\begin{aligned} \text{Minimize } Z = & \sum_{k=1}^T \left(\frac{1}{(1+i_r)^k} \right) \sum_{x=1}^{Nw} C^q(x)q(x, k) + \sum_{x=1}^{Nw} C^{IP}(x)IP(x) + \text{Max} \left\{ D \left(\sum_{x=1}^{Nw^i} q(x, k) \right) \right\}_{k=1}^T \\ & + \text{Max} \left\{ E \left(\sum_{x=1}^{Nw^e} q(x, k) \right) \right\}_{k=1}^T + \text{Max} \left\{ CL \left(\sum_{x=1}^{Nw^i} q(x, k) \right) \right\}_{k=1}^T \end{aligned}$$

- $CL \left(\sum_{x=1}^{Nw^i} q(x, k) \right)$ = Well cleaning cost which is a function of the total injection rate (\$)
- Material cost and Pump cost were added in the well installation cost as it is a constant value



The cost factor and optimized cost



Approximate cost for the cleaning of well by surge block method

Factor	Cost
Material cost	\$150/block
Pump cost	\$2000
Average wage rate (Bureau of Labour Statistics, 2016)	\$25.61/hr

Cost function coefficient 'CL' (excluding instrument and material cost)

Coefficient	Value with frequency of cleaning for one well
CL (cleaning cost)	$C_{0-3.78 \text{ L/s}} = \921.96 (6 times/year)
	$C_{3.78-6.30 \text{ L/s}} = \614.64 (4 times/year)
	$C_{6.30-8.82 \text{ L/s}} = \460.98 (3 times/year)



The objective function- if increase of injection rates is the option

Comparison of total remediation cost for time varying pumping strategy for the possibility of well failure due to extreme well clogging.

Optimization algorithm	Pumping strategy	Number of wells	Total cost (\$)
(Shieh and Peralta, 2005)	Time varying	i_1, i_2, i_4, e_1	163,300
(Kumar et al., 2013)	Time varying	i_1, i_2, i_4, e_1	160,684
ELM-PSO	Time varying	i_1, i_2, i_4, e_1	158,229
ELM-PSO (with cleaning)	Time varying	i_1, i_2, i_4, e_1	160, 503

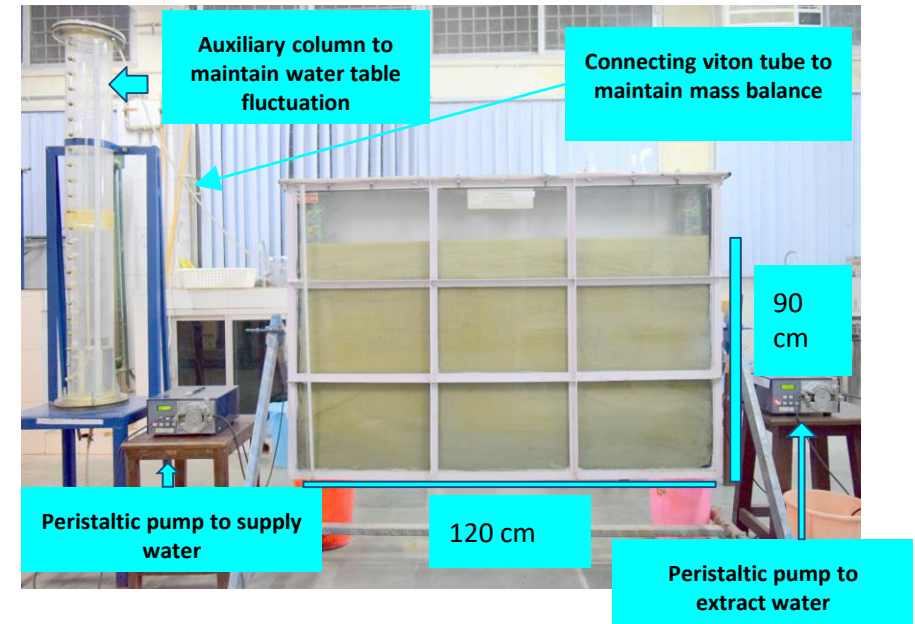
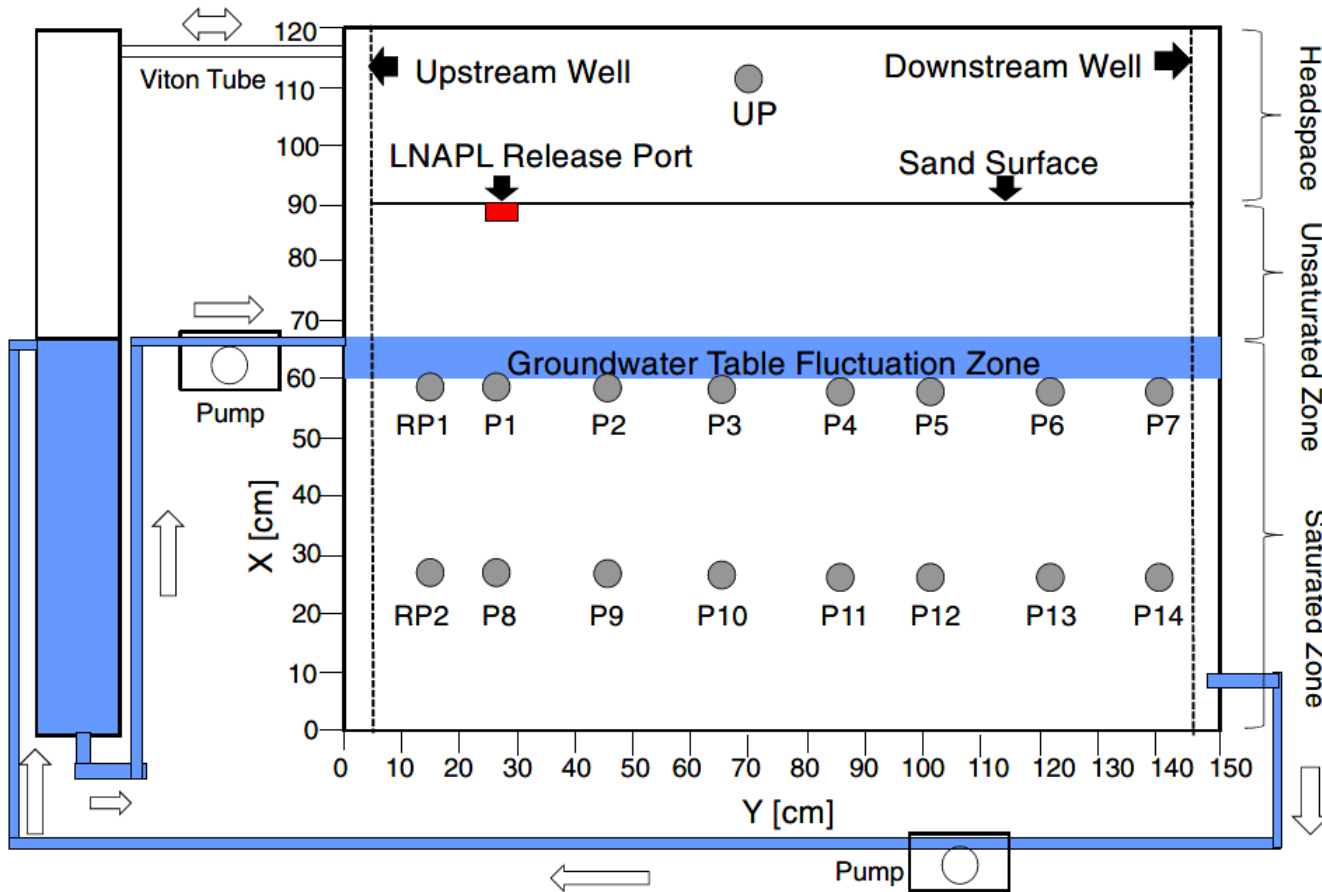
- The study suggest that the cleaning of the injection well is the best choice.
- The cost obtained is higher than what was projected in the earlier studies, however with this system the cost is more realistic and feasible.



Role of groundwater fluctuations and environmental parameters on bioremediation

- How groundwater table fluctuations affect the toluene plume?
- Is there any impact on biodegradation rates?
- Toluene concentration and microbial growth.
- Soil moisture and temperature.

Experimental setup and selected level of fluctuations



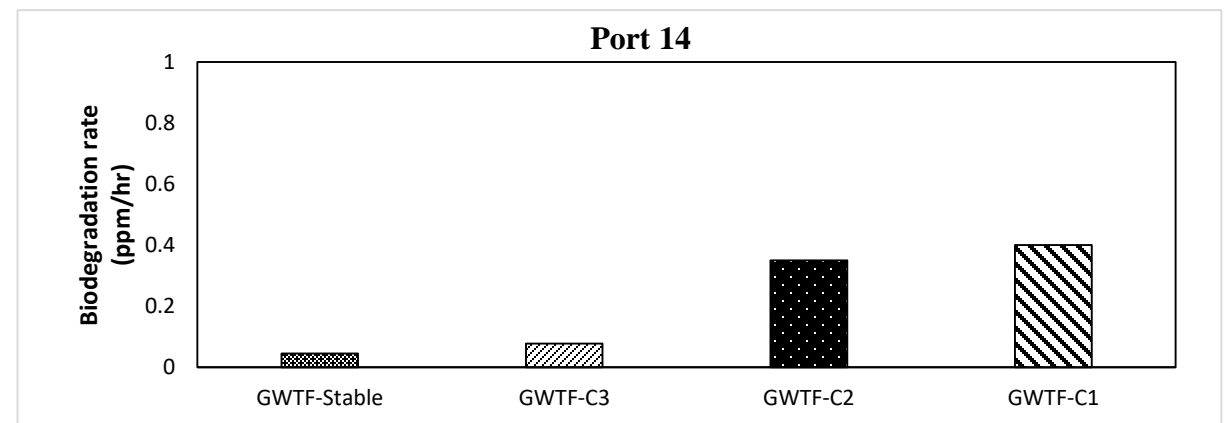
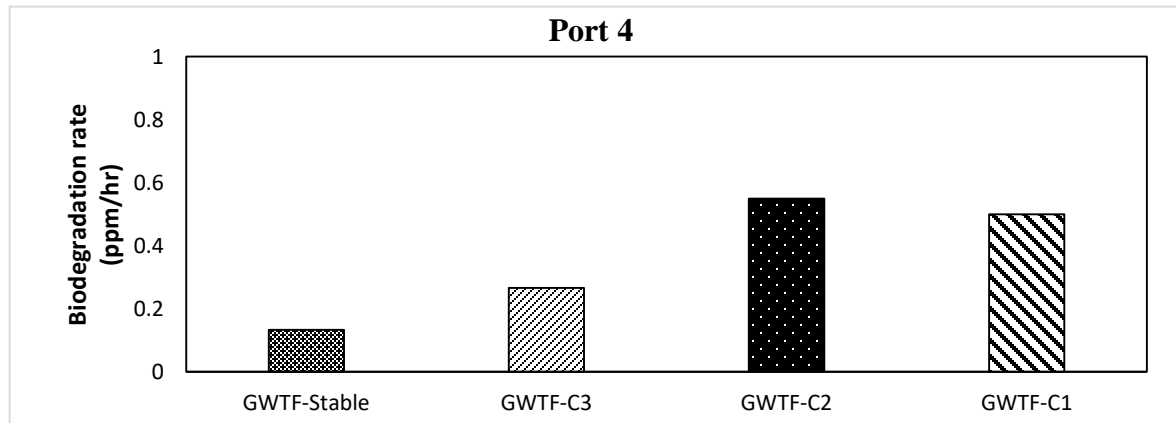
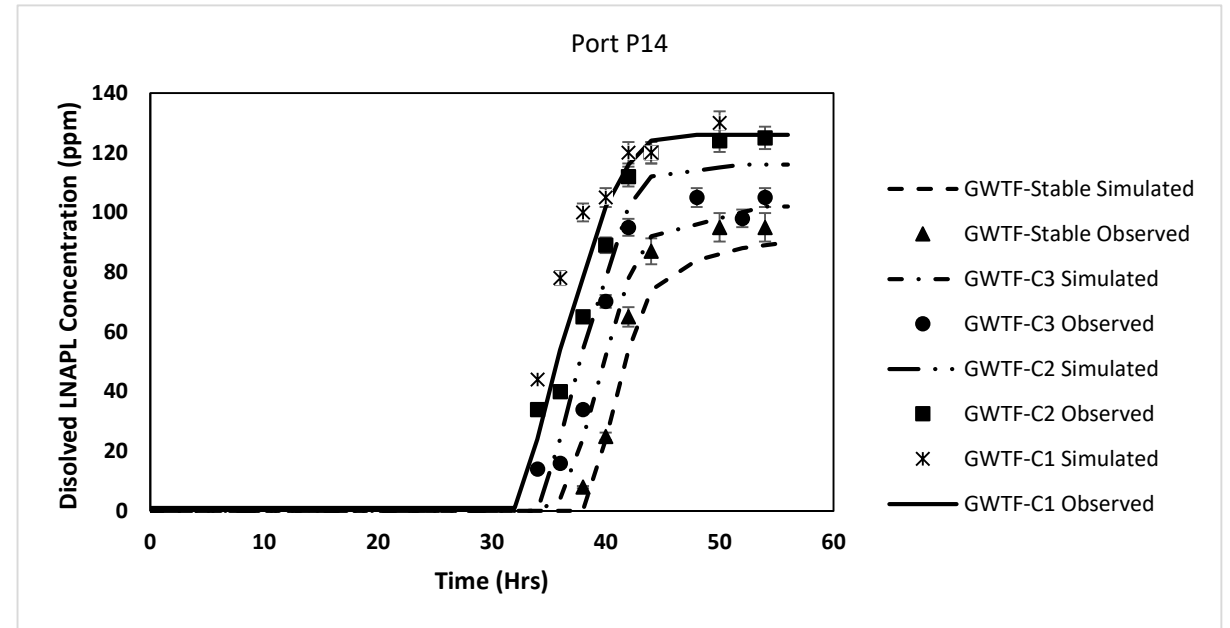
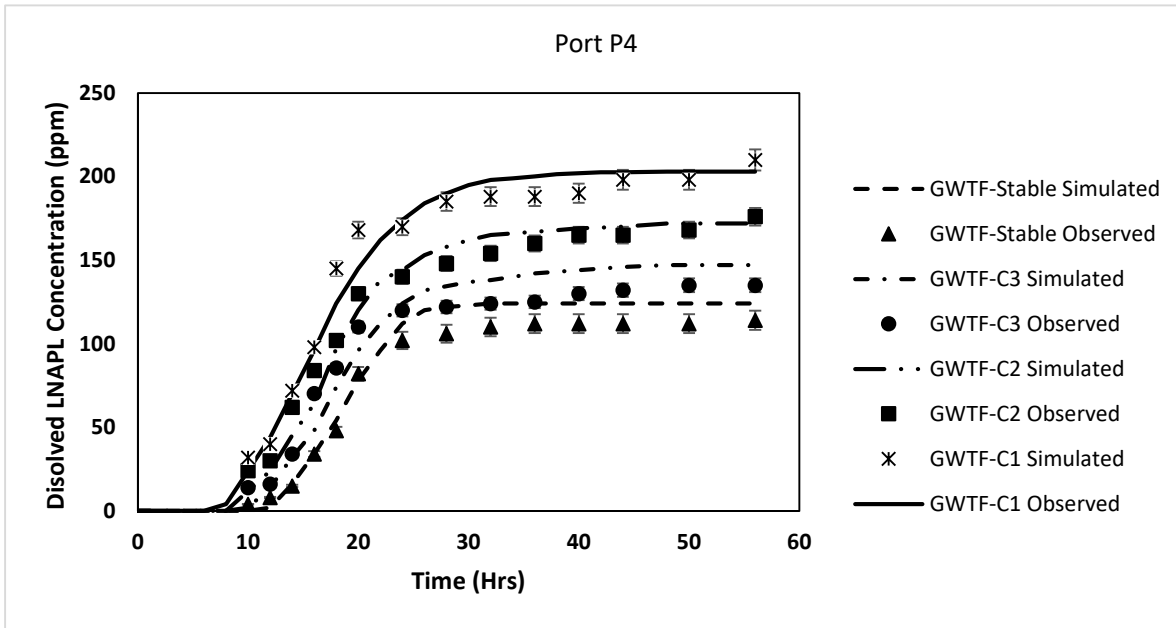
Selected level of fluctuations and pumping rates

Conditions	Inflow pumping		Outflow pumping		Total duration (h)	Pumping rate (mL/h)
	Rise (h)	Fall	Rise	Fall (h)		
C1 Rapid fluctuation	1	—	—	1	2	2,475.0
C2 General fluctuation	2	—	—	2	4	1,237.5
C3 Slow fluctuation	4	—	—	4	8	6,18.7

Gupta, P. K., Yadav, B., & Yadav, B. K. (2019). Assessment of LNAPL in subsurface under fluctuating groundwater table using 2D sand tank experiments. *Journal of Environmental Engineering*, 145(9), 04019048.



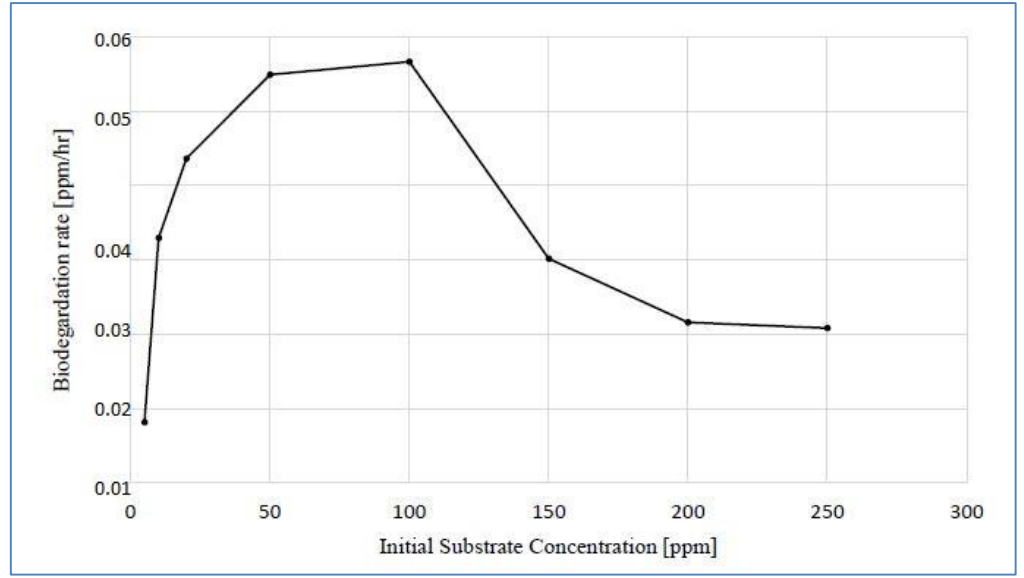
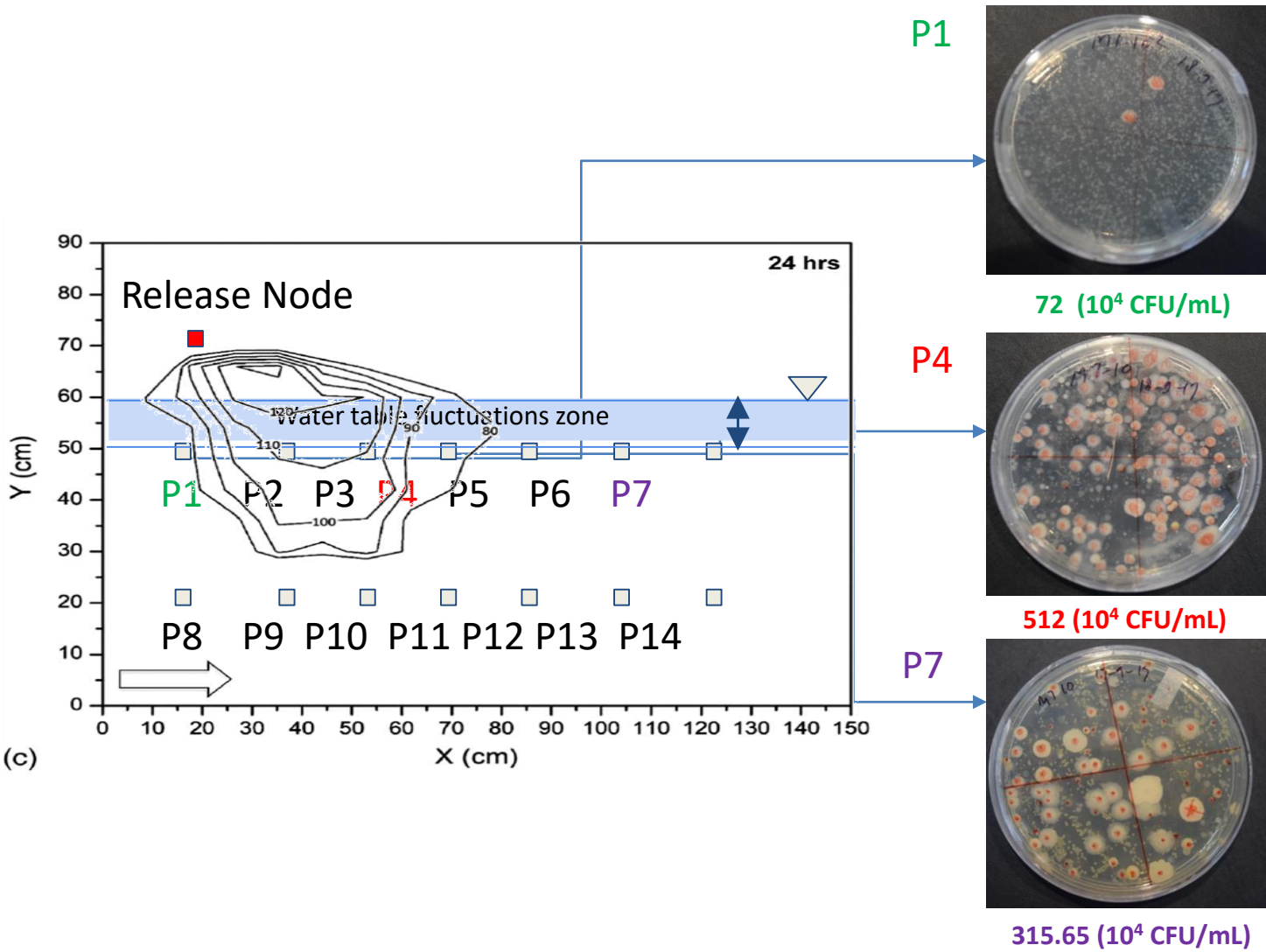
Transport of dissolved LNAPL



Gupta, P. K., Yadav, B., & Yadav, B. K. (2019). Assessment of LNAPL in subsurface under fluctuating groundwater table using 2D sand tank experiments. *Journal of Environmental Engineering*, 145(9), 04019048.



Microbial growth at different locations



Biodegradation rates

Gupta, P. K., Yadav, B., & Yadav, B. K. (2019). Assessment of LNAPL in subsurface under fluctuating groundwater table using 2D sand tank experiments. *Journal of Environmental Engineering*, 145(9), 04019048.



Impact of various environmental conditions on biodegradation rate



To estimate the biodegradation rate of dissolved Toluene moving towards groundwater through partially saturated zone having **different soil moisture level under normal and cold environmental conditions**

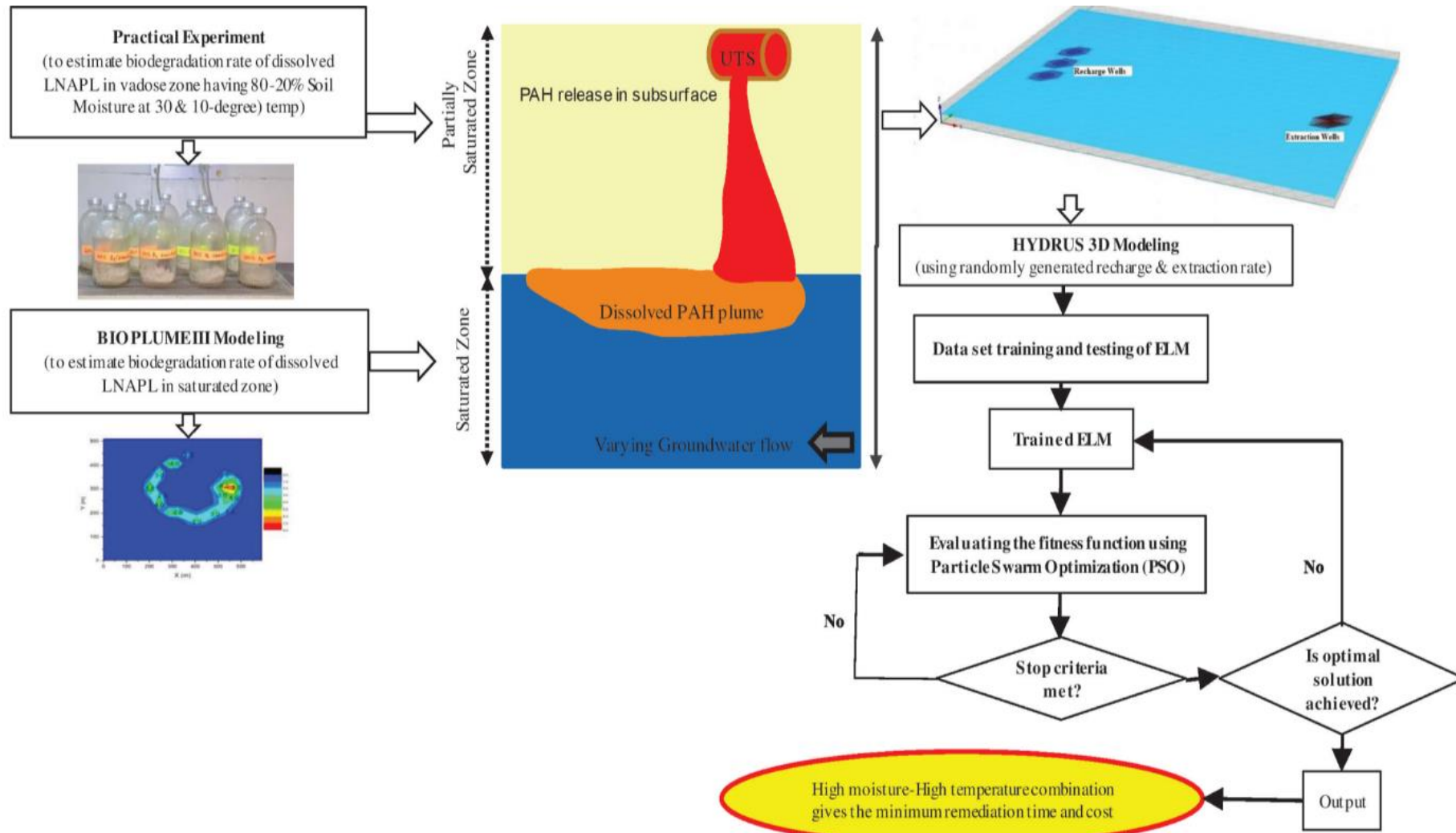


Batch system having different soil-moisture conditions.

Moisture Levels	Temperature	Total degradation time [hours] in batch system	Rate of Biodegradation [mg/L hr]
80%	10±0.5 ⁰ C	72	0.0025
	30±2 ⁰ C	42	0.0154
60%	10±0.5 ⁰ C	105	0.0018
	30±2 ⁰ C	75	0.0120
40%	10±0.5 ⁰ C	120	0.0010
	30±2 ⁰ C	84	0.0092
20%	10±0.5 ⁰ C	128	0.0008
	30±2 ⁰ C	90	0.0028



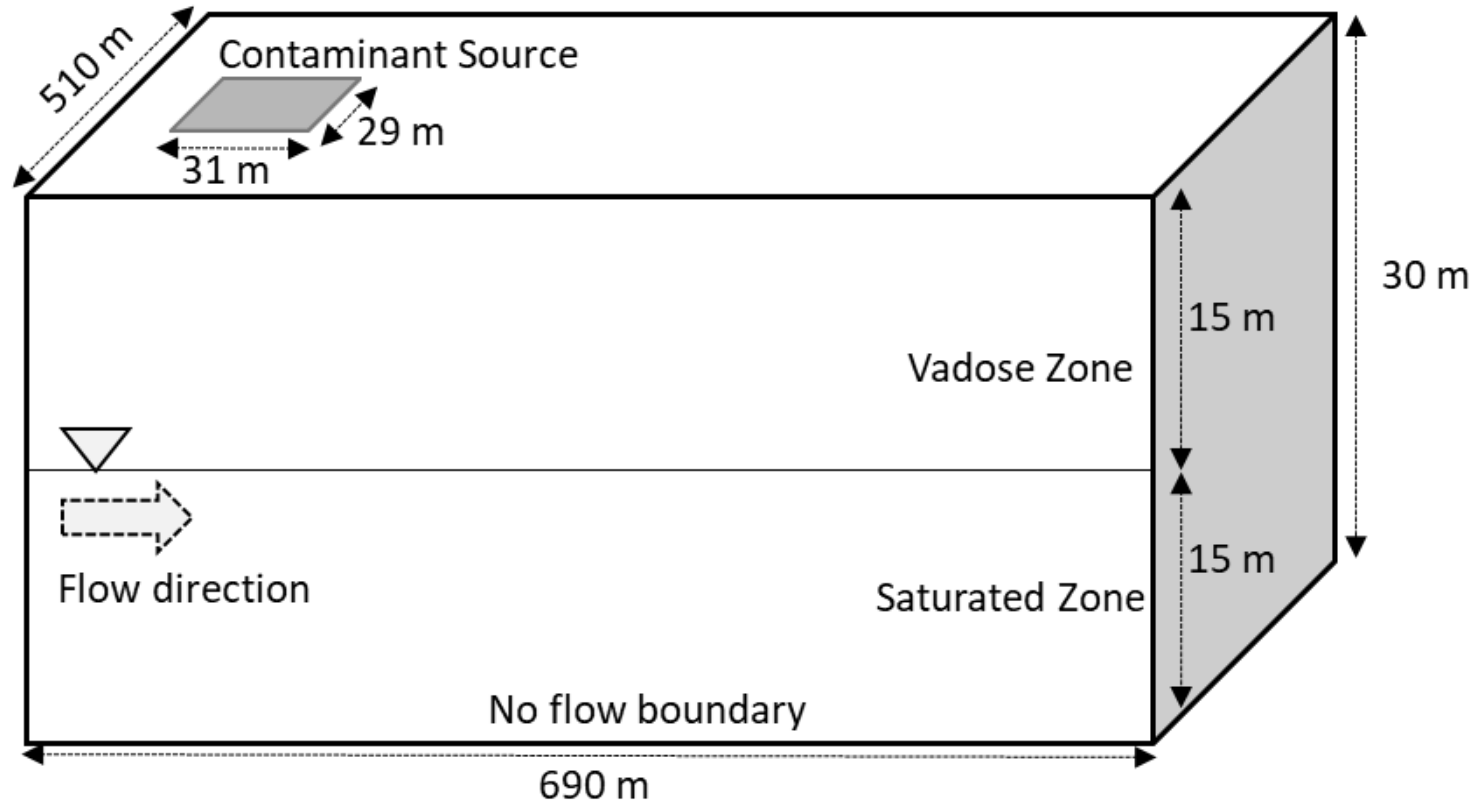
Remediation system for removal of Toluene from groundwater and partially saturated zone



Gupta, P. K., Yadav, B., Yadav, B. K., Sushkova, S., & Basu, S. (2021). Engineered Bioremediation of NAPL Polluted Sites: Experimental and Simulation-Optimization Approach under Heterogeneous Moisture and Temperature Conditions. *Journal of Environmental Engineering*, 147(8), 04021023.)



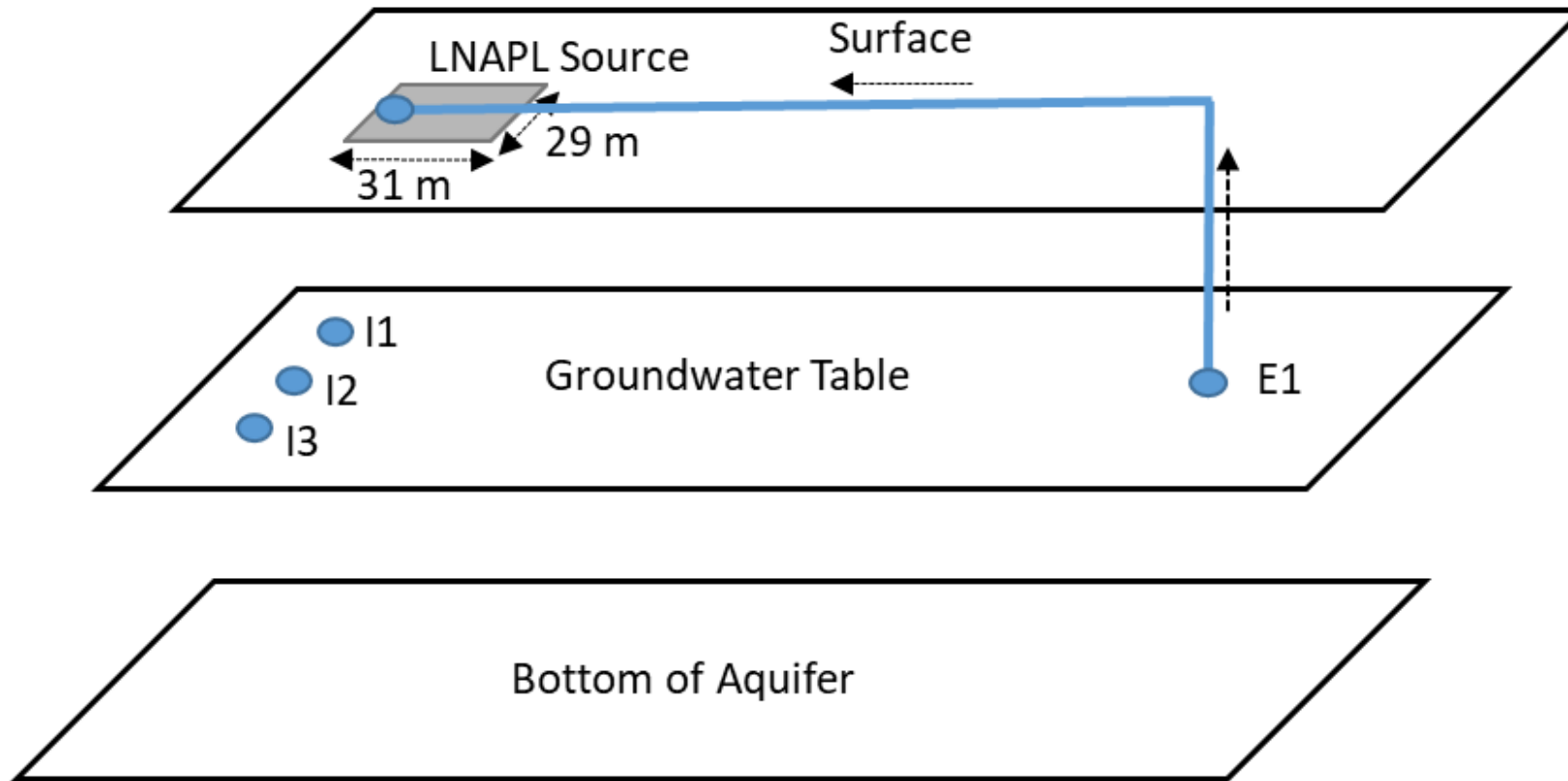
Study Domain- partially saturated and saturated zones



- The steady state condition was considered throughout the simulation.
- Homogeneously distributed sand was considered as porous media.
- Constant pumping rates were taken

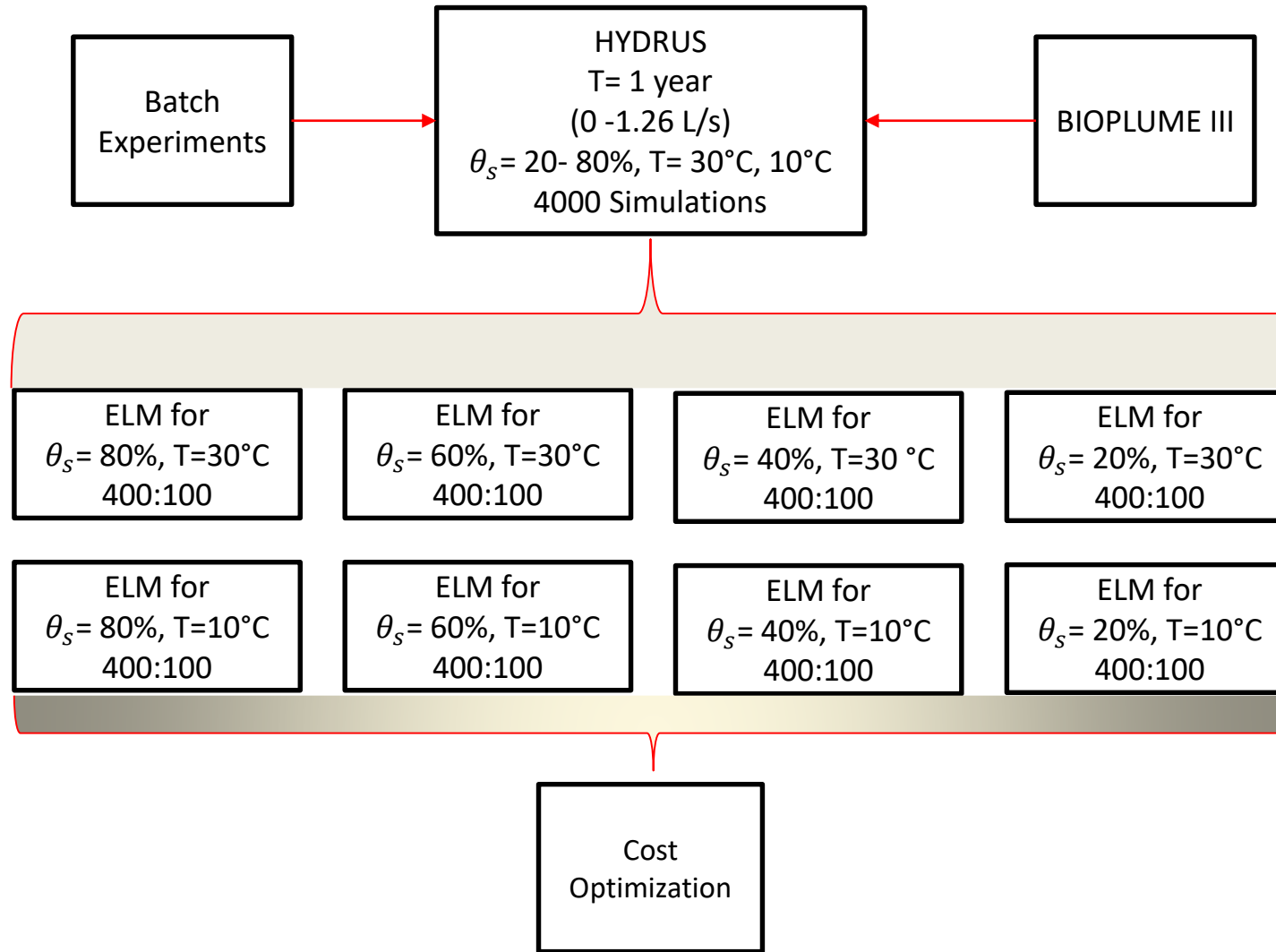


Injection/Extraction well and Recharge flux location





Trained surrogate simulator to replace HYDRUS 2D/3D





Objective function for constant pumping rates



Minimize
$$F = W_F \sum_{e=1}^{N_w} C_{p_e} \cdot p_e + \sum_{e=1}^{N_w} C_{I p_e} \cdot I p_e + D \left[\sum_{e=1}^{N_i} p_e \right] + E \left[\sum_{e=1}^{N_e} p_e \right]$$

$$W_F = \left[(1 + i_r)^T - 1 \right] / \left[i_r (1 + i_r)^T \right]$$

Minimize Concentration = C_{\max}

Subject to:-

$$0 \leq C_{ow} \leq C_{st}$$

$$ow = 1, 2, \dots, N_o$$

$$H_{i \min} \leq H_e \leq H_{i \max}$$

$$e = 1, 2, \dots, N_i$$

$$H_{e \min} \leq H_e \leq H_{e \max}$$

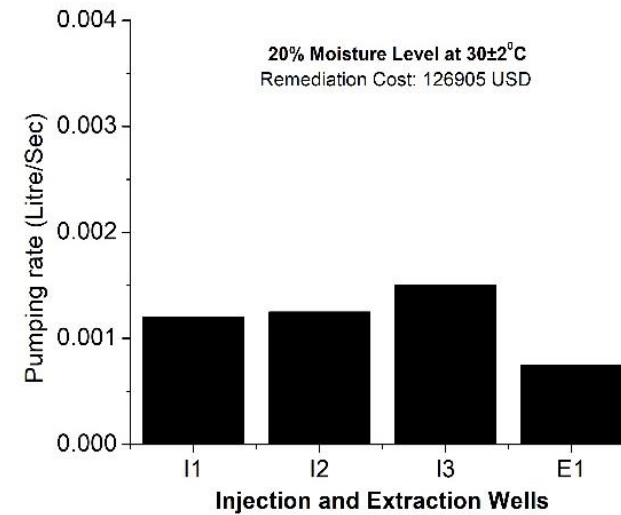
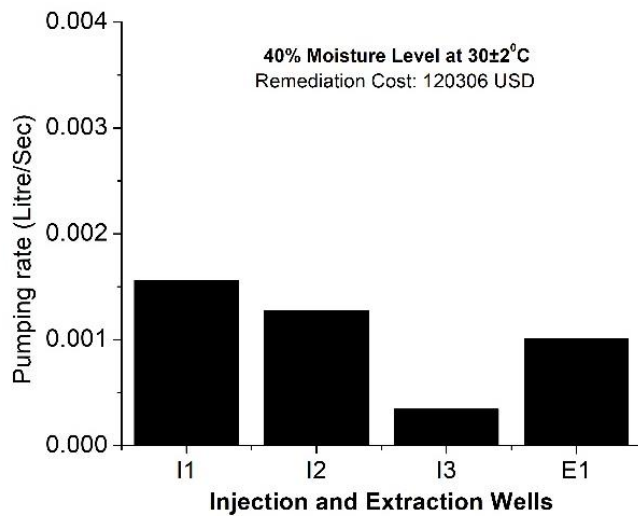
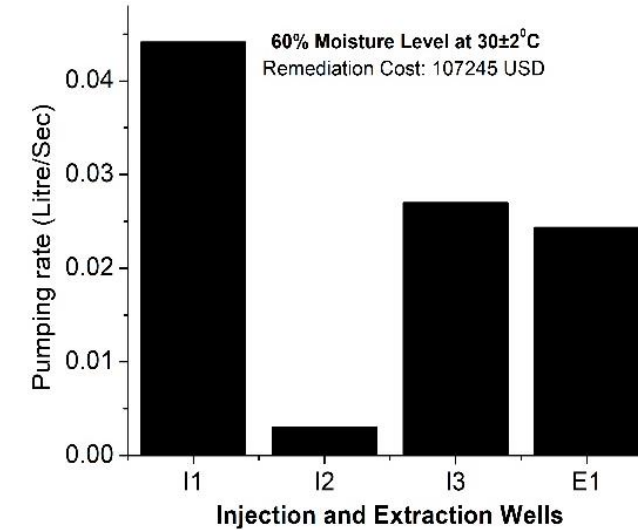
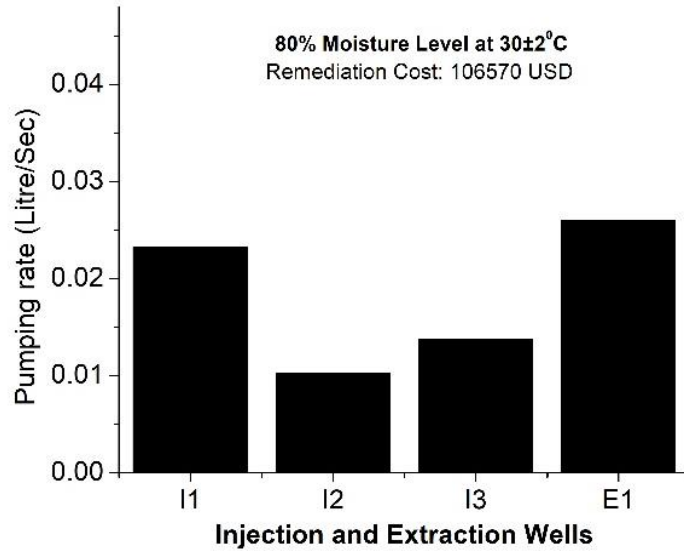
$$e = 1, 2, \dots, N_e$$

$$p_{\min} \leq p_e \leq p_{\max}$$

$$e = 1, 2, \dots, N_w$$

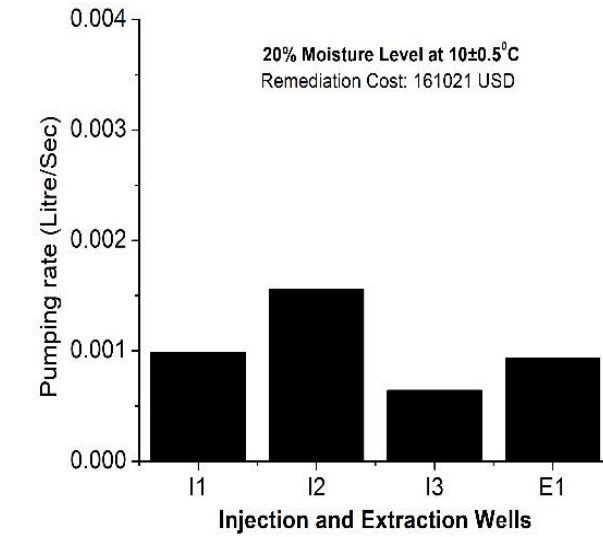
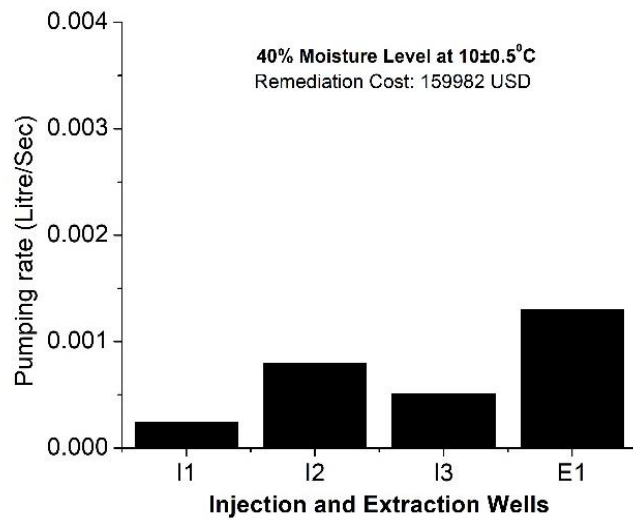
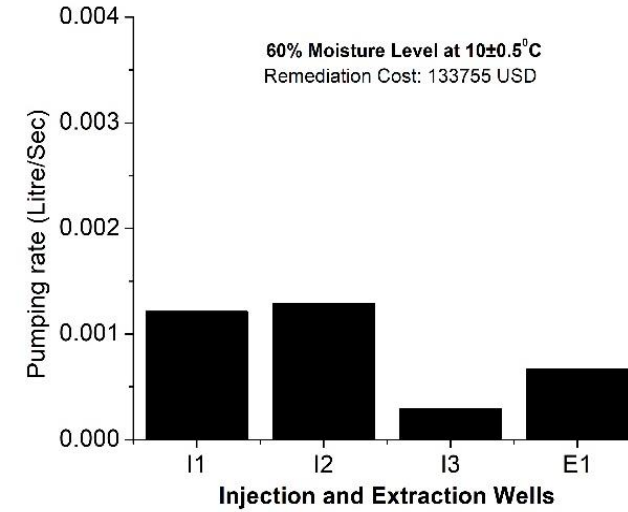
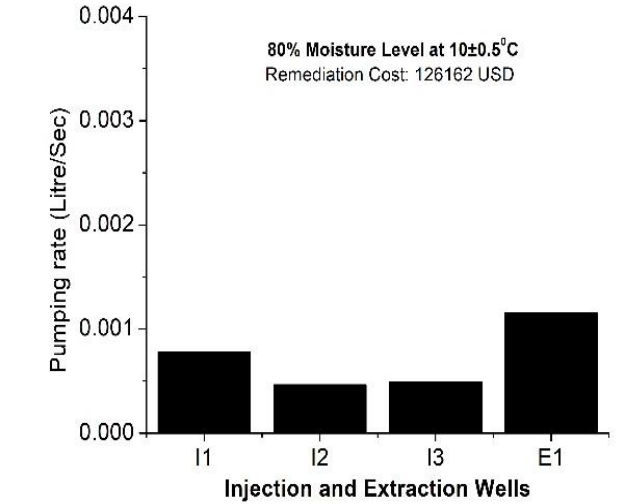


Optimized injection and extraction rates at 30 °C





Optimized injection and extraction rates at 10 °C

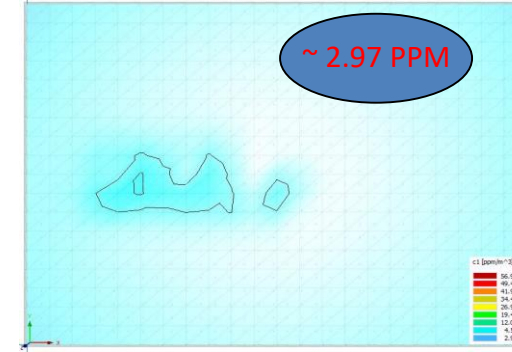
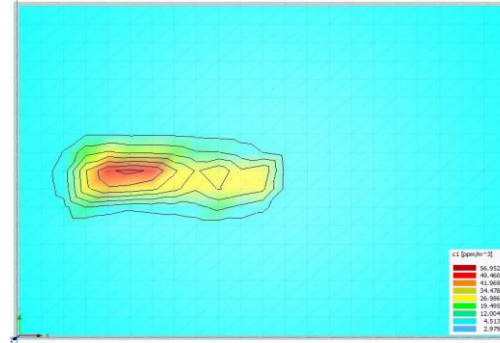
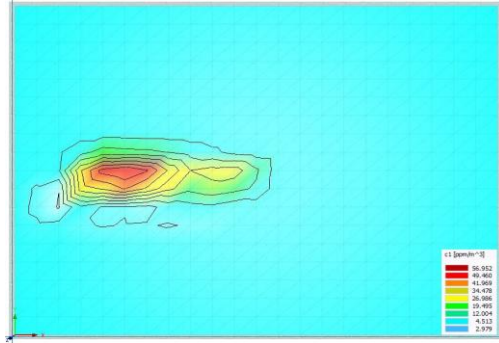




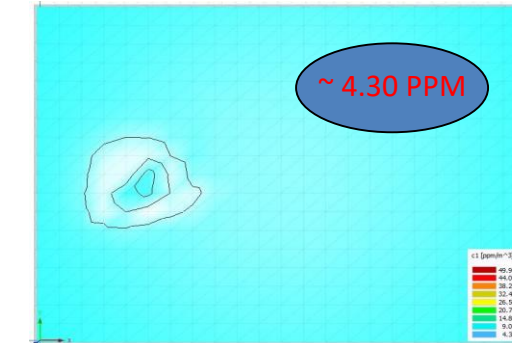
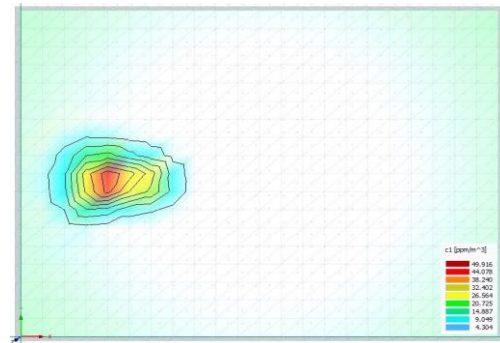
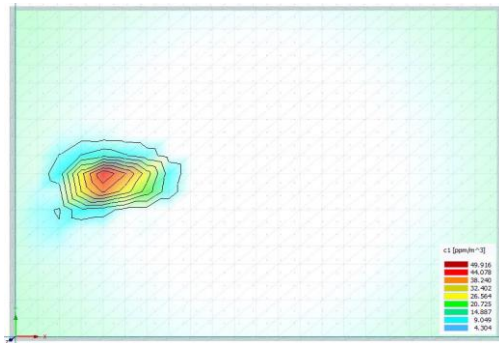
Validation of the optimized injection and extraction rates at 30 °C



80% and temperature 30°C



60% and temperature 30°C



5 days

180 days

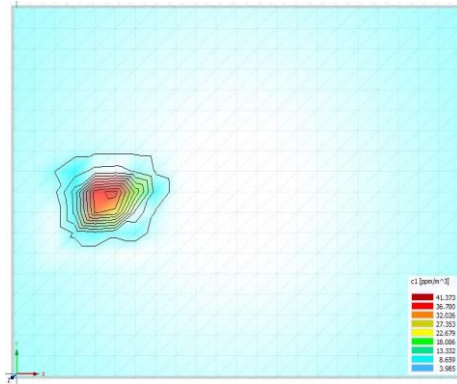
365 days



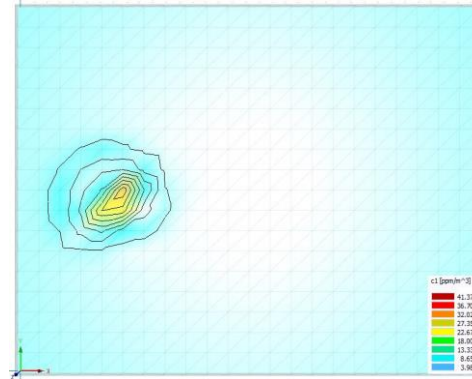
Validation of the optimized injection and extraction rates at 30 °C



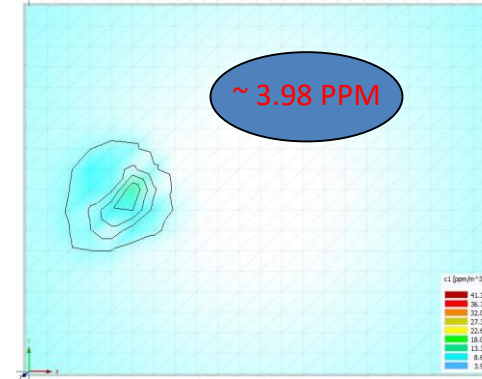
40% and temperature 30°C



5 days

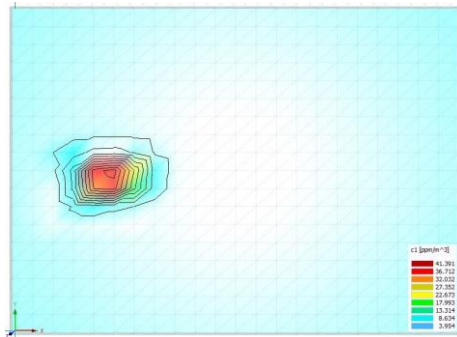


365 days

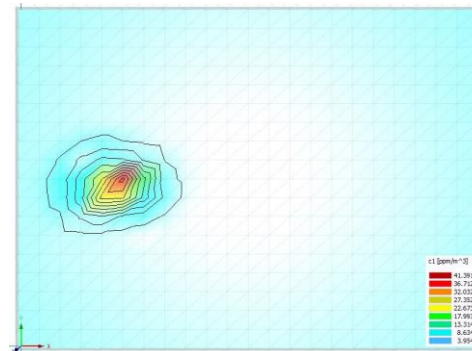


455 days

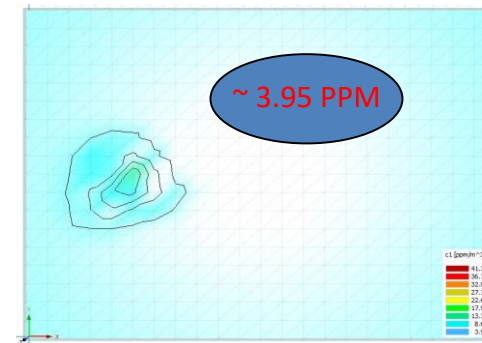
20% and temperature 30°C



5 days



455 days

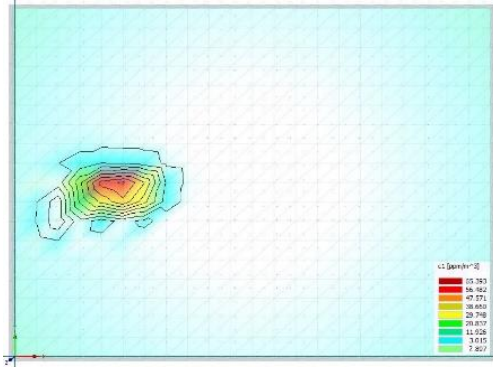


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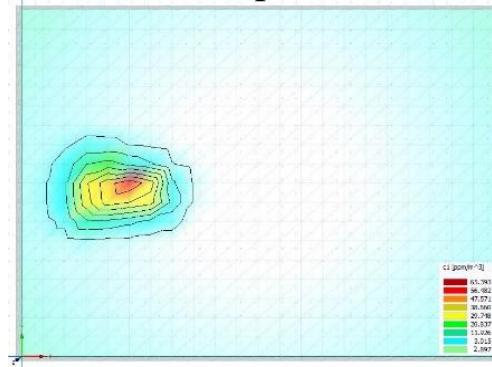


Validation of the optimized injection and extraction rates at 10 °C

80% and temperature 10°C



5 days

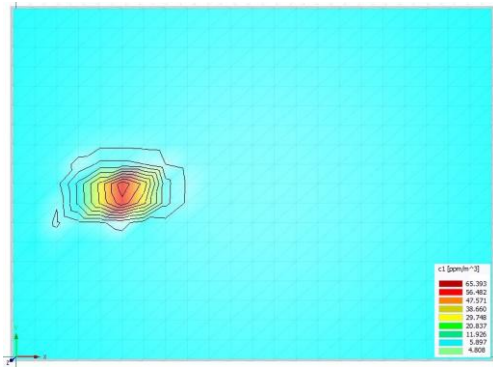


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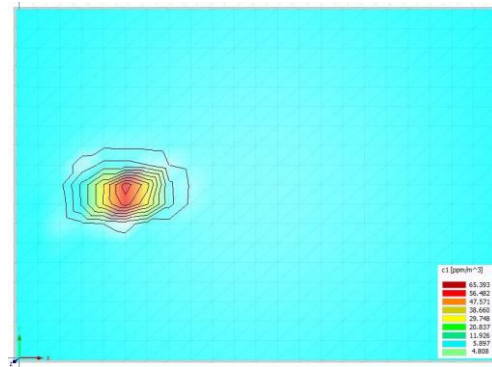


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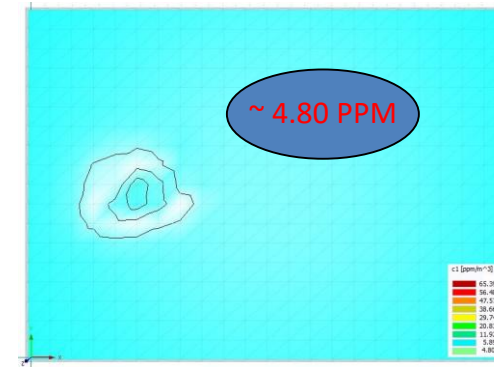
60% and temperature 10°C



5 days



455 days



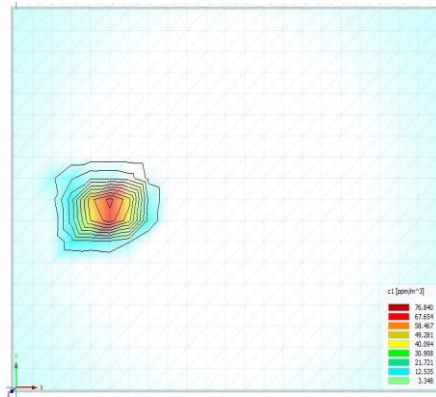
730 days



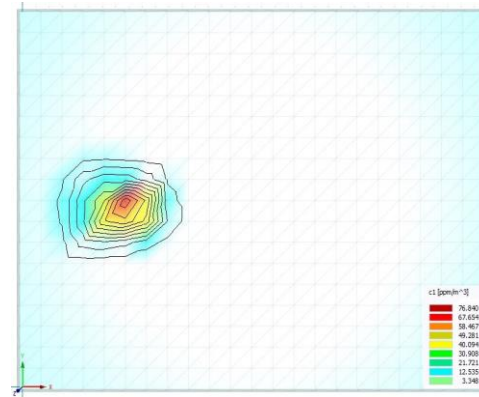
Validation of the optimized injection and extraction rates at 10 °C



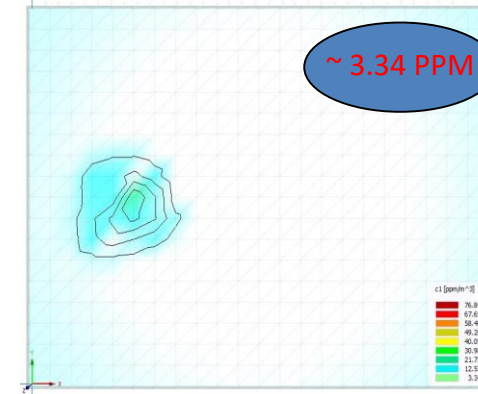
40% and temperature 10°C



5 days

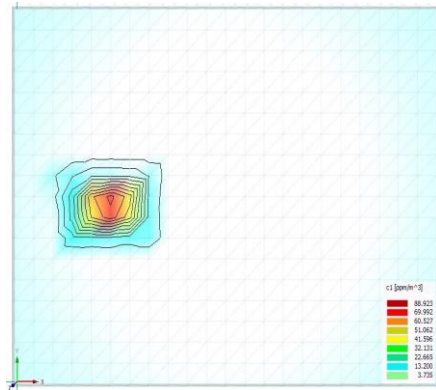


455 days

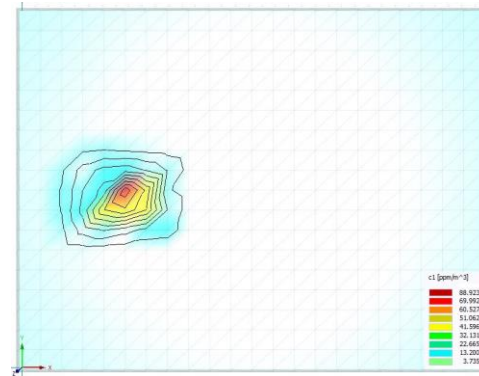


545 days

20% and temperature 10°C



5 days



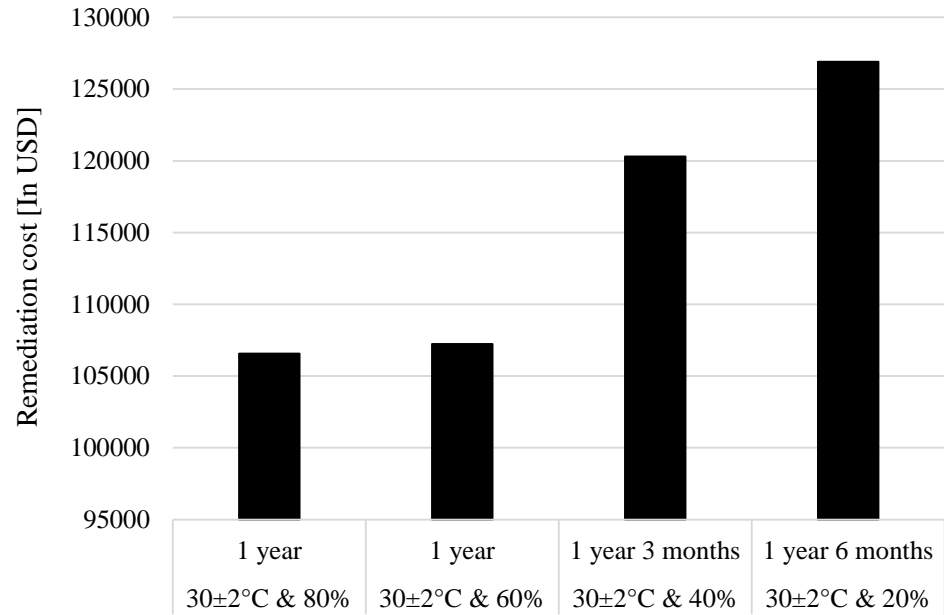
455 days



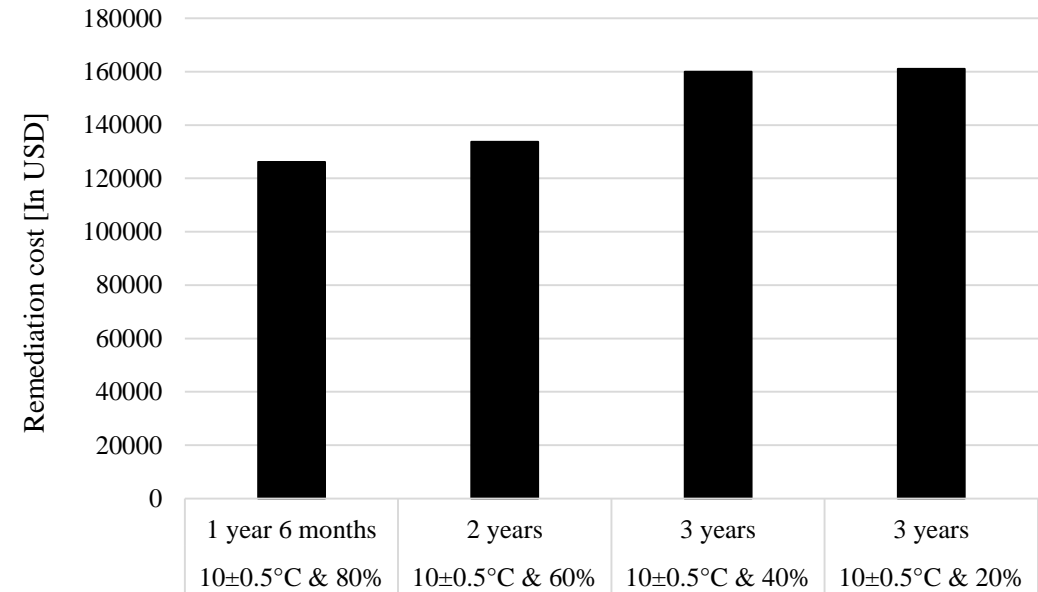
730 days



Optimized remediation system cost



Site conditions along with Remediation period



Site conditions along with Remediation period

High moisture-
High temperature
combination gives
the minimum cost



Summary



- In-situ bioremediation is the effective strategy for remediation of water contaminated with the petroleum hydrocarbons causing least site disturbance and minimum cost.
- The simulation optimization approach can solve the management problem. The approach of data based modeling can be very useful in hybrid simulation-optimization formulation.
- The developed approach can be generalized in case the remediation time changes, site constraints changes etc.
- The study also suggest that the more realistic and feasible design can be formulated by extending the optimization scope (well cleaning)
- The integrated approach of experimental, numerical and data based modeling gives the flexibility to characterise the site condition more effectively and accurately
- The similar approach can be extended to study the impact of other hydrological and hydrogeological variables on fate and transport of contaminants
- The scope and accuracy of data based modeling can be extended using various data mining techniques.



References



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2. Yadav, B*, Ch, S., Mathur, S., & Adamowski, J. Estimation of in-situ bioremediation system cost using a hybrid Extreme Learning Machine (ELM)-particle swarm optimization approach. *Journal of Hydrology*, 543, 373-385, (2016).
3. Gupta, P. K., Yadav, B., & Yadav, B. K. Assessment of LNAPL in subsurface under fluctuating groundwater table using 2D sand tank experiments. *Journal of Environmental Engineering*, 145(9), 04019048, (2019).
4. Gupta, P. K., Yadav, B., Yadav, B. K., Sushkova, S., & Basu, S. (2021). Engineered Bioremediation of NAPL Polluted Sites: Experimental and Simulation-Optimization Approach under Heterogeneous Moisture and Temperature Conditions. *Journal of Environmental Engineering*, 147(8), 04021023.)

A high-speed photograph of a water droplet suspended in mid-air above a pool of water. The droplet is perfectly spherical and reflects light, creating a bright highlight. Below it, the water surface is disturbed, forming a series of concentric ripples that spread outwards. The background is a soft, out-of-focus blue gradient.

Thank You