A software integrating sophisticated transport analytical model, GIS, and human health risk assessment for comprehensive site evaluation of groundwater contaminated with chlorinated solvents

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Outline

- Introduction
- Methodology
- Results and discussions
- Conclusions and future work

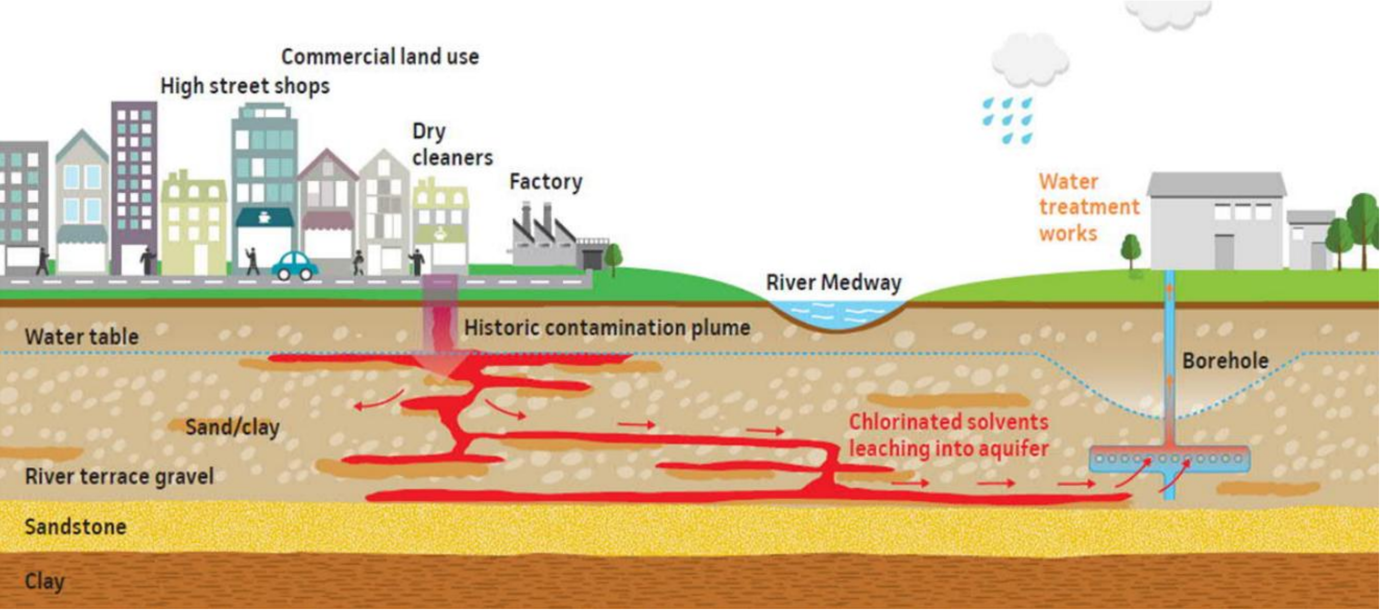
Groundwater contamination

Groundwater resources are important. However, the contamination of the subsurface environment pose threats to human health.

Chlorinated solvents are common contaminants found in contaminated groundwater.

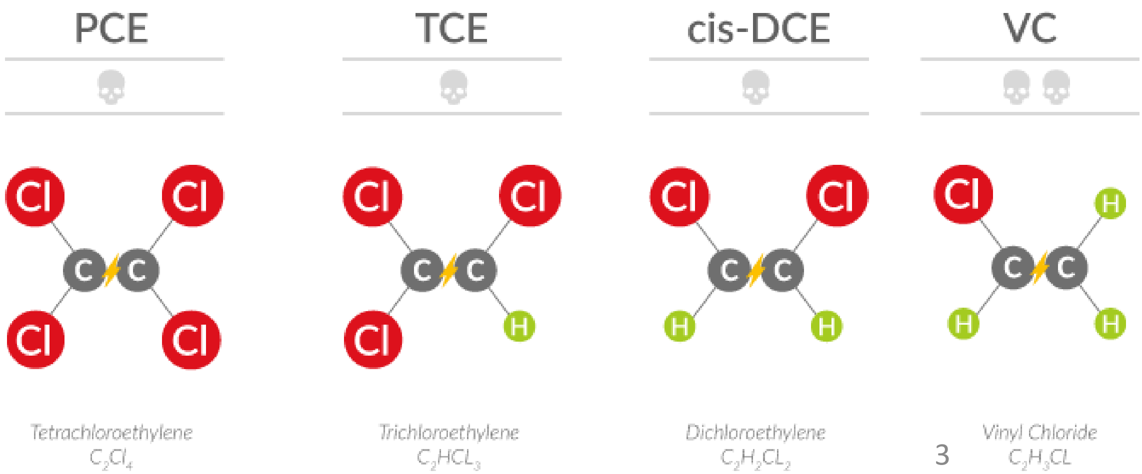
- Used for dry cleaning, metal degreasing
- Dense non-aqueous phase liquids (DNAPLs)
- Carcinogenic

→ **Contaminated site evaluation**



Subsurface environmental contamination

Chlorinated solvents



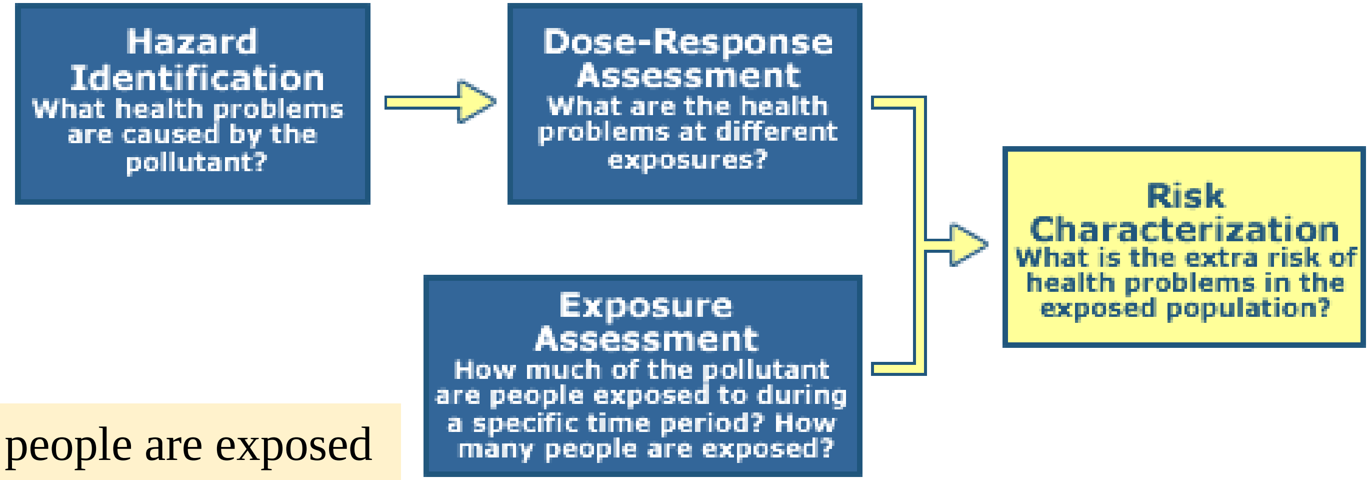
Human health risk assessment (HHRA)

- HHRA is the process to estimate the potential adverse health effects in humans who are exposed to chemicals in contaminated environmental media.

- HHRA helps in decision-making for site remediation and risk management, also can help governments to deliver technical knowledge to the public.

How much dosage cause people sick:
Reference dose, RfD; Cancer slope factor, SF

Contaminants of concern
Site extent
Geology information
Hydrology information
…



How, where, and how long people are exposed

Four steps of human health risk assessment process

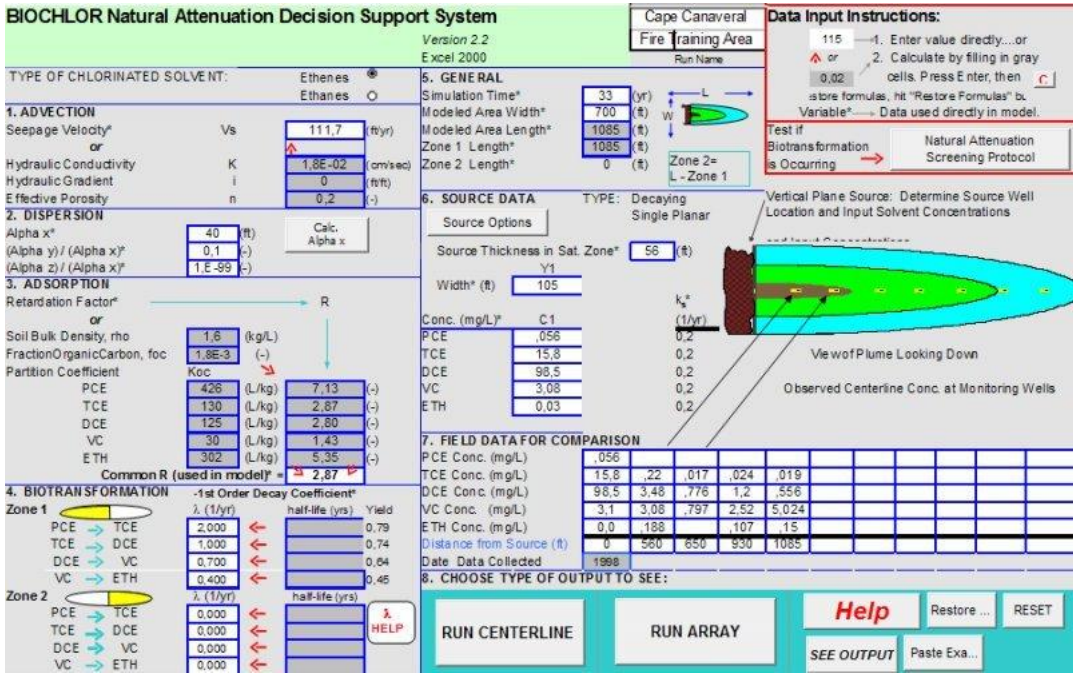
Previous contaminants transport analytical solution software

- BIOCHLOR
  - Excel-based table software.
  - Most used software simulates remediation by natural attenuation released in 2000.

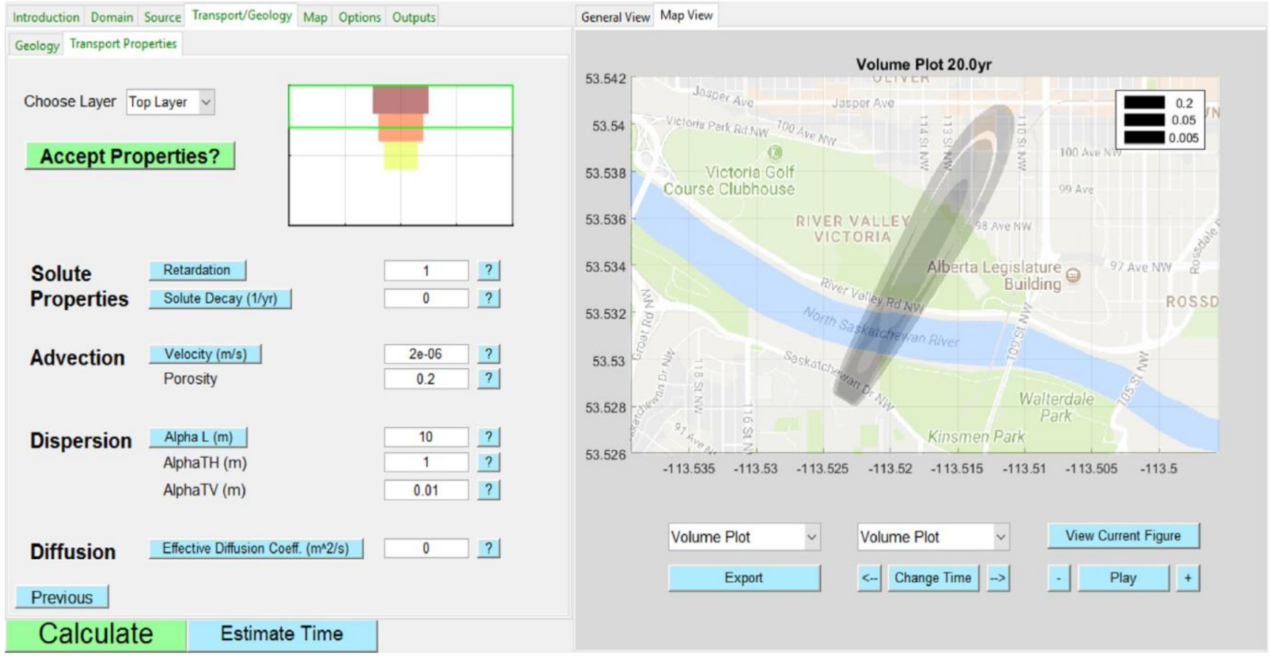
All contaminants can only use the same retardation factor.

- HYDROSCAPE
  - MATLAB-based window software.
  - With map view result.
  - Released in 2017.

Only can simulate single contaminant.



BIOCHLOR interface

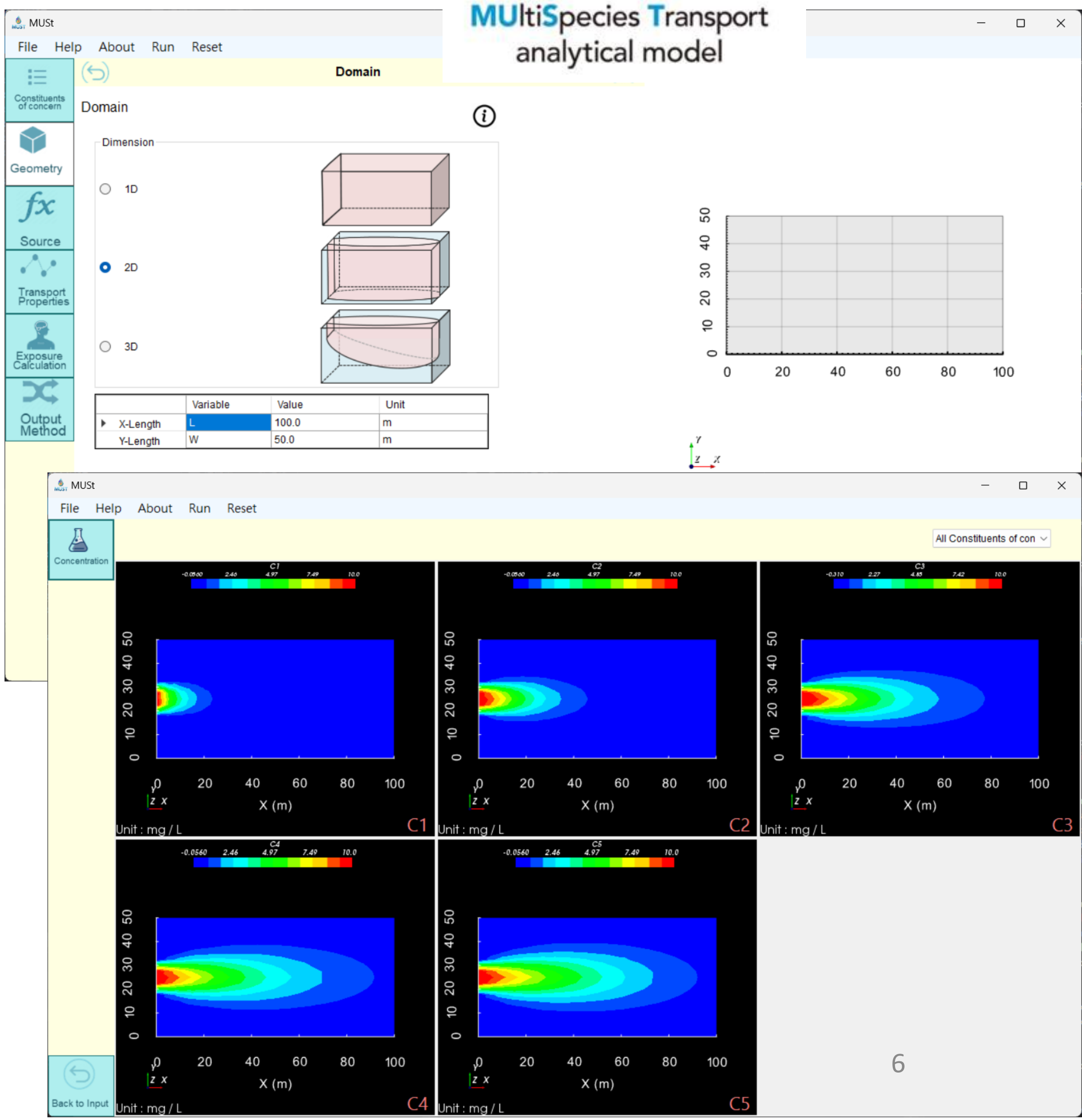


HYDROSCAPE interface

MUSt software

MUSt (**MU**lti**S**pecies **t**ransport analytical model):

- Using analytical solutions (Liao et al., 2021) for simulating transport of chlorinated solvent contaminant and its degradation products, without the limitations of those previous software.
- Integrated with human health risk assessment for groundwater ingestion.
- With user-friendly interface and multiple visualize output results.

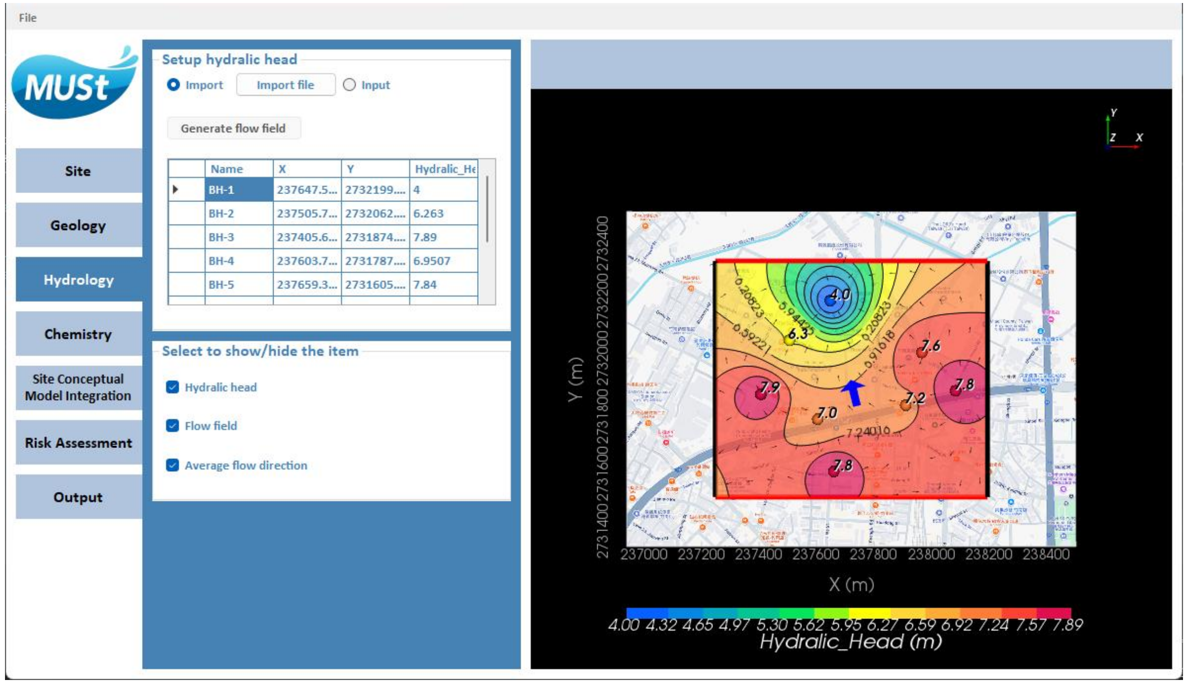


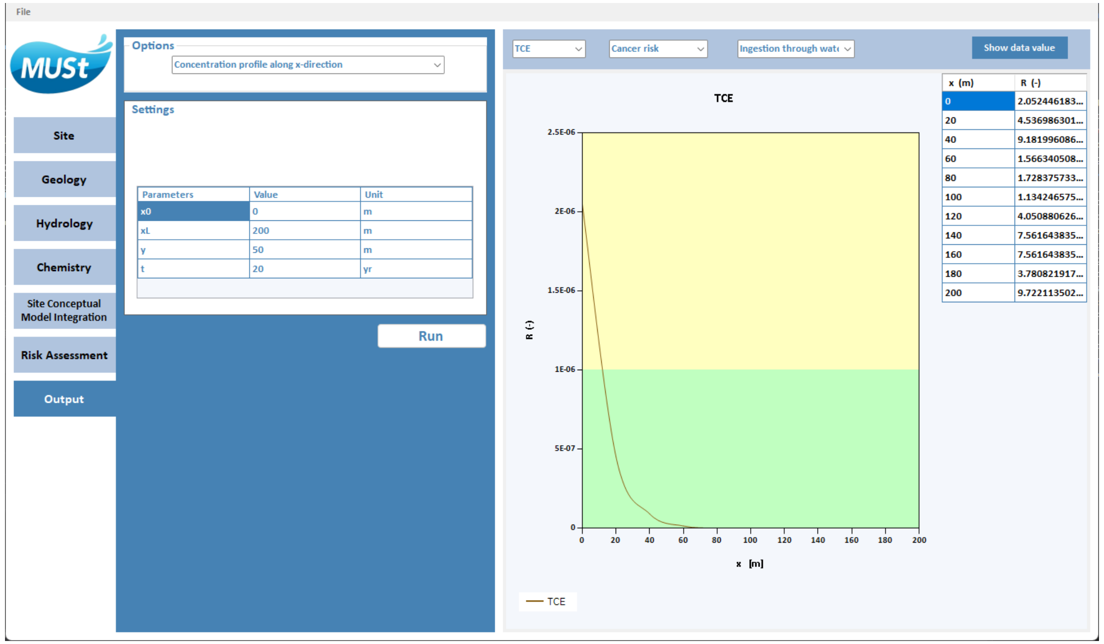
What other features may be needed?

- Site information management module
  - Multiple exposure pathways

Why new features?

- Site information management module:
  - Improve the efficiency
  - Better management of data
- Multiple exposure pathways:
  - Accurate Dose Estimation
  - Provide a solid scientific basis

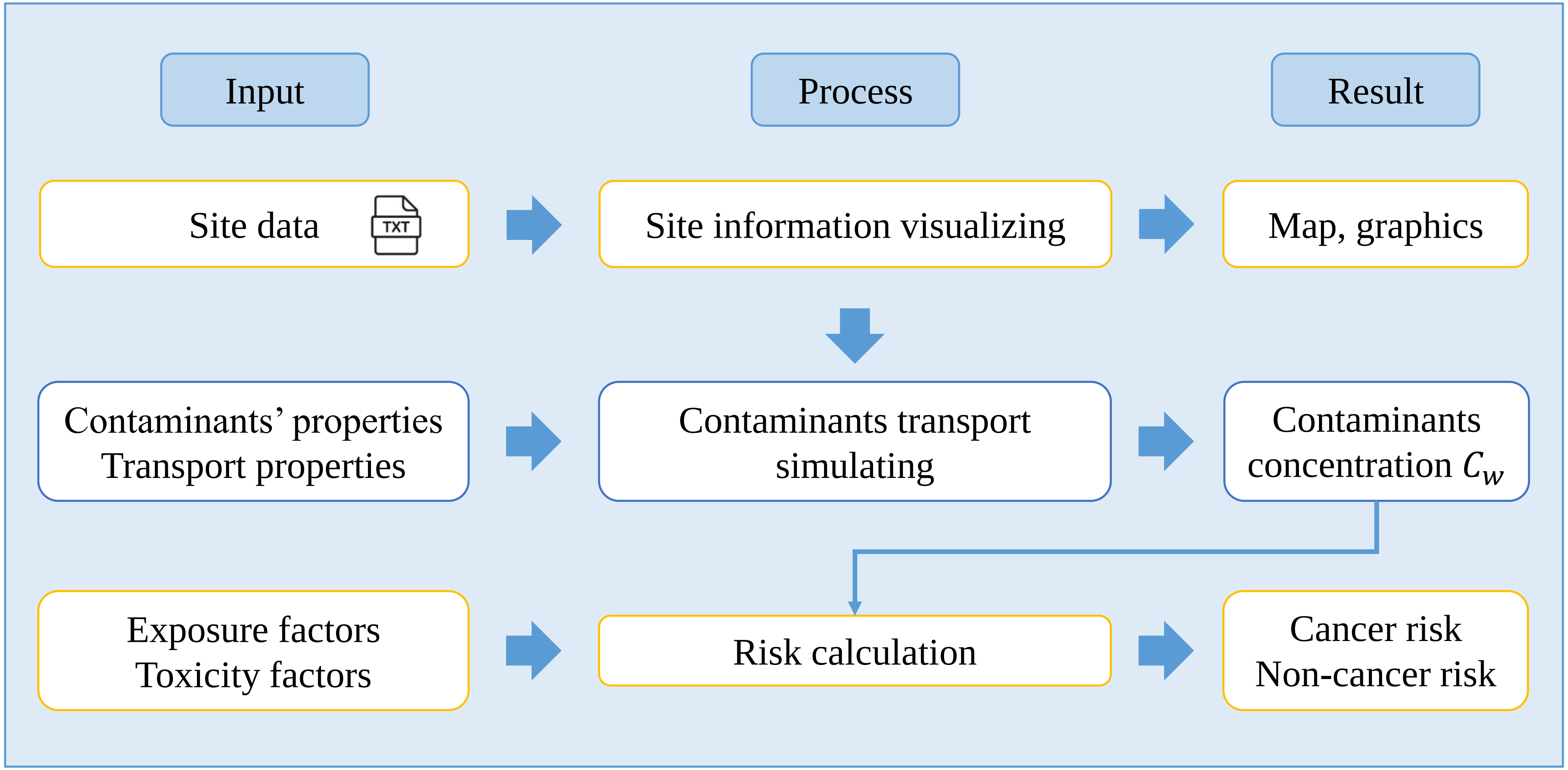




Objective

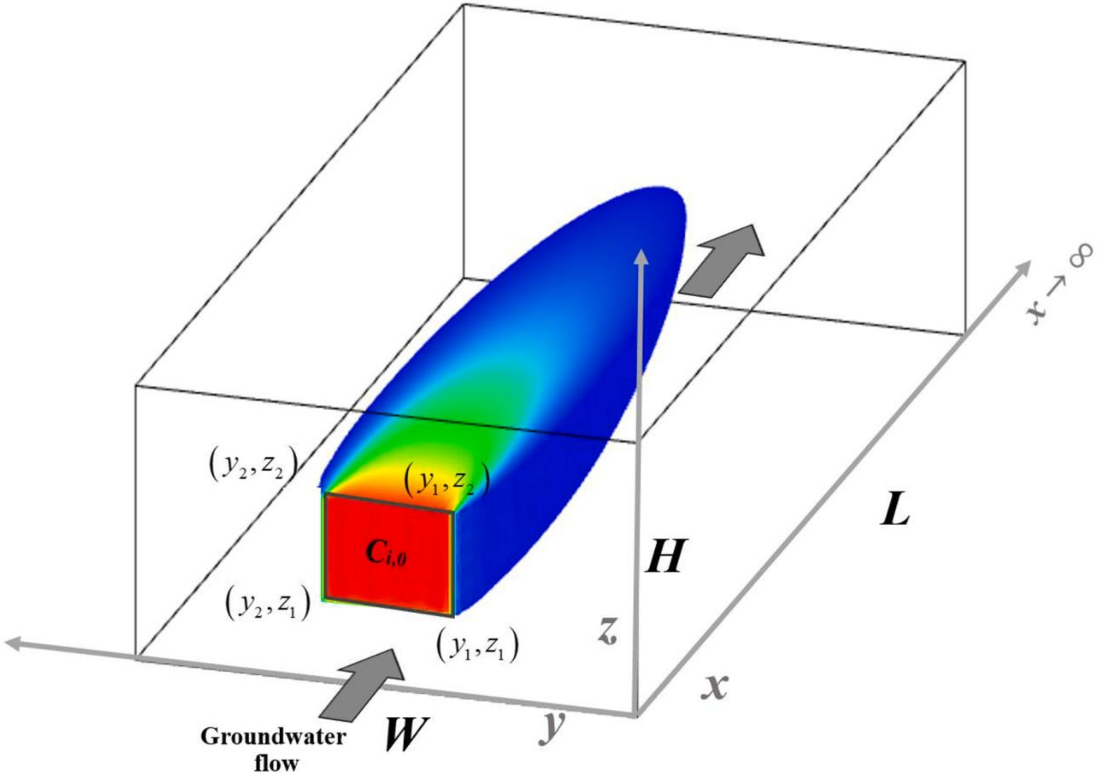
- This study enhances existing software MUSt, integrating advanced functionalities for managing and visualizing site information (GIS), and expands the human health risk assessment module to consider multiple exposure pathways.

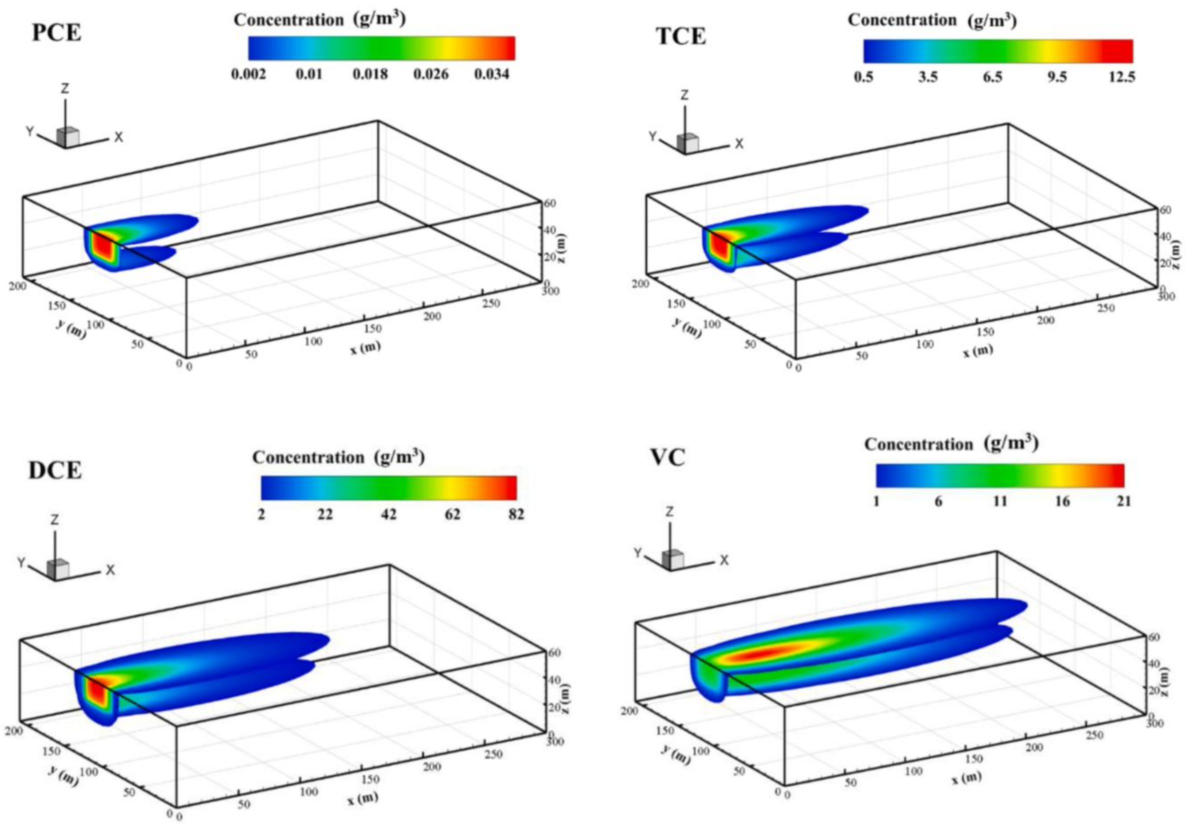
Software usage flow chart



Contaminant transport model

- MUSt software base on the three-dimensional multispecies ADEs from Liao et al., 2021:





$C_i(x, y, z, t)$: concentration(mg/L)
x, *y*, *z*: spatial coordinates(m), *t*: time(year)
v: constant pore-water velocity in the *x* direction(m/year)
D_x, D_y, D_z: dispersion coefficients(m^2 /year)
R_i: retardation factor (-)
μ_i: first-order degradation reaction rate constant(1/year)
$g_{i-1 \to i}$: yield coefficient(-)

Exposure dose calculation and exposure pathways

[1] USEPA, 1989
[2] Andelman, 1990

Exposure dose (average daily dose, *ADD*) are calculated as:

- Groundwater ingestion[1]: $ADD = C_w \times \frac{IR \times EF \times ED}{BW \times AT}$
- Groundwater inhalation through shower[2]: $ADD = (C_{a1} \times IR_s \times t_1 + C_{a2} \times IR_s \times t_2) \times \frac{EV_s \times EF \times ED}{BW \times AT}$

  where $C_{a1} = \frac{1}{2} \times \frac{C_w \times f \times F_s \times t_1}{V_a} \times CF, C_{a2} = \frac{C_w \times f \times F_s \times t_2}{V_a} \times CF$
- Groundwater inhalation through indoor washing[1]: $ADD = C_a \times \frac{IR_w \times EF \times ED}{BW \times AT}$

  where $C_a = \frac{C_w \times f \times F_W}{V_h \times ER \times MC} \times CF$
- Groundwater dermal contact through shower or washing[1]: $ADD = DA \times SA \times \frac{EV \times EF \times ED}{BW \times AT}$

For $t \leq 2.4\tau$

$$DA = 2 \times FA \times K_p \times C_w \times \sqrt{6 \times \frac{\tau \times t}{\pi}} \times CF$$

For $t > 2.4\tau$

$$DA = FA \times K_p \times C_w \times \left[\frac{t}{1+B} + 2 \times \tau \left(\frac{1 + 3 \times B + 3 \times B^2}{(1+B)^2}\right)\right] \times CF$$

ADD: average daily dose (mg/kg-day)
C_w : contaminant concentration in groundwater (mg/L)
EF: exposure frequency (days/year)
ED: exposure duration (years)
BW: body weight (kg); *AT*: average lifetime (days)

Parameters in ADD calculation

IR: water ingestion rate (L/day)
IR_s: shower inhalation rate ($m^3/hour$), IR_w: inhalation rate (m^3/day)
EV: event frequency (events/day), EV_s: shower event frequency (events/day)
C_a: contaminant concentration in air (mg/m^3)
C_{a1}: contaminant concentration in air while shower (mg/m^3), C_{a2}: contaminant concentration in air after shower (mg/m^3)
t_1: shower time ($hour$), t_2: the time still stays in bathroom after shower ($hour$)
V_a: bathroom volume (L), V_h: house volume (L)
F_s: shower water flow rate (L/hour), F_w: daily water usage (L/day)
f: evaporation fraction (-)
ER: indoor air exchanged rate (air changes/day)
MC: air mixture coefficient (-)
DA: exposure dose in single event (mg/cm^2)
FA: absorb fraction (-)
SA: skin surface area (cm^2)
K_p: skin permeability coefficient (cm/hour)
τ: lag time per event (hour)
B: Relative permeability coefficient ratio of the contaminant from the stratum corneum to the epidermis (-)
t: time of skin contact in single event (hour)
CF: unit transfer factor (L/m^3 or L/cm^3)

Risk calculation

- Non-carcinogenic and carcinogenic risk indexes are calculated as:
  - Non-carcinogenic: $R_{ep} = \frac{ADD}{RfD_{ep}}$
  - Carcinogenic: $R_{ep} = ADD \times SF_{ep}$

  ep = oral, inhalation, dermal contact

Transfer function

Inhalation:

$$RfD_{oral} = RfC \times \frac{IR_{inh}}{BW}$$

$$SF_{oral} = SF_{inh} \times \frac{BW}{IR_{inh}}$$

Dermal contact:

$$RfD_{dermal} = RfD_{oral} \times ABS_{GI}$$

$$SF_{dermal} = \frac{SF_{oral}}{ABS_{GI}}$$

- The total non-carcinogenic and carcinogenic risk are calculated as:

$$R_{total} = R_{oral} + R_{inh} + R_{dermal}$$

ADD: average daily dose (mg/kg-day)

RfD: reference dose (mg/kg-day); SF: cancer slope factor ($\frac{1}{\text{mg/kg−day}}$)

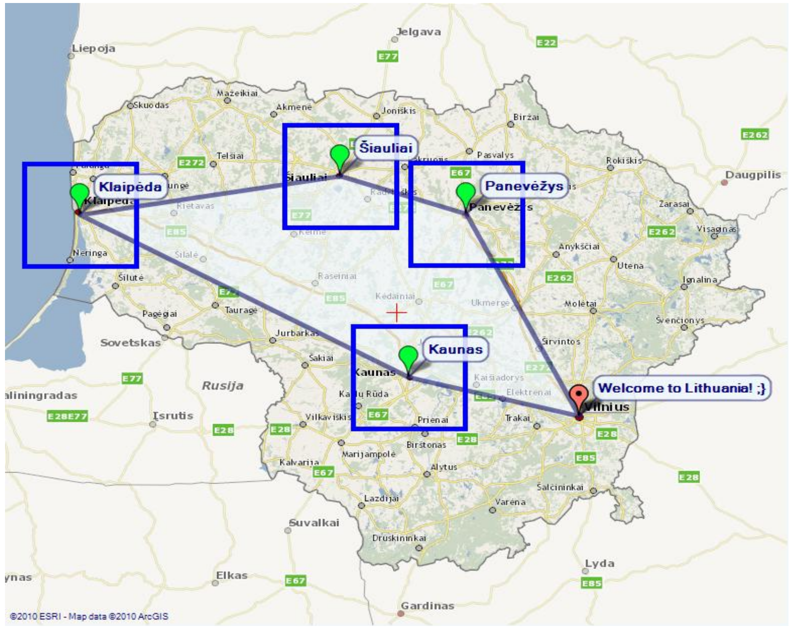
RfC: inhalation reference dose(mg/m^3); IR: inhalation rate(m^3/day)

ABS_{GI}: fraction of chemicals absorbed in the gastrointestinal tract(-)

Development tools

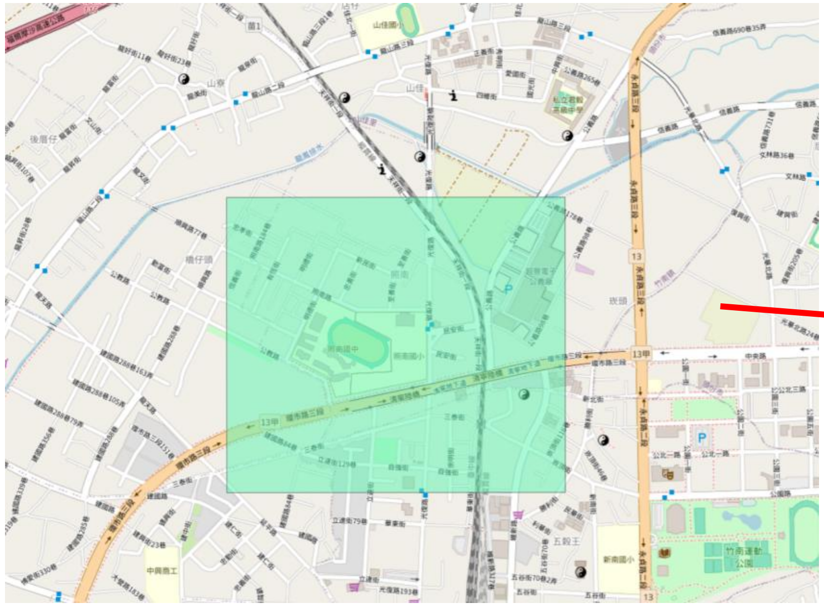
- .NET is a platform provides a large class library, enabling developers to create high-performance applications.
- Csharp is the most popular programming language in .NET which can build a wide range of applications from desktop to mobile.

- Visualization toolkit is a library for 3D computer graphics, image processing, and scientific visualization.
- Widely used in fields like medical imaging, computational fluid dynamics, and geological data visualization.



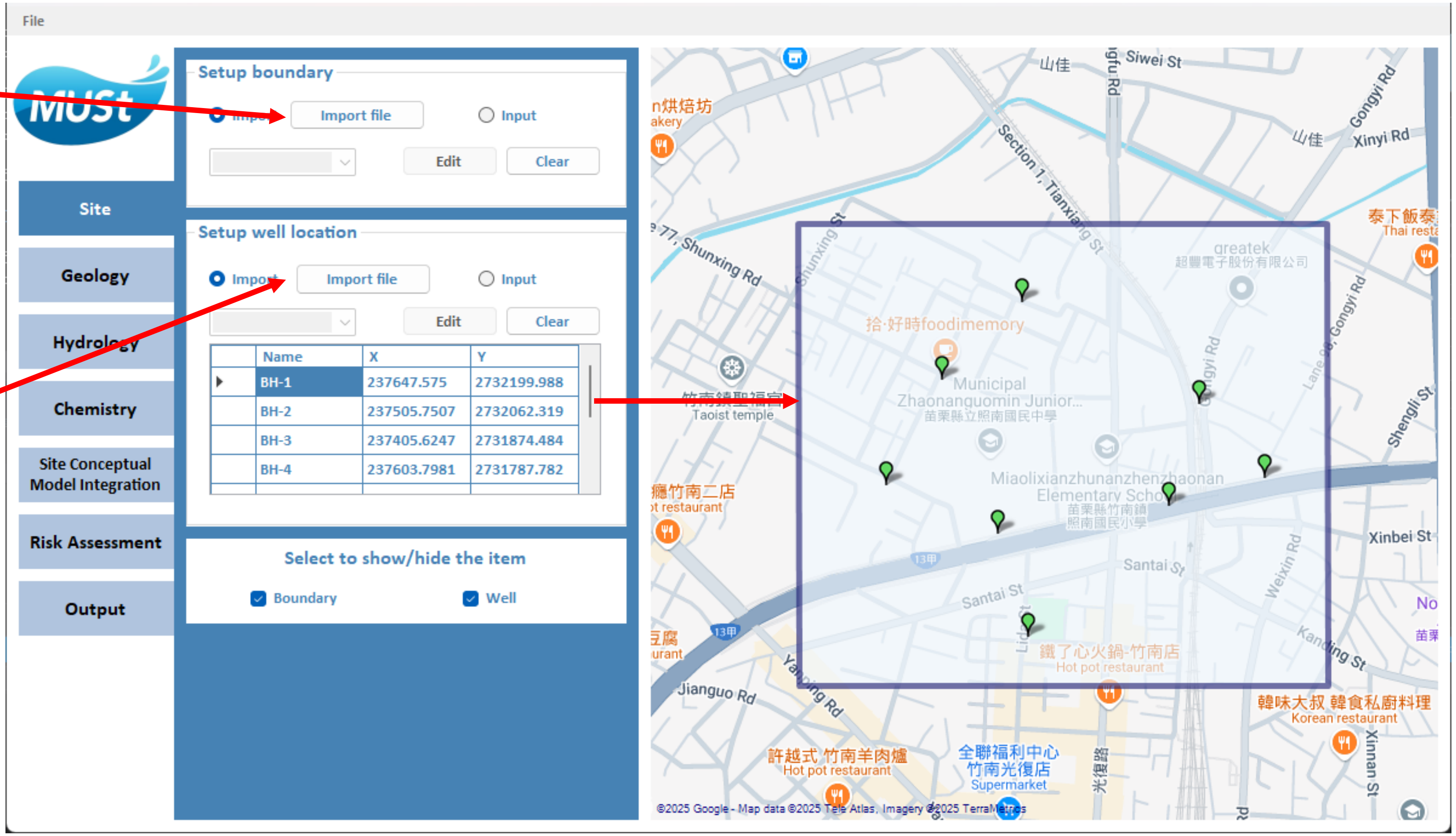
- Gmap.NET is a library in .NET provides interactive maps from various providers, supports creating objects on map.

User interface : Site

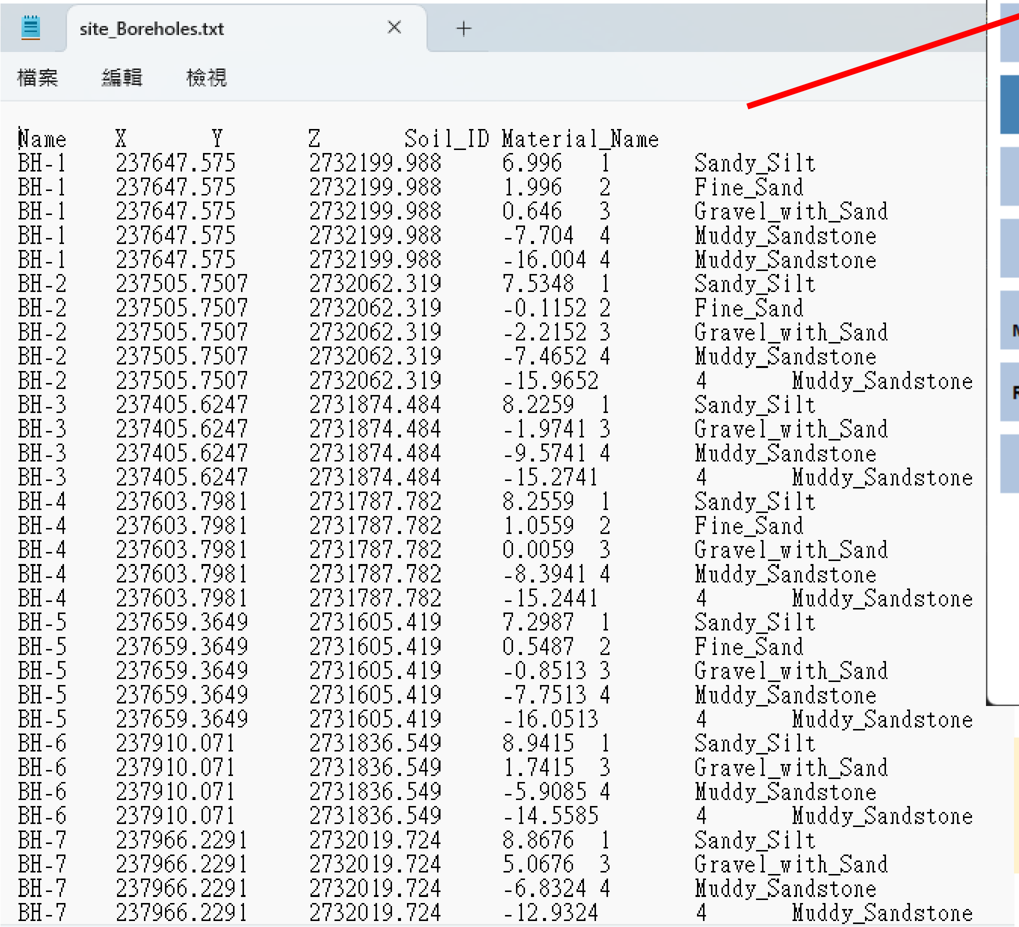


By importing shapefile and text file,
the boundary of the site and the well location can be shown on the map.

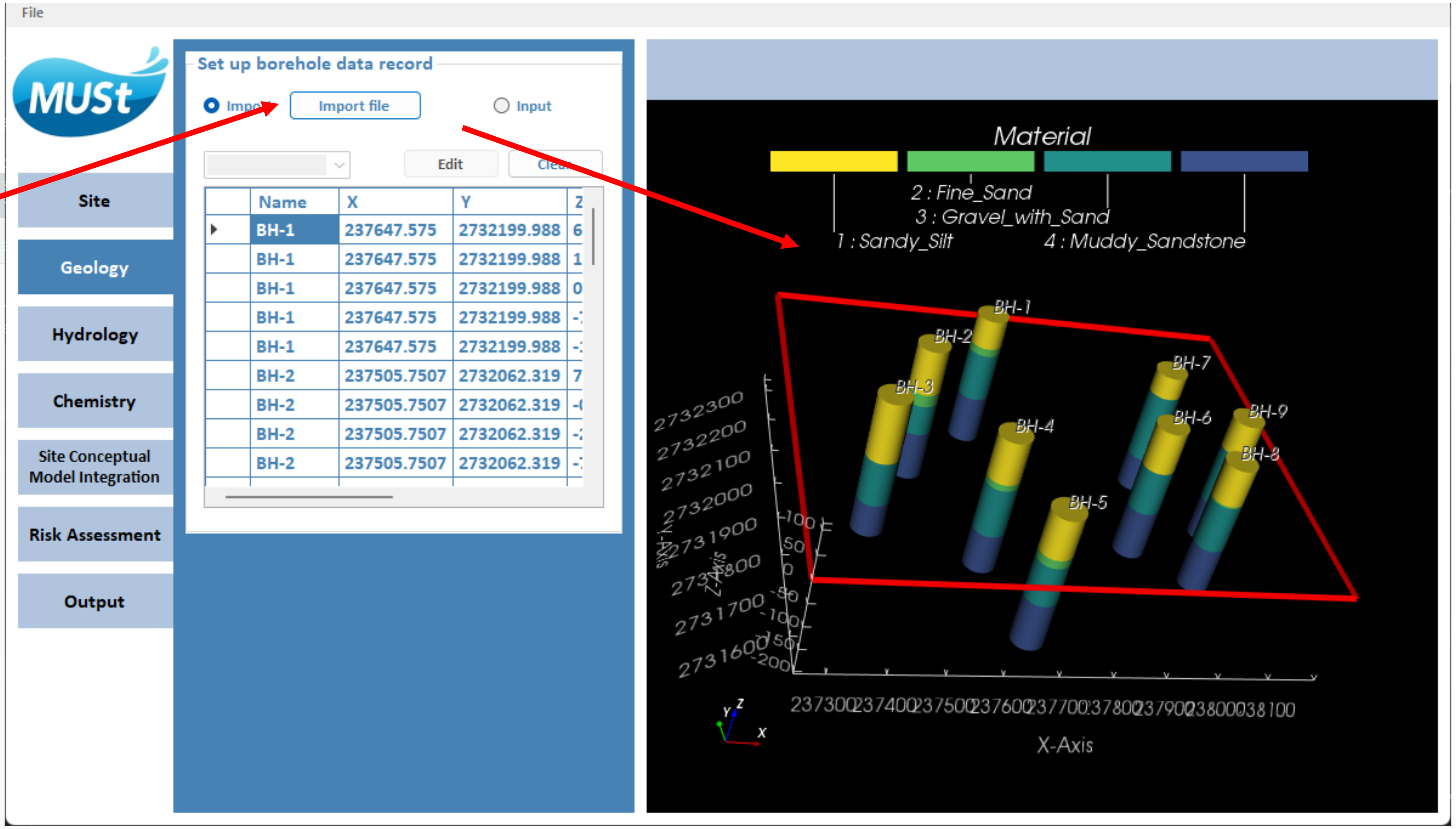
Name	X	Y
BH-1	237647.575	2732199.988
BH-2	237505.7507	2732062.319
BH-3	237405.6247	2731874.484
BH-4	237603.7981	2731787.782
BH-5	237659.3649	2731605.419
BH-6	237910.071	2731836.549
BH-7	237966.2291	2732019.724
BH-9	238083.3117	2731886.543



User interface : Geology

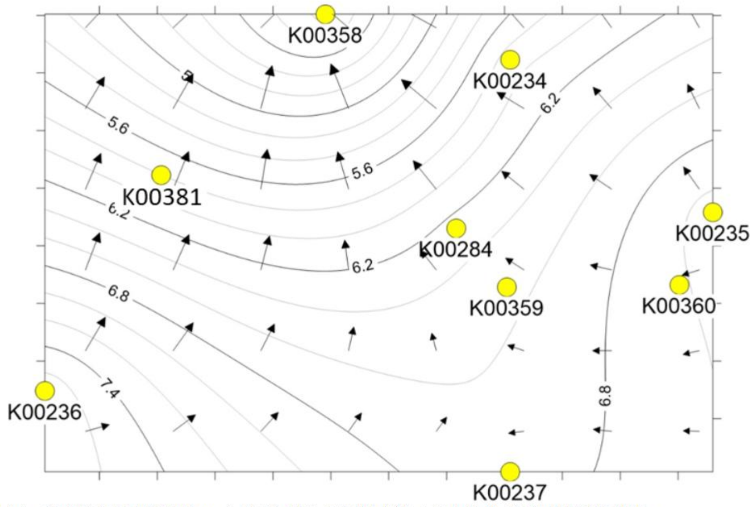

site_Boreholes.txt
檔案 編輯 檢視

Name	X	Y	Z	Soil_ID	Material_Name
BH-1	237647.575	2732199.988	6.996	1	Sandy_Silt
BH-1	237647.575	2732199.988	1.996	2	Fine_Sand
BH-1	237647.575	2732199.988	0.646	3	Gravel_with_Sand
BH-1	237647.575	2732199.988	-7.704	4	Muddy_Sandstone
BH-1	237647.575	2732199.988	-16.004	4	Muddy_Sandstone
BH-2	237505.7507	2732062.319	7.5348	1	Sandy_Silt
BH-2	237505.7507	2732062.319	-0.1152	2	Fine_Sand
BH-2	237505.7507	2732062.319	-2.2152	3	Gravel_with_Sand
BH-2	237505.7507	2732062.319	-7.4652	4	Muddy_Sandstone
BH-2	237505.7507	2732062.319	-15.9652	4	Muddy_Sandstone
BH-3	237405.6247	2731874.484	8.2259	1	Sandy_Silt
BH-3	237405.6247	2731874.484	-1.9741	3	Gravel_with_Sand
BH-3	237405.6247	2731874.484	-9.5741	4	Muddy_Sandstone
BH-3	237405.6247	2731874.484	-15.2741	4	Muddy_Sandstone
BH-4	237603.7981	2731787.782	8.2559	1	Sandy_Silt
BH-4	237603.7981	2731787.782	1.0559	2	Fine_Sand
BH-4	237603.7981	2731787.782	0.0059	3	Gravel_with_Sand
BH-4	237603.7981	2731787.782	-8.3941	4	Muddy_Sandstone
BH-4	237603.7981	2731787.782	-15.2441	4	Muddy_Sandstone
BH-5	237659.3649	2731605.419	7.2987	1	Sandy_Silt
BH-5	237659.3649	2731605.419	0.5487	2	Fine_Sand
BH-5	237659.3649	2731605.419	-0.8513	3	Gravel_with_Sand
BH-5	237659.3649	2731605.419	-7.7513	4	Muddy_Sandstone
BH-5	237659.3649	2731605.419	-16.0513	4	Muddy_Sandstone
BH-6	237910.071	2731836.549	8.9415	1	Sandy_Silt
BH-6	237910.071	2731836.549	1.7415	3	Gravel_with_Sand
BH-6	237910.071	2731836.549	-5.9085	4	Muddy_Sandstone
BH-6	237910.071	2731836.549	-14.5585	4	Muddy_Sandstone
BH-7	237966.2291	2732019.724	8.8676	1	Sandy_Silt
BH-7	237966.2291	2732019.724	5.0676	3	Gravel_with_Sand
BH-7	237966.2291	2732019.724	-6.8324	4	Muddy_Sandstone
BH-7	237966.2291	2732019.724	-12.9324	4	Muddy_Sandstone



By importing text file,
the borehole record can be shown as the cylinder inside the boundary.

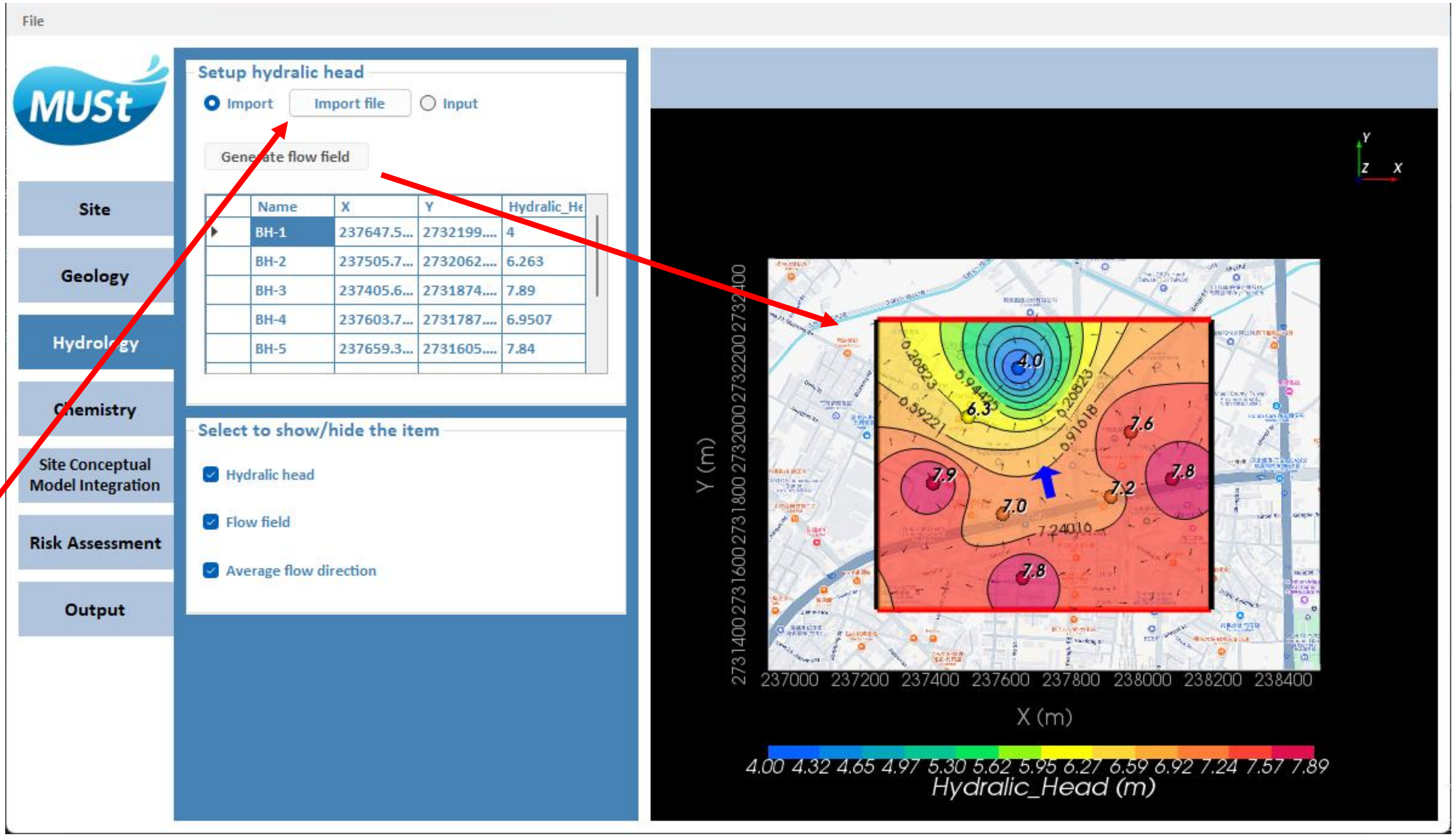
User interface : Hydrology



資料來源：行政院環境保護署(109 年)污染場址高解析度調查與生物整治適用性試驗計畫。

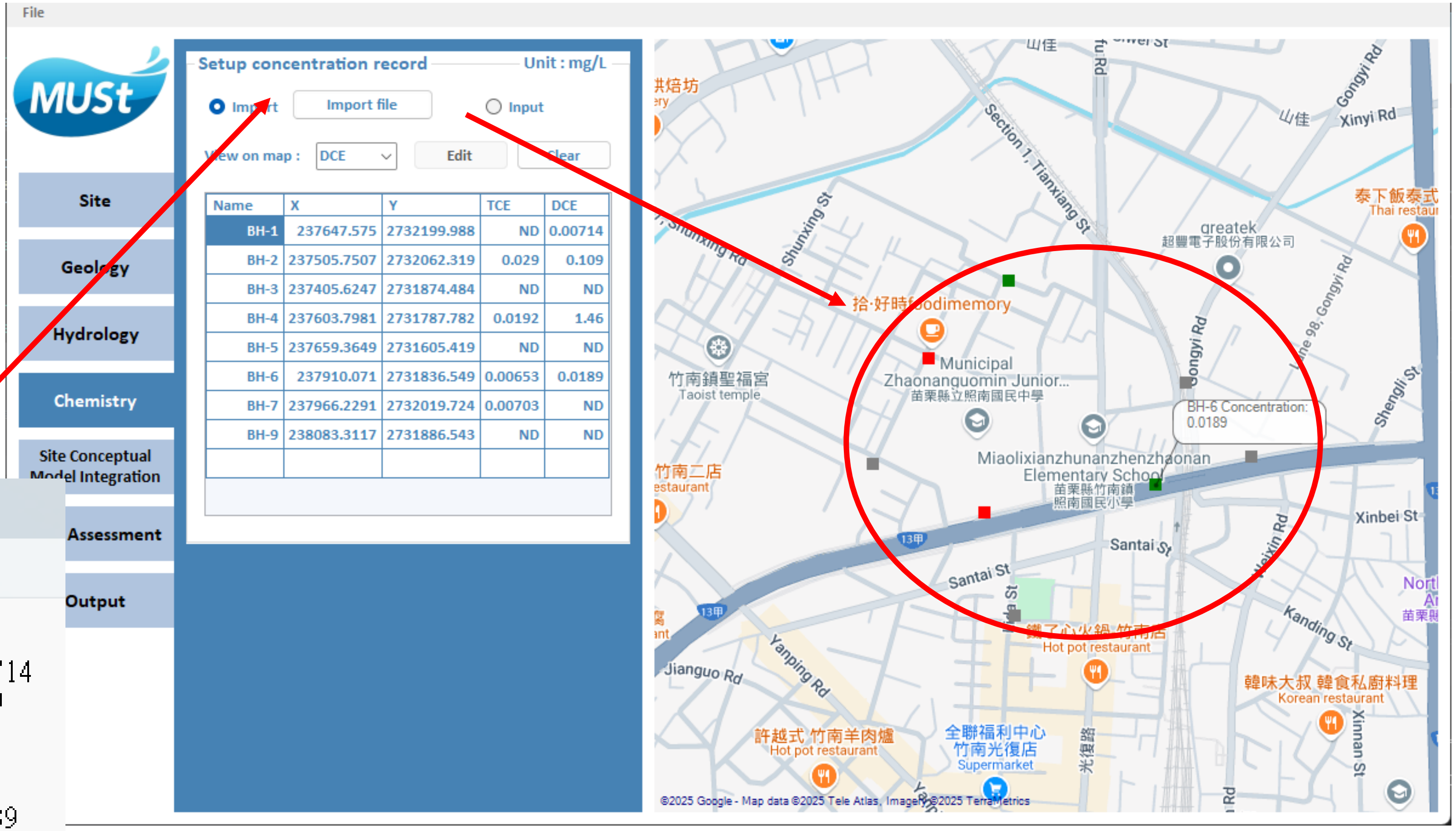
圖 4.3- 11　場址周邊地下水流向推估(108 年資料)

Name	X	Y	Hydralic_Head
BH-1	237647.575	2732199.988	4
BH-2	237505.7507	2732062.319	6.263
BH-3	237405.6247	2731874.484	7.89
BH-4	237603.7981	2731787.782	6.9507
BH-5	237659.3649	2731605.419	7.84
BH-6	237910.071	2731836.549	7.1887
BH-7	237966.2291	2732019.724	7.5657
BH-9	238083.3117	2731886.543	7.85



By importing text file,
the hydraulic head record can be shown on the map picture,
also to generate flow field and average flow direction.

User interface : Chemistry



site_Concentration.txt

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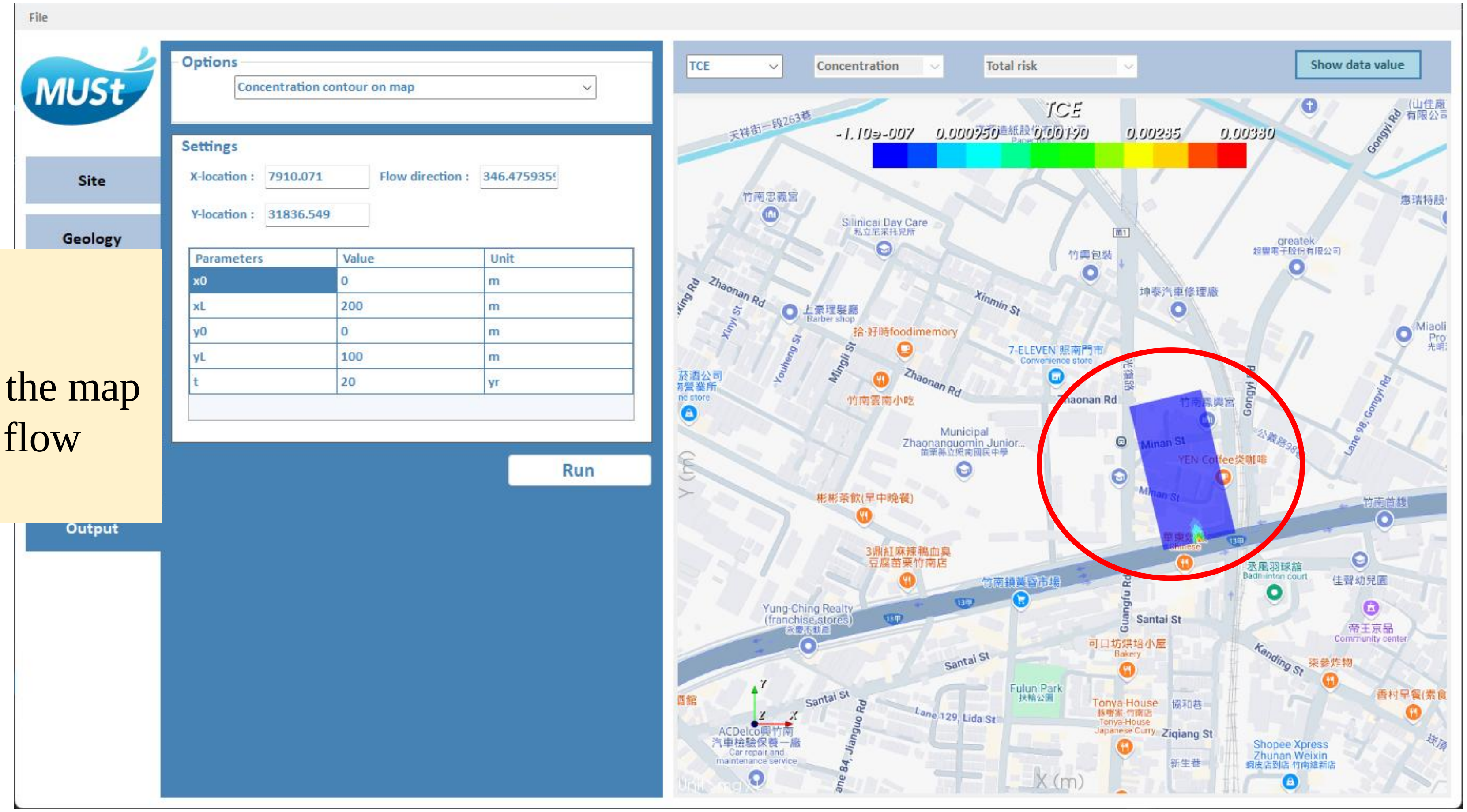
Name	X	Y	TCE	DCE
BH-1	237647.575	2732199.988	ND	0.00714
BH-2	237505.7507	2732062.319	0.029	0.109
BH-3	237405.6247	2731874.484	ND	ND
BH-4	237603.7981	2731787.782	0.0192	1.46
BH-5	237659.3649	2731605.419	ND	ND
BH-6	237910.071	2731836.549	0.00653	0.0189
BH-7	237966.2291	2732019.724	0.00703	ND
BH-9	238083.3117	2731886.543	ND	ND

By importing text file, the contaminant concentration record can be shown on map with colors.

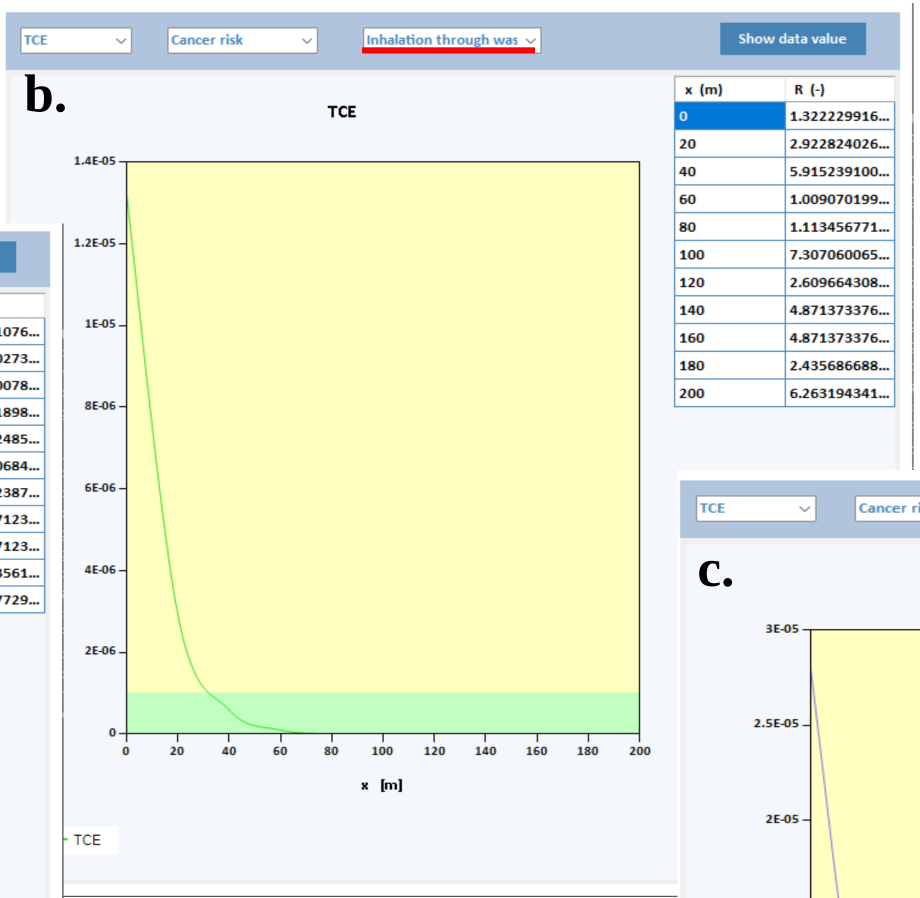
User interface : Output

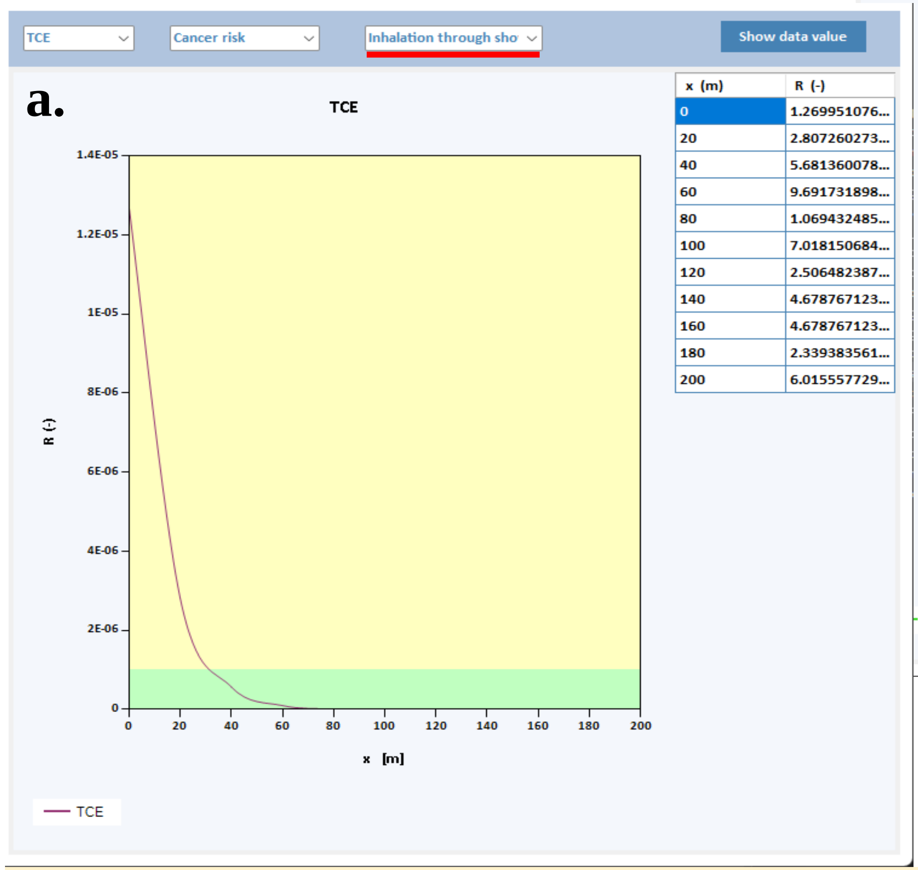
New result option:

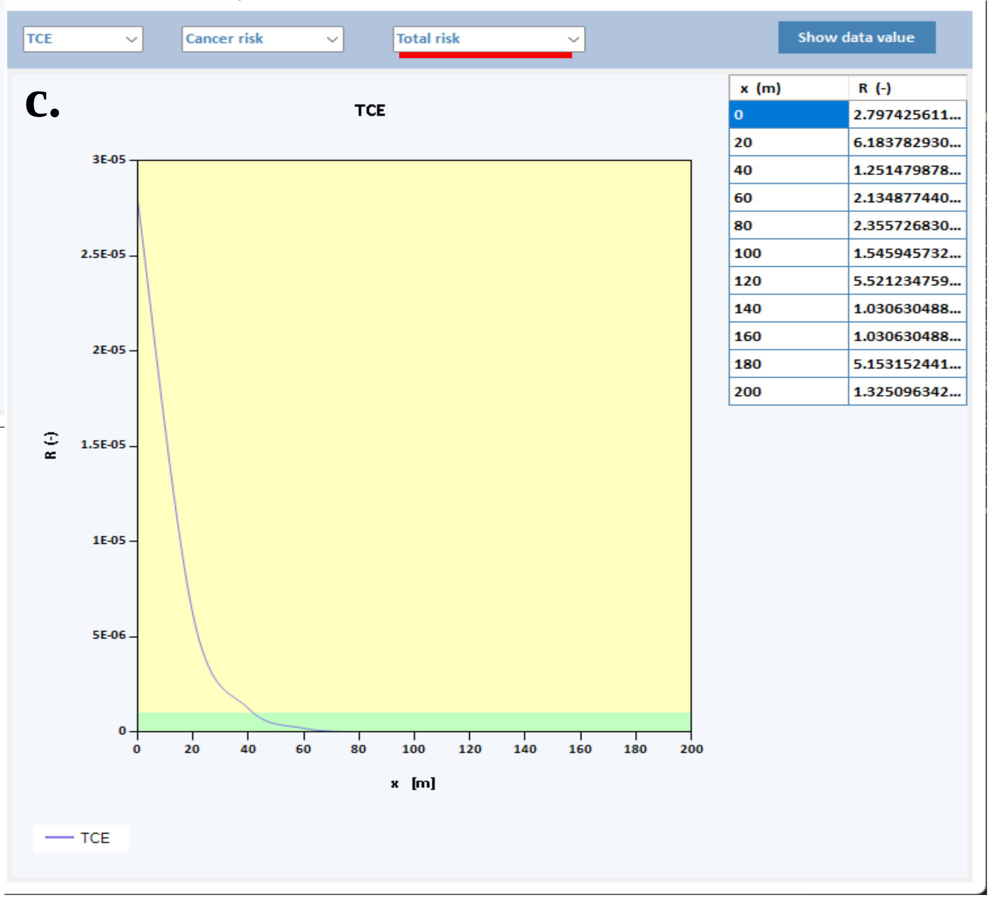
Apply the concentration contour on the map with specified location and average flow direction.



User interface : Output







New result option:

a. Inhalation through shower using groundwater
b. Inhalation through indoor washing using groundwater
c. Total risk

Conclusions and future work

- This study enhance the software's ability, incorporate geographic, geological, hydrological, and chemical visualizations, while also consider multiple exposure pathways. These improvements provide a comprehensive framework for site evaluation and decision-making.

- The new version software can improve the efficiency of site management while enhancing risk communication, enabling more informed decisions and fostering better stakeholder engagement.

- Future work :
  - Improve the risk calculation function with more exposure pathways considered.
  - Add probabilistic method into software for the more complex contaminated site evaluation.

Thank you for your attention!

Reference

- United States Environmental Protection Agency : https://www.epa.gov/
- Exact analytical solutions with great computational efficiency to three-dimensional multispecies advection-dispersion equations coupled with a sequential first-order reaction network : https://www.sciencedirect.com/science/article/pii/S0309170821001731
- HYDROSCAPE: A new versatile software program for evaluating contaminant transport in groundwater : https://www.sciencedirect.com/science/article/pii/S235271101730050X
- 103年環保署 土壤及地下水污染場址健康風險評估方法

$$D_x\frac{\partial^2 C_1(x,y,z,t)}{\partial x^2}+D_y\frac{\partial^2 C_1(x,y,z,t)}{\partial y^2}+D_z\frac{\partial^2 C_1(x,y,z,t)}{\partial z^2}-v\frac{\partial C_1(x,y,z,t)}{\partial x},$$

$$-\mu_1 R_1 C_1(x,y,z,t)=R_1\frac{\partial C_1(x,y,z,t)}{\partial t},\ 0\le x\le\infty,\ 0\le y\le W,\ 0\le z\le H \quad (1a)$$

$$D_x\frac{\partial^2 C_i(x,y,z,t)}{\partial x^2}+D_y\frac{\partial^2 C_i(x,y,z,t)}{\partial y^2}+D_z\frac{\partial^2 C_i(x,y,z,t)}{\partial z^2}-v\frac{\partial C_i(x,y,z,t)}{\partial x},$$

$$-\mu_i R_i C_i(x,y,z,t)+g_{i-1\rightarrow i}\mu_{i-1}R_{i-1}C_{i-1}(x,y,z,t)=R_i\frac{\partial C_i(x,y,z,t)}{\partial t}$$

$$0\le x\le\infty,\ 0\le y\le W,\ 0\le z\le H \quad i=2,3,4,5 \quad (1b)$$

I.C.

$$C_i(x,y,z,t=0)=0\ \ 0\le x\le\infty,\ 0\le y\le W,\ 0\le z\le H \quad i=1,2,3,4,5 \quad (2)$$

B.C.

$$C_i(x=0,y,z,t)=C_{i,0}[H(y-y_1)-H(y-y_2)]\cdot[H(z-z_1)-H(z-z_2)] \quad i=1,2,3,4,5 \quad (3a)$$

$$-D_x\frac{\partial C_i(x=0,y,z,t)}{\partial x}+vC_i(x=0,y,z,t)$$

$$=vC_{i,0}[H(y-y_1)-H(y-y_2)]\cdot[H(z-z_1)-H(z-z_2)] \quad i=1,2,3,4,5 \quad (3b)$$

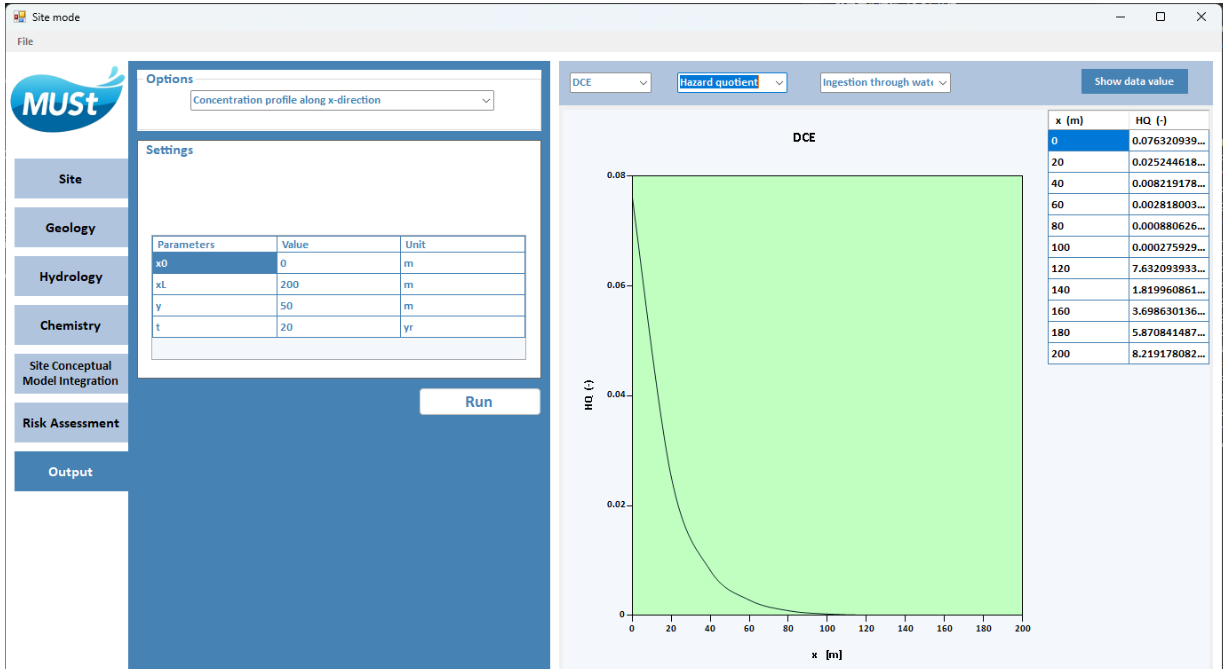
$$C_i(x\rightarrow\infty,y,z,t)=0 \quad i=1,2,3,4,5 \quad (4)$$

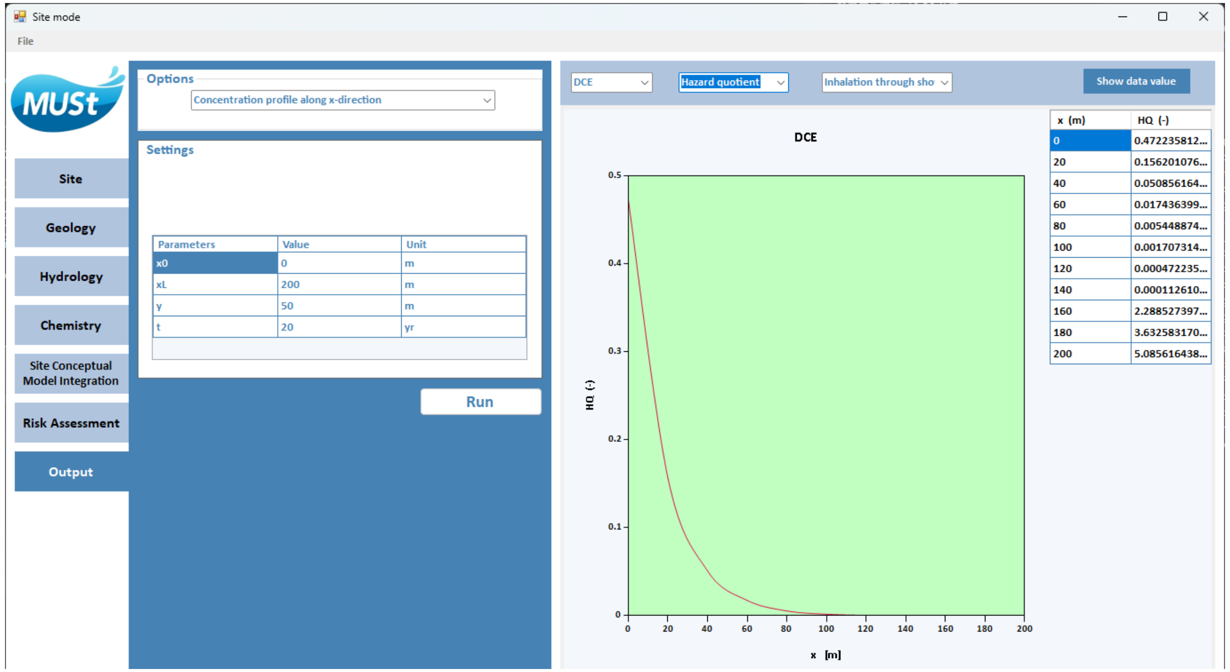
$$\frac{\partial C_i(x,y=0,z,t)}{\partial y}=0 \quad i=1,2,3,4,5 \quad (5)$$

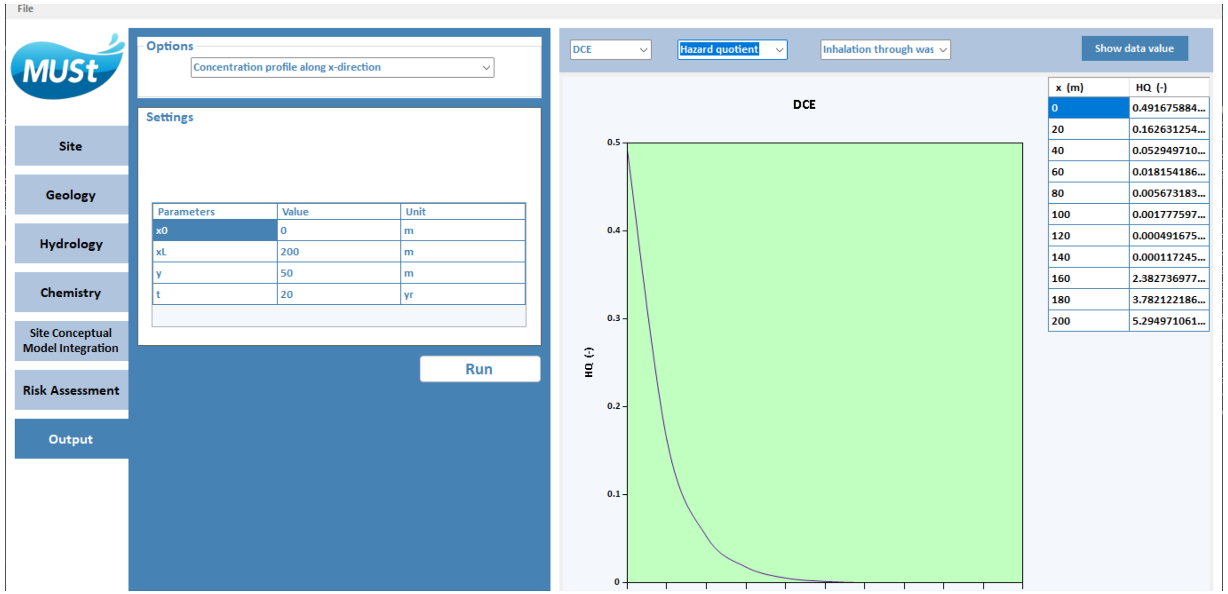
$$\frac{\partial C_i(x,y=W,z,t)}{\partial y}=0 \quad i=1,2,3,4,5 \quad (6)$$

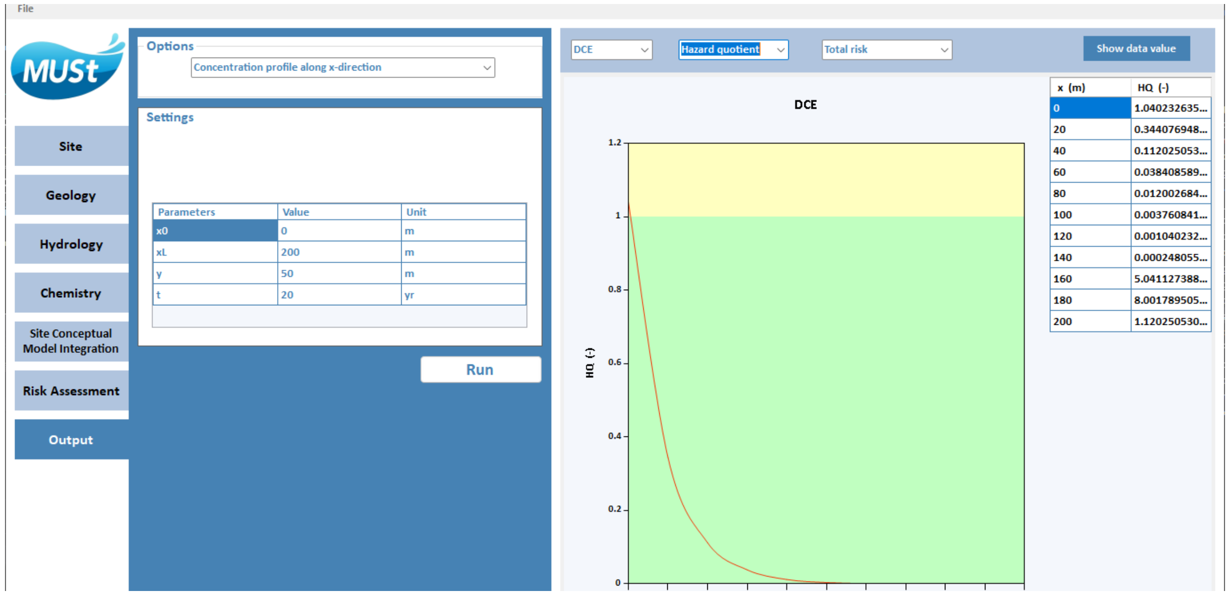
$$\frac{\partial C_i(x,y,z=0,t)}{\partial z}=0 \quad i=1,2,3,4,5 \quad (7)$$

$$\frac{\partial C_i(x,y,z=H,t)}{\partial z}=0 \quad i=1,2,3,4,5 \quad (8)$$


Site mode
File
MUSt
Options
Concentration profile along x-direction
Settings
Parameters | Value | Unit
x0 | 0 | m
xL | 200 | m
y | 50 | m
t | 20 | yr
Site
Geology
Hydrology
Chemistry
Site Conceptual Model Integration
Risk Assessment
Output
Run
DCE
Hazard quotient
Ingestion through wat
Show data value
DCE
HQ (-)
x [m]
x (m) | HQ (-)
0 | 0.076320939...
20 | 0.025244618...
40 | 0.008219178...
60 | 0.002818003...
80 | 0.000880626...
100 | 0.000275929...
120 | 7.632093933...
140 | 1.819960861...
160 | 3.698630136...
180 | 5.870841487...
200 | 8.219178082...


Site mode
File
MUSt
Options
Concentration profile along x-direction
Settings
Parameters | Value | Unit
x0 | 0 | m
xL | 200 | m
y | 50 | m
t | 20 | yr
Site
Geology
Hydrology
Chemistry
Site Conceptual Model Integration
Risk Assessment
Output
Run
DCE
Hazard quotient
Inhalation through sho
Show data value
DCE
HQ (-)
x [m]
x (m) | HQ (-)
0 | 0.472235812...
20 | 0.156201076...
40 | 0.050856164...
60 | 0.017436399...
80 | 0.005448874...
100 | 0.001707314...
120 | 0.000472235...
140 | 0.000112610...
160 | 2.288527397...
180 | 3.632583170...
200 | 5.085616438...


File
MUSt
Options
Concentration profile along x-direction
Settings
Parameters | Value | Unit
x0 | 0 | m
xL | 200 | m
y | 50 | m
t | 20 | yr
Site
Geology
Hydrology
Chemistry
Site Conceptual Model Integration
Risk Assessment
Output
Run
DCE
Hazard quotient
Inhalation through was
Show data value
DCE
HQ (-)
x (m) | HQ (-)
0 | 0.491675884...
20 | 0.162631254...
40 | 0.052949710...
60 | 0.018154186...
80 | 0.005673183...
100 | 0.001777597...
120 | 0.000491675...
140 | 0.000117245...
160 | 2.382736977...
180 | 3.782122186...
200 | 5.294971061...


File
MUSt
Options
Concentration profile along x-direction
Settings
Parameters | Value | Unit
x0 | 0 | m
xL | 200 | m
y | 50 | m
t | 20 | yr
Site
Geology
Hydrology
Chemistry
Site Conceptual Model Integration
Risk Assessment
Output
Run
DCE
Hazard quotient
Total risk
Show data value
DCE
HQ (-)
x (m) | HQ (-)
0 | 1.040232635...
20 | 0.344076948...
40 | 0.112025053...
60 | 0.038408589...
80 | 0.012002684...
100 | 0.003760841...
120 | 0.001040232...
140 | 0.000248055...
160 | 5.041127388...
180 | 8.001789505...
200 | 1.120250530...

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Original software publication

HYDROSCAPE: A new versatile software program for evaluating contaminant transport in groundwater

Sean P. Funk *, Danny Hnatyshin, Daniel S. Alessi

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contaminant	cancer
四氯乙烯PCE	Bladder cancer, liver cancer, kidneys cancer and blood system related cancers
三氯乙烯TCE	Kidney, liver, and lymphoma
氯乙烯VC	Liver cancer, brain cancer, lung cancer, blood cancer