Utilizing THMC and MUSt Software for Remediation and Management of Contaminants with PRB

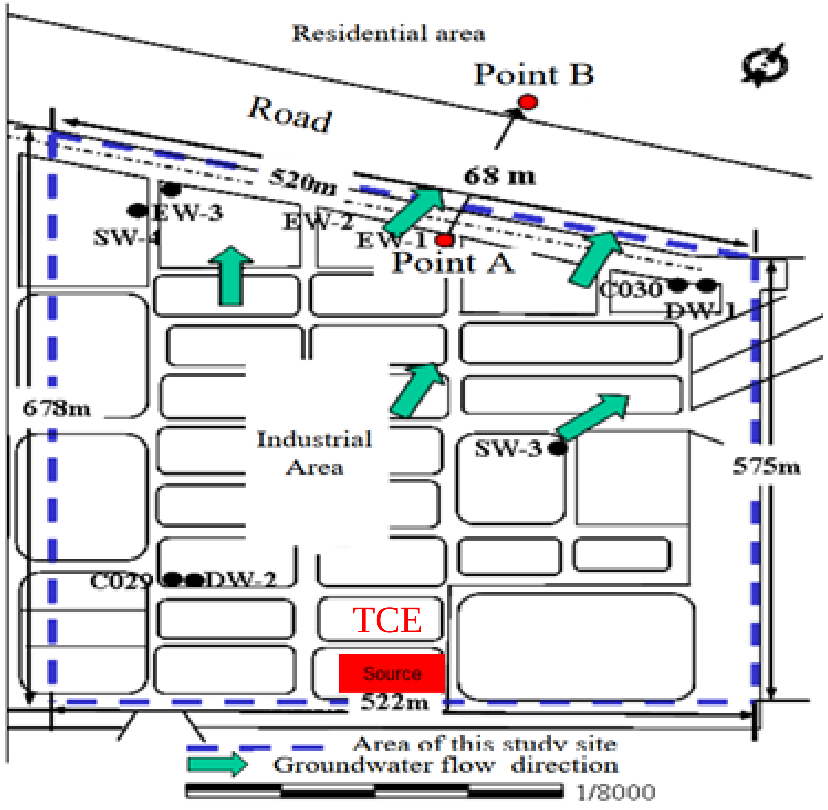
Student: Thi-Tuyet-Han Nguyen
Advisor: Prof. Jui-Sheng Chen
Date: 2025/04/11

Outline

- Introduction
- Methodology
- Results and Discussion
- Conclusions
- Future work

Motivation

A risk management study was conducted at a chlorinated solvent chemical spill site in southern Taiwan.



Schematic diagram of the studied site
(Tsai et al., 2012)

The calculated risk levels exceeded the target cancer risk of 10^{-6} set by Taiwan's Soil and Groundwater Remediation Act

Health risk assessment point

Assessment point	The status of land use	The distance from the contaminated site (m)	Cancer risk benchmark (personal)
Inside the contaminated area (point A)	Industrial area	0	$>10^{-6}$
Outside the contaminated area (point B)	Residential area	68	

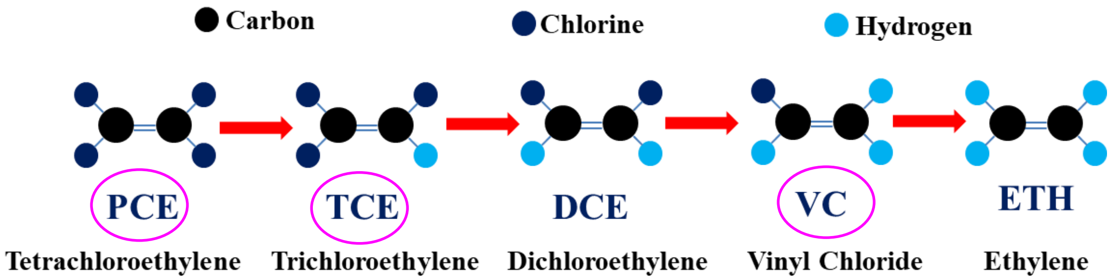
Environmental Protection Administration, Taiwan R.O.C (Taiwan EPA)

Appropriate remedial actions are required to lower the risk to below the target level.

Chlorinated solvent

Chlorinated solvents (PCE, TCE, DCE, etc.) are widespread groundwater contaminants often released as dense nonaqueous phase liquids (DNAPLs).

The biodegradation pathway of the chlorinated solvent



These compounds, widely used in industrial processes and dry cleaning, pose several remediation challenges:

Toxicity and Health Risks:

Chlorinated solvents are known carcinogens and can adversely impact human health, even at low concentrations.

Migration and Plume Complexity:

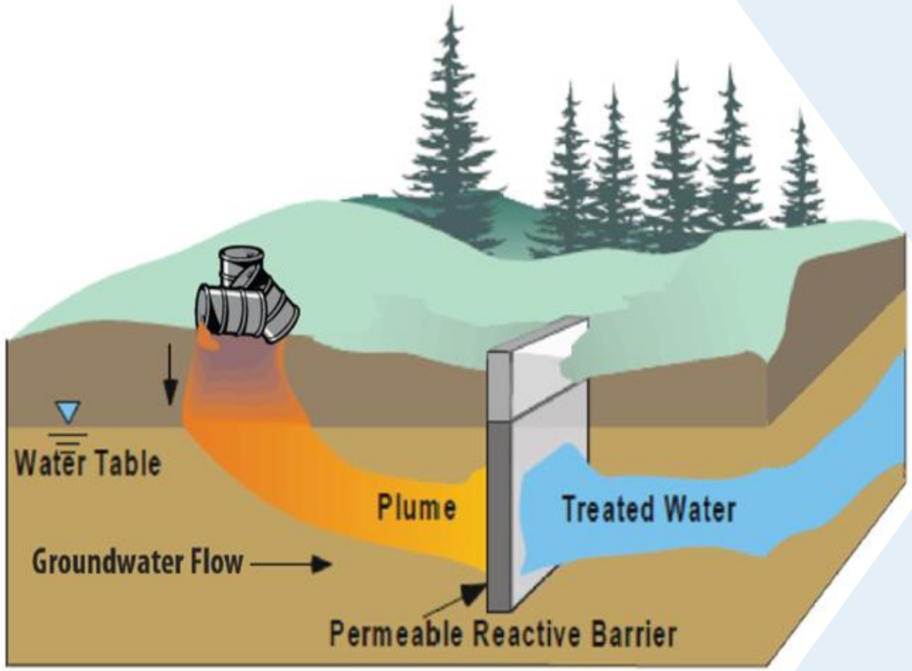
Chlorinated solvents move downward and laterally in groundwater, forming dense, hard-to-predict and remediate plumes

Environmental Persistence:

Under some site conditions, these chemicals resist natural degradation, allowing them to remain in the environment for decades.

Permeable Reactive Barrier (PRB)

Permeable Reactive Barrier (PRB) is an in situ technology used to treat groundwater contaminants.



Permeable Reactive Barrier (PRB)

Reactive materials

Zero-valent iron (ZVI)
Activated alumina
Activated carbon
Pea gravel, limestone, sawdust

The primary removal methods

(1) Chemical reaction
(2) Sorption and precipitation
(3) Reactions involving biological mechanisms

Advantages

- No ground space
- Low operation cost
- Longevity (30 years)
- Energy-saving

Objective

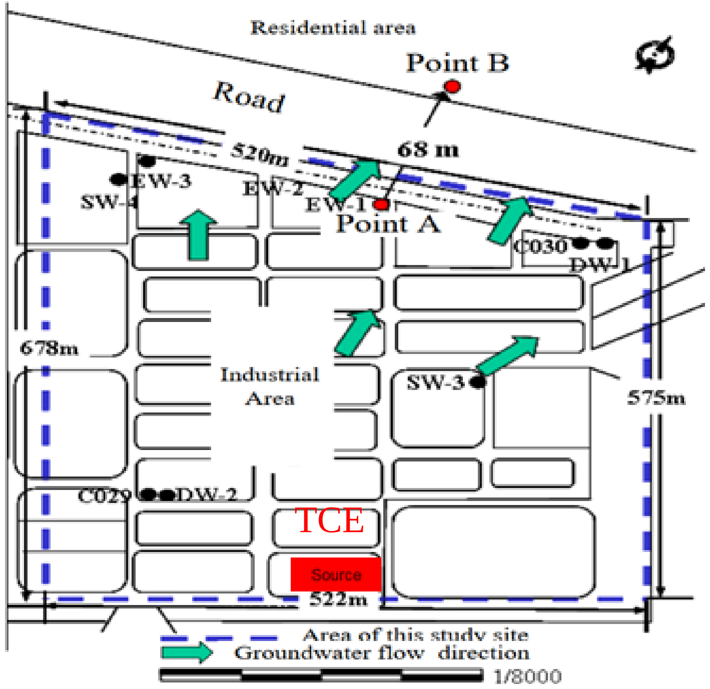
Utilizing THMC and MUSt software for remediation and management of contaminants with PRB

+ Design and implement a PRB using the THMC model, and assess its performance by integrating flow simulations and reactive transport.

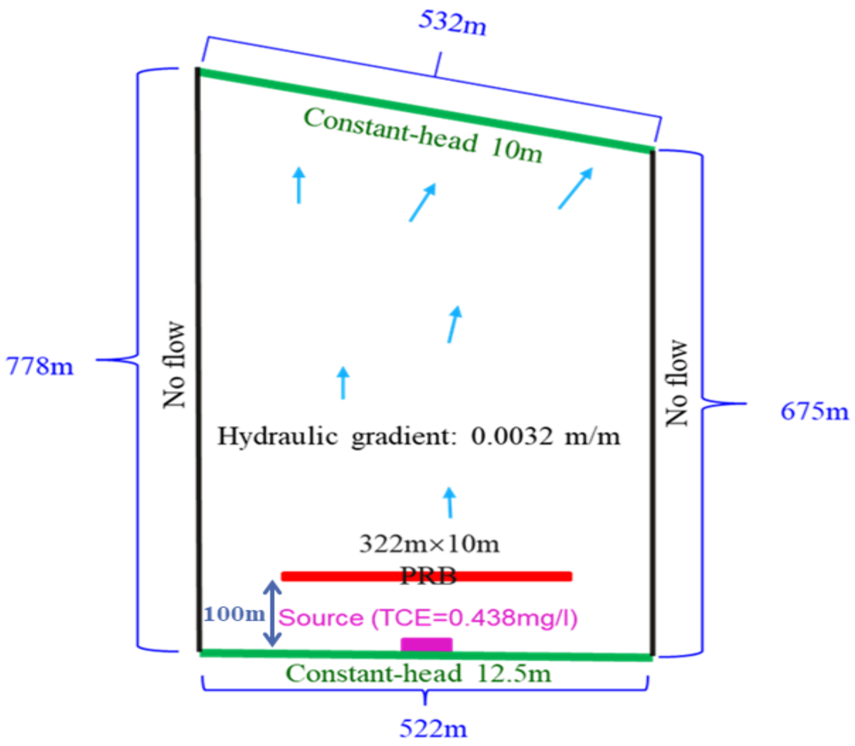
+ Health risk assessment with MUSt software

+ Evaluate whether PRB is applicable in this area.

Conceptual model



PRBs containing zero-valent iron (ZVI) as the reactive medium



Hydrological parameters and boundary conditions

	Aquifer	PRB
Hydraulic conductivity (K)	81 (m/day)	216 (m/day)
Porosity	0.3	0.6
Boundary conditions	No flow: left, right Constant-head (Dirichlet) Upstream and Downstream	Upgradient: background ground water concentrations

Reaction
$Fe^0 + H_2O + 0.5O_2 \rightarrow Fe^{2+} + 2OH^-$
$Fe^0 + 2H_2O \rightarrow Fe^{2+} + H_2 + 2OH^-$
$4Fe^0 + 7H_2O + NO_3^- \rightarrow 4Fe^{2+} + 10OH^- + NH_4^+$
$Fe^0 + 1/3\ TCE + H^+ \rightarrow Fe^{2+} + 1/3\ ETH + 1/2\ Cl^-$
$SO_4^{2-} + 4H_2 \rightarrow HS^- + OH^- + 3H_2O$
$HCO_3^- \leftrightarrow H^+ + CO_3^{2-}$
$H_2O \leftrightarrow H^+ + OH^-$

Governing equation

Groundwater flow model

The steady-state flow through the aquifer and PRB

$$\nabla . \left[K.(\nabla h + \frac{p}{p_0} \nabla z) \right] = 0$$

K: hydraulic conductivity (L/T)
h: pressure head (L), z: potential head (L)
p: fluid density with dissolved biogeochemical concentrations (M/L^3)
p_0: referenced fluid density at zero biogeochemical concentration (M/L^3)

Reactive transport model

$$\frac{\partial \theta C_i}{\partial t} + \underbrace{\boxed{\nabla(\theta C_i V_f)}}_{\text{Advection}} + \underbrace{\boxed{\nabla J_i}}_{\text{Dispersion \& diffusion}} = \underbrace{\boxed{\theta r_i}}_{\text{Reactions}}$$

C_i: concentration of the ith species (M/L^3)
V_f : fluid velocity (L/T)
r_i: production rate of species i per unit volume from all reactions ($(M/L^3)/T$)
θ : effective porosity
J_i: surface flux due to dispersion and diffusion [$(M/T)/L^2$]

METHODOLOGY

Health risk assessment

TCE concentration from the THMC model will be applied to the MUSt model

MUltiSpecies transport analytical model

The lifetime average daily dose (USEPA 2004):

$$ADD = C_w \times \left[\frac{IR \times EF \times ED}{BW \times AT \times 365 day/year}\right]$$

Lifetime cancer-causing carcinogenic risk indexes for the direct oral ingestion exposure case were calculated (USEPA 2004):

$$TR_{carinogenic} = ADD \times SF$$

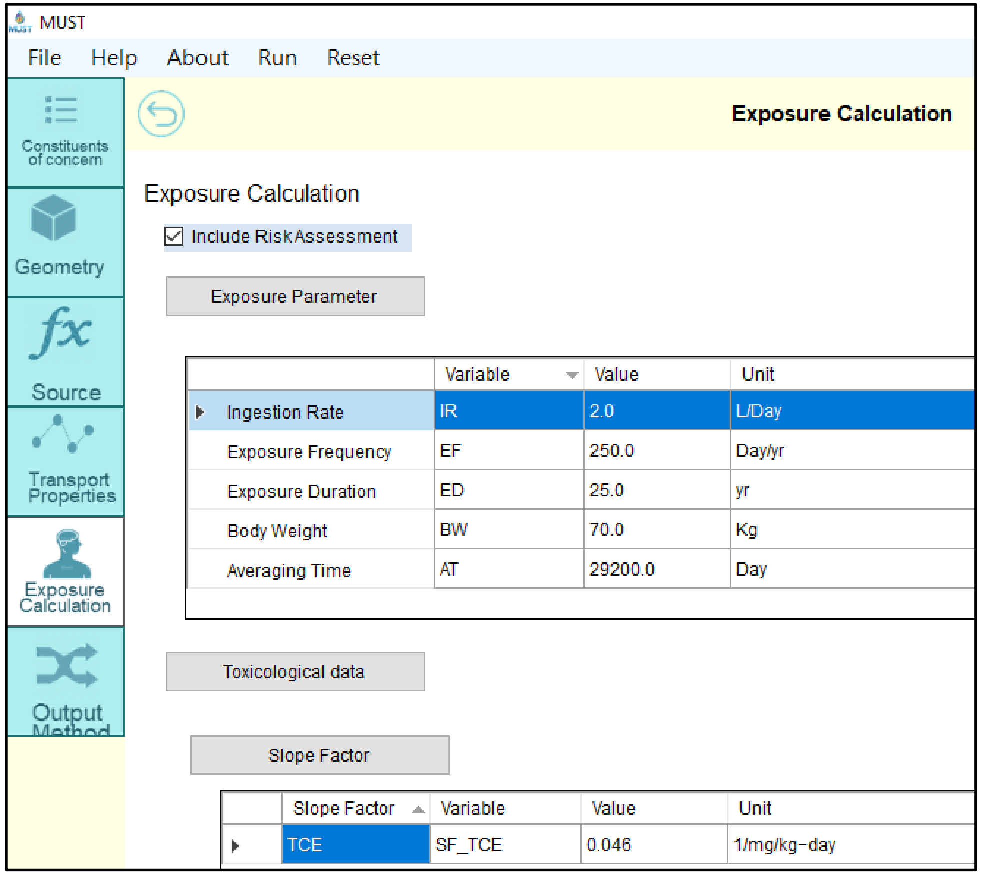
$TR < 10^{-6}$: *Low risk*

$10^{-4} < TR$: *High risk*

$10^{-6} \leq TR \leq 10^{-4}$: *Medium risk*

C_w: estimated long-term contaminant concentration (mg/L)	*ED*: exposure duration (years)
IR: water ingestion rate (L/day)	*BW*: body weight (kg)
EF: exposure frequency (day/year)	*AT*: average lifetime (years)
	SF: slope factor (1/mg/kg-day)

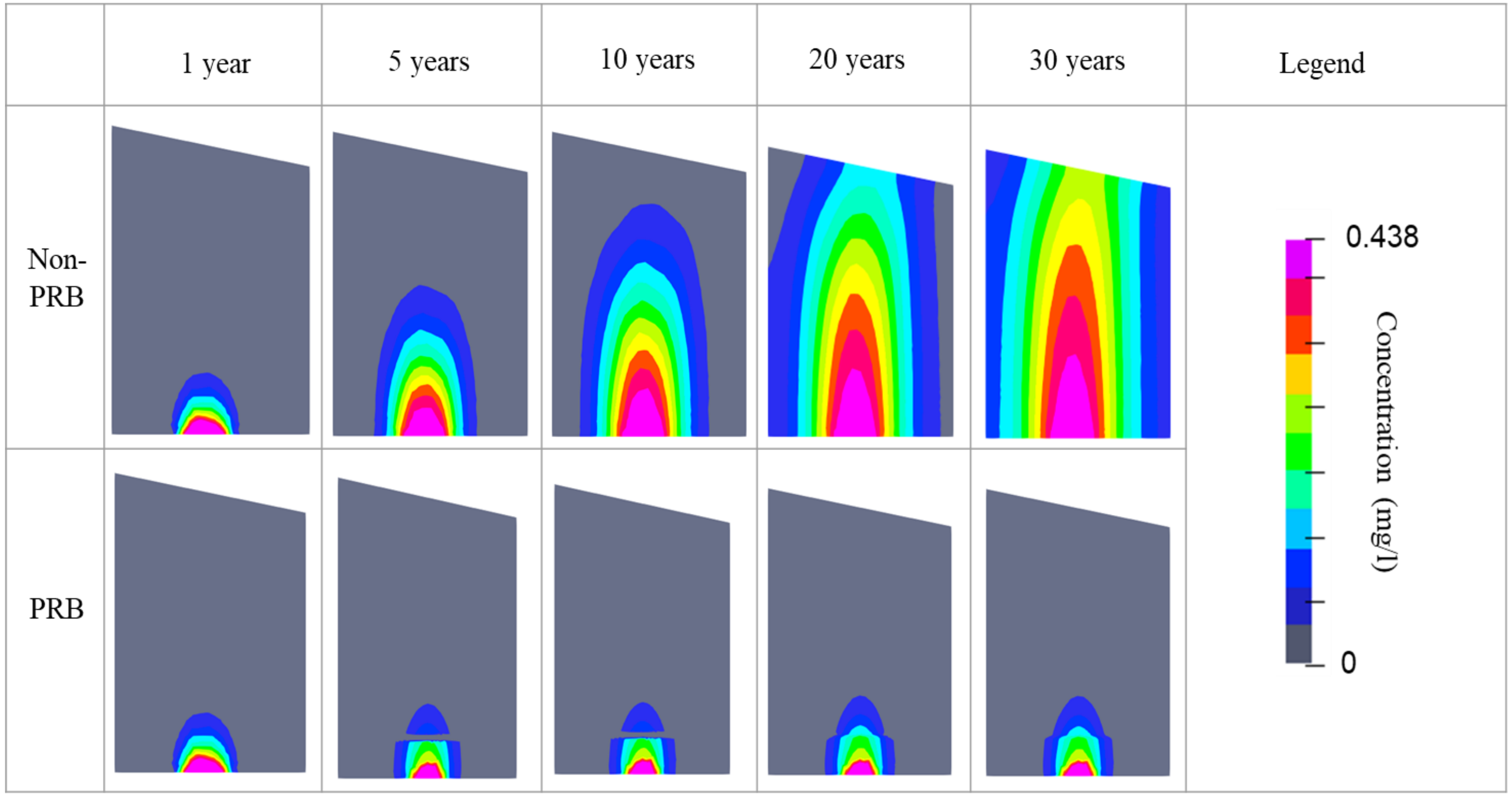
Set up value in MUSt software



SF is from USEPA Integrated Risk Information System (IRIS)

Remediation efficiency of PRB with THMC model

PRB systems can significantly reduce TCE by treating groundwater in situ as it flows through reactive materials, providing a long-term, passive remediation solution



TCE concentration results at the PRB and non-PRB by the THMC model

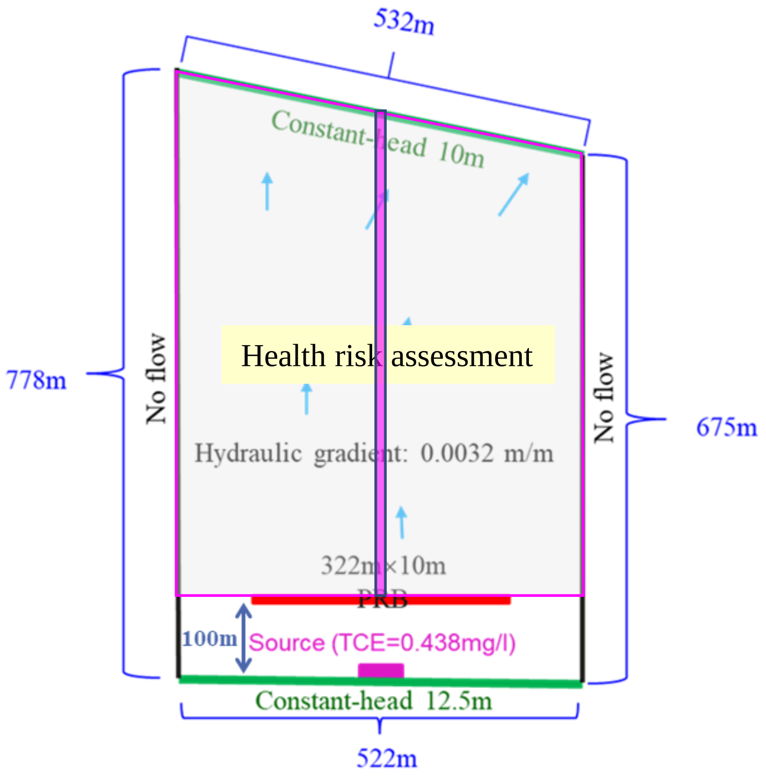
- The concentration of TCE decreases as the groundwater passes through the barrier.

- The degradation process transforms harmful TCE into non-toxic ETH, reducing contaminant levels in the aquifer

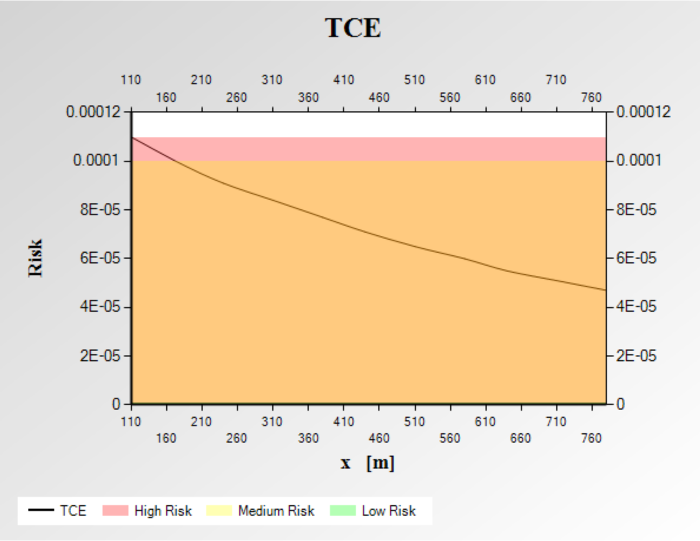
$$Fe^{0}(s)+\frac{1}{3}TCE+H^{+}\rightarrow Fe^{+2}\,\frac{1}{3}ETH+\frac{1}{2}Cl^{-}$$

Health risk assessment with MUSt software

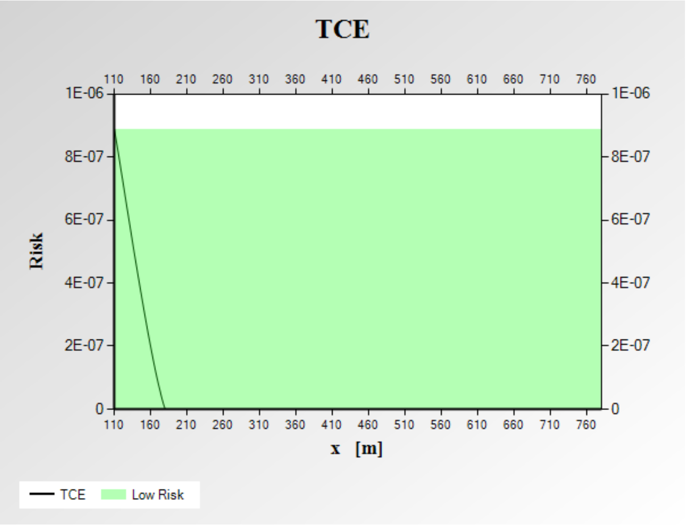
PRB help decrease area health hazards to minor levels



Non-PRB



PRB



Health risk assessment results by MUSt model between PRB and non-PRB for 30 years

CONCLUSIONS

- THMC modeling evaluates PRB performance by simulating flow and chemical reactions, showing significant TCE reduction as groundwater passes through ZVI.

- The MUSt health risk evaluation indicates that PRBs may reduce health risks to low levels.

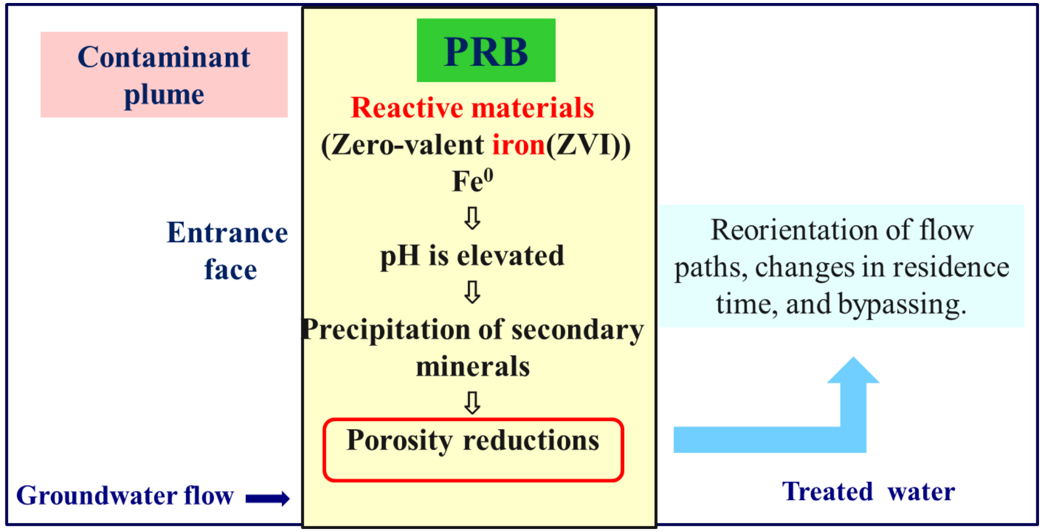
→ PRB is an effective remediation method that can be applied to this site

- THMC and MUSt models help to monitor PRB performance over time, providing practical methods for managing contaminants and optimizing PRB operation.

FUTURE WORK

Porosity reduction ranges from 0.0007 to 0.03 per year and depends on in situ geochemistry and flow conditions (Li et al., 2006).

- Continue to collect concentrations of species in groundwater in this site to run models to evaluate porosity reduction and evaluate influencing factors



Reaction[a]	Mineral formed[a]
$CaCO_3 \leftrightarrow Ca^{2+} + CO_3^{2-}$	Calcite/Aragonite
$CaMg(CO_3)_2 \leftrightarrow Ca^{2+} + Mg^{2+} + 2CO_3^{2-}$	Ca–Mg–carbonate
$MgCO_3 \leftrightarrow Mg^{2+} + CO_3^{2-}$	Magnesite
$Mg(OH)_2 \leftrightarrow Mg^{2+} + 2OH^-$	Brucite
$MnCO_3 \leftrightarrow Mn^{2+} + CO_3^{2-}$	Rhodochrosite
$Mn(OH)_2 \leftrightarrow Mn^{2+} + 2OH^-$	Pyrochroite
$FeCO_3 \leftrightarrow Fe^{2+} + CO_3^{2-}$	Siderite
$Fe(OH)_2 \leftrightarrow Fe^{2+} + 2OH^-$	Ferrous Hydroxide
$FeS + H_2O \leftrightarrow Fe^{2+} + HS^- + OH^-$	Ferrous Sulfide

a. Li et al. (2006)

- Calibrate the model after PRB is completed on the site

Thank you for your listening