MUSt 2: A site management module and health risk assessment integrated multispecies transport analytical solution software for management of groundwater chlorinated solvents contaminated site

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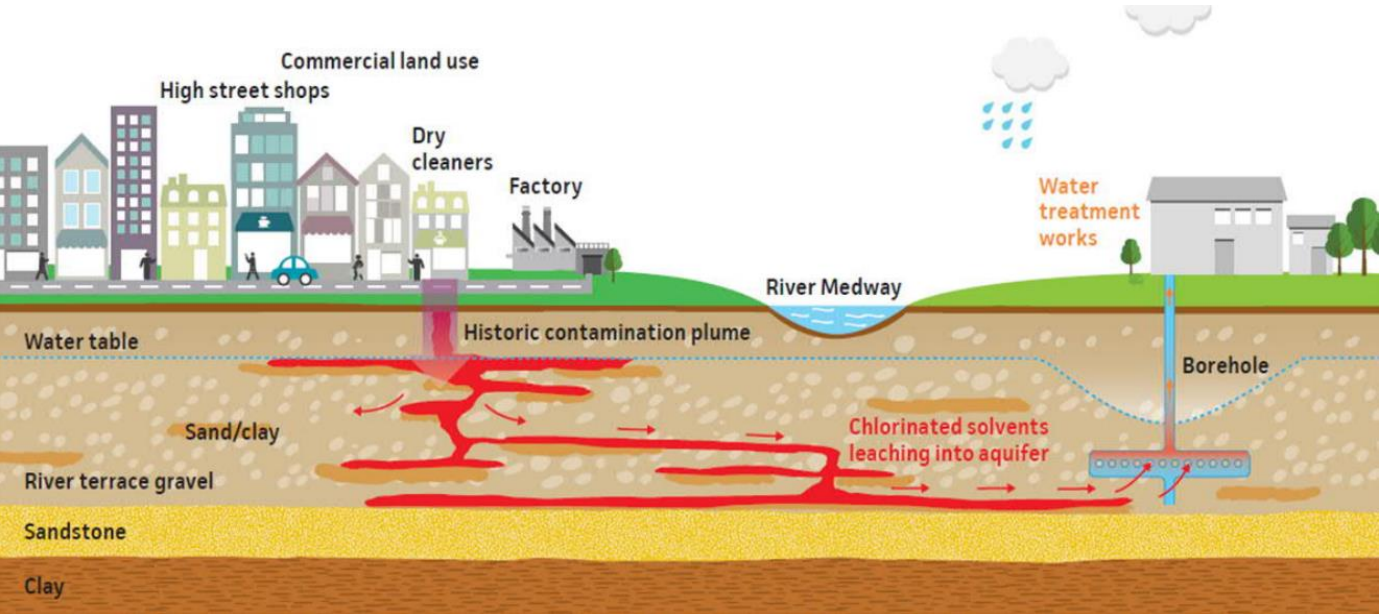
Outline

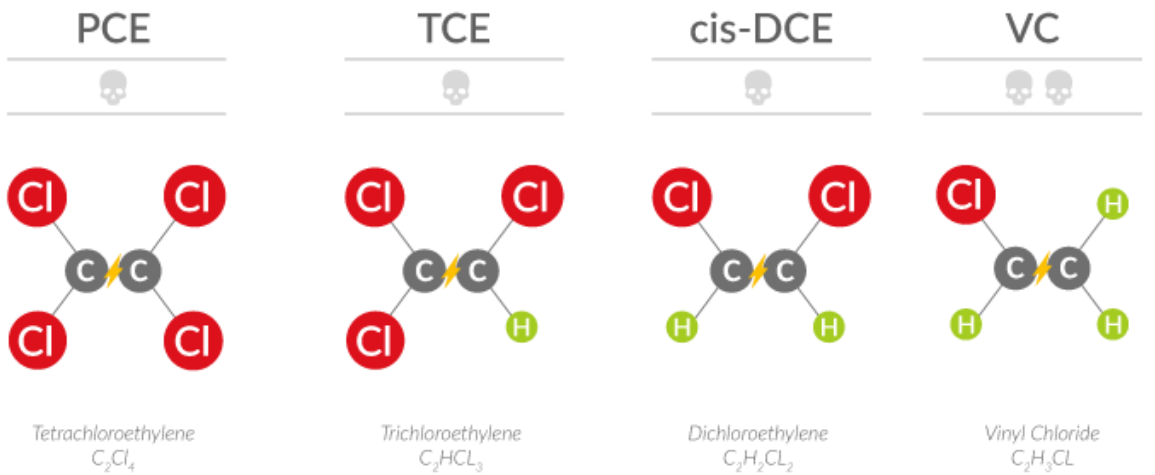
- Introduction
- Material and method
- Preliminary results
- Conclusions and future work

Groundwater contaminants

- There are many contaminated sites worldwide, and the contamination of the subsurface environment pose threats to human health.

- Chlorinated solvents like tetrachloroethene (PCE) and trichloroethene (TCE) are common contaminants in groundwater that cause different kinds of cancer.





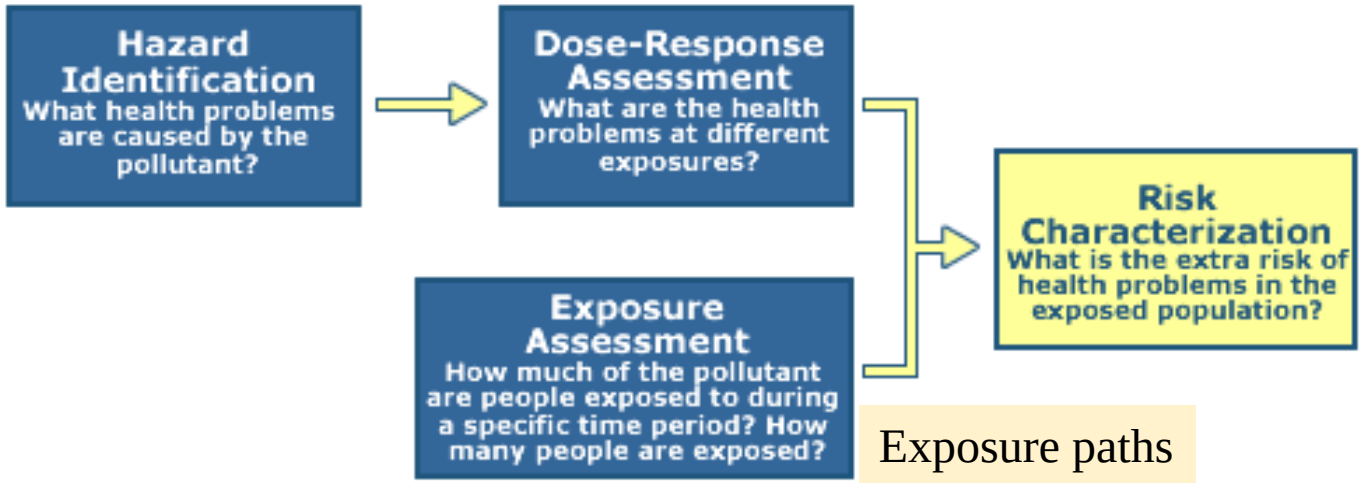
Human health risk assessment (HHRA)

- HHRA is the process to estimate the probability of adverse health effects in humans who may be exposed to chemicals in contaminated environmental media.

- HHRA can be the reference of the remedial actions, also can help governments to deliver technical knowledge to the public.

How much dosage cause people sick

Conceptual site model :
Site range
Contaminants
Hydrology & Geology
…

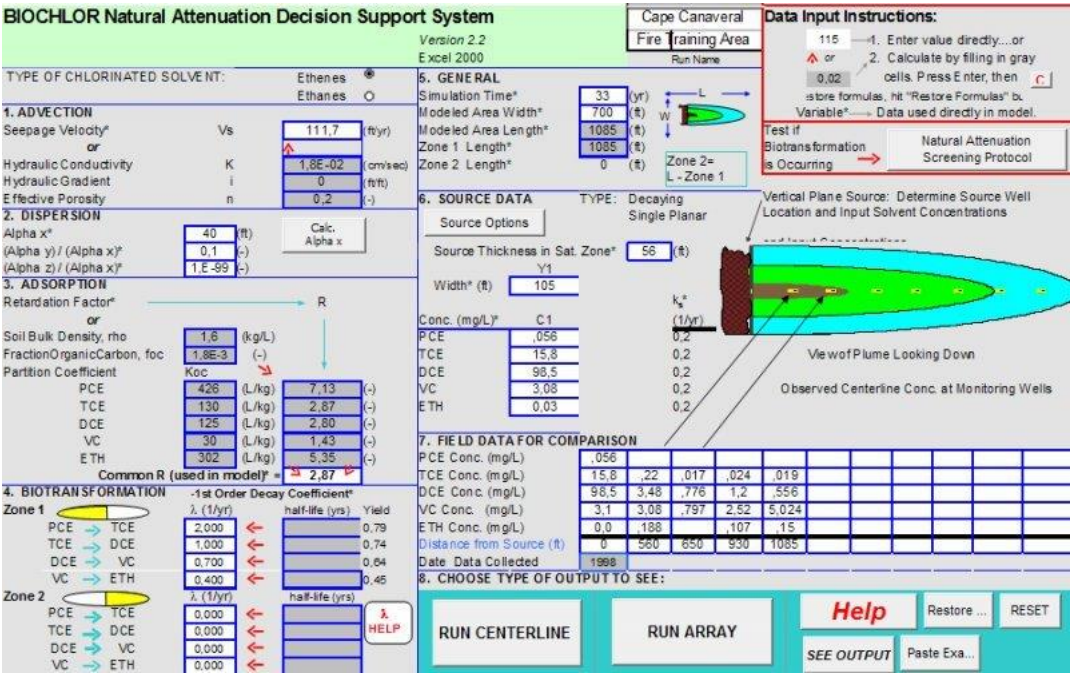


Exposure paths

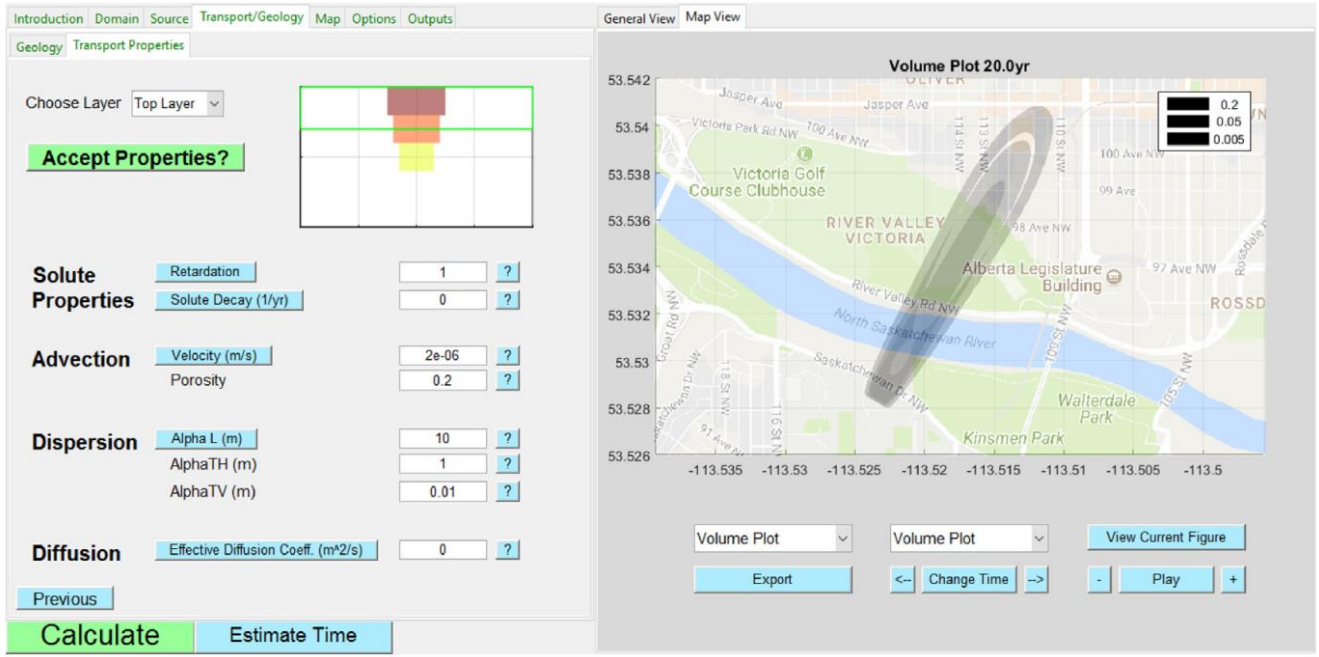
Four steps of human health risk assessment process

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.
  - Released in 2017.
  - Only can simulate single contaminant.



MUSt software

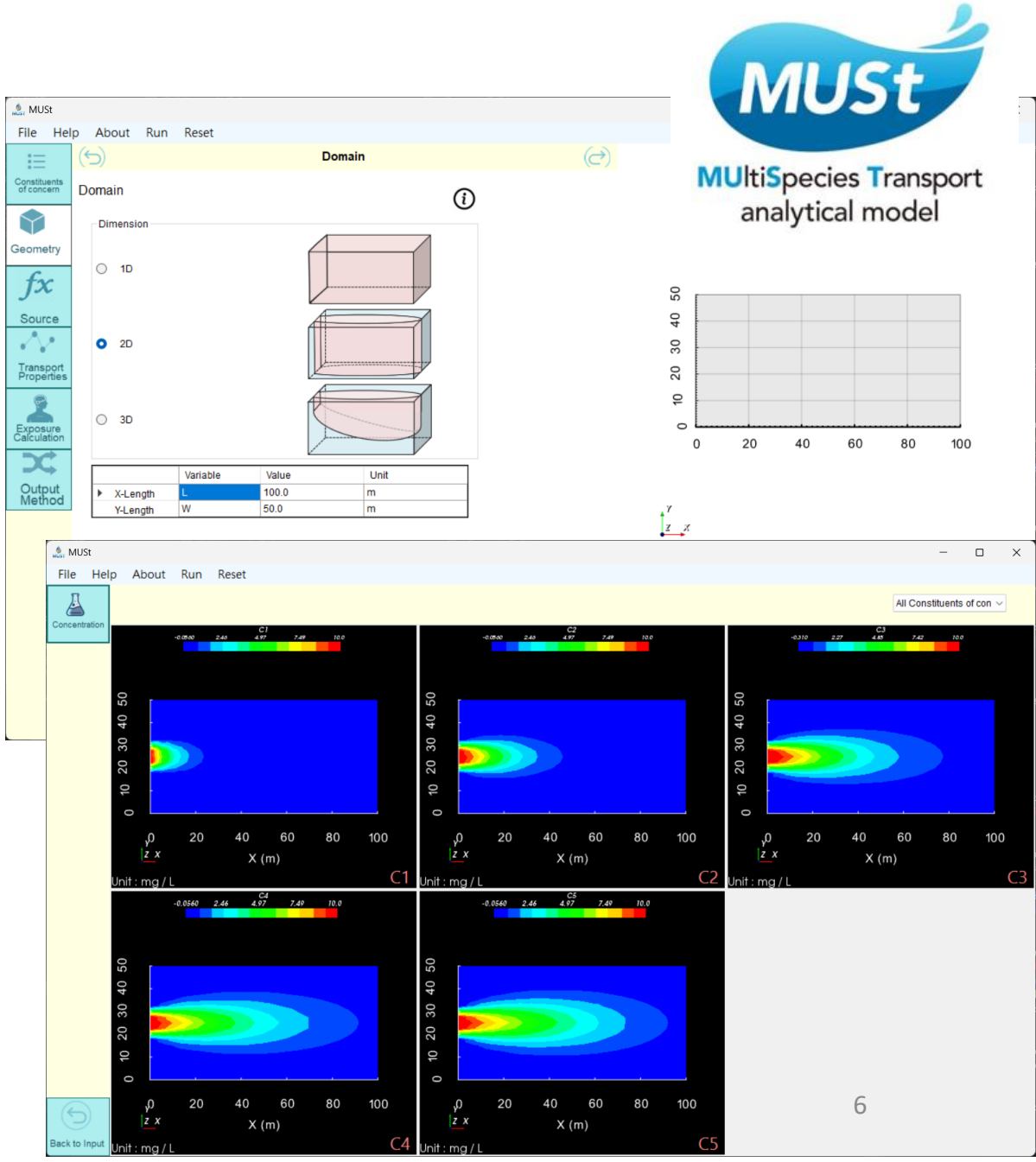
- MUSt (**MU**lti**S**pecies **t**ransport analytical model) is a software based on analytical solutions (Liao et al., 2021) for simulating transport of chlorinated solvent contaminant and its byproducts, integrated with health risk assessment.

- Developed from our lab, fixed the disadvantages of those previous software.

- Featuring with user-friendly interface, health risk assessment and multiple visualize output results.

What other features may be needed?

Site information management



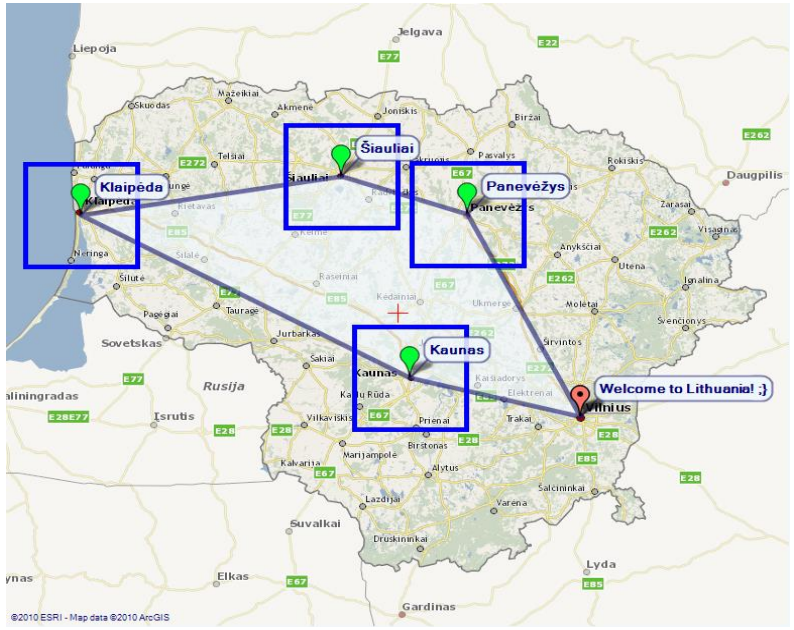
Objective

- To develop a new version of MUSt software (MUSt 2), extends the site management module, help users better know the information of the contaminated site and have better evaluation:
  - Manage and visualize the data collected from site.
  - Data combine with map view.

Material

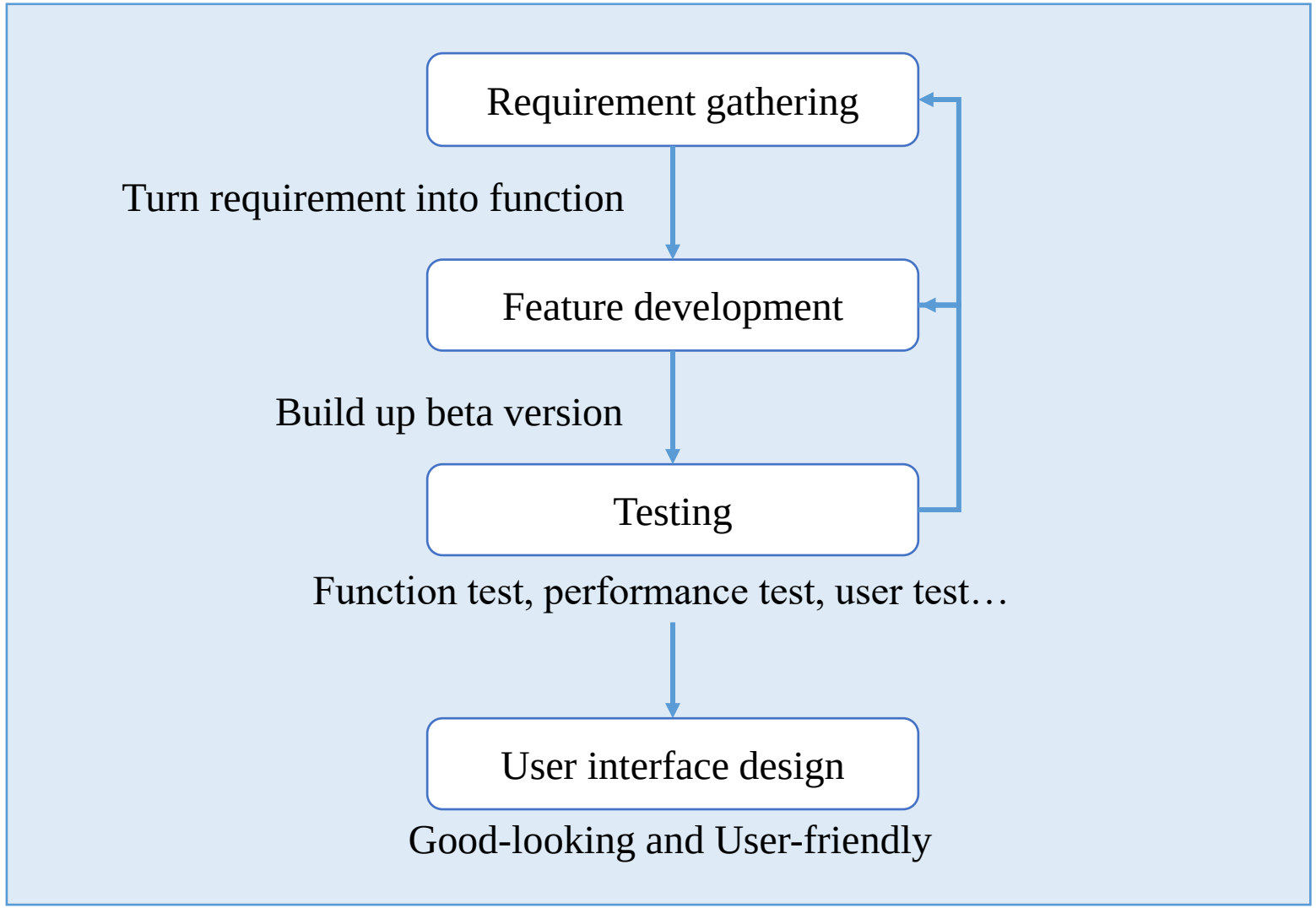
- .NET is a platform provides a large class library, enabling developers to create high-performance applications.
- Csharp is the most popular programming language in .NET which can build a wide range of applications from desktop to mobile.

- 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.

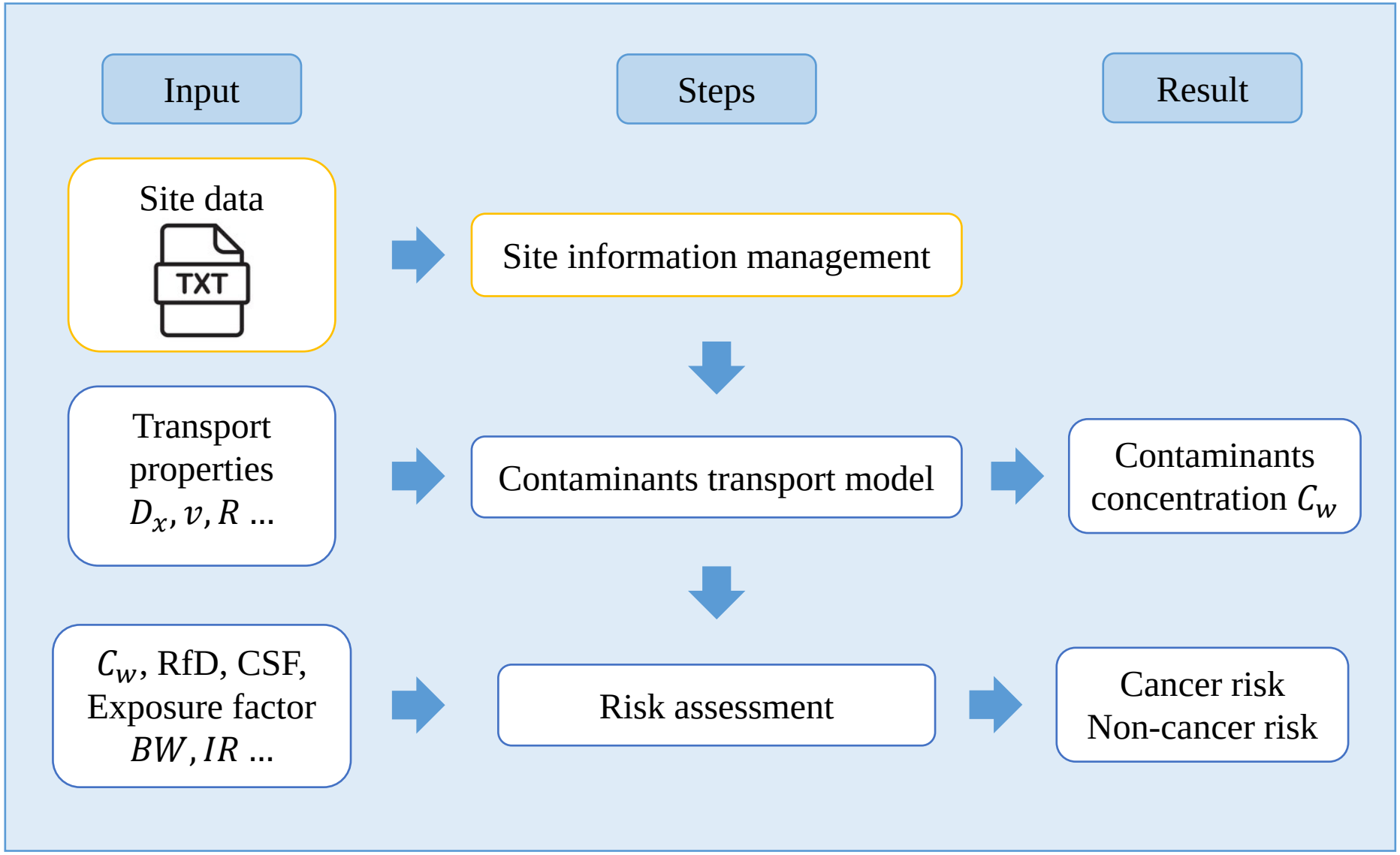


- Gmap.NET is a library in .NET provides interactive maps from various providers, supports creating objects on map.

Software development flow chart



Software usage flow chart



D_x: longitudinal dispersivity
v: groundwater velocity
R: retardation factor
IR: water ingestion rate (L/day)
BW: body weight (kg)
RfD: reference dose
CSF: cancer slope factor

User interface : Site

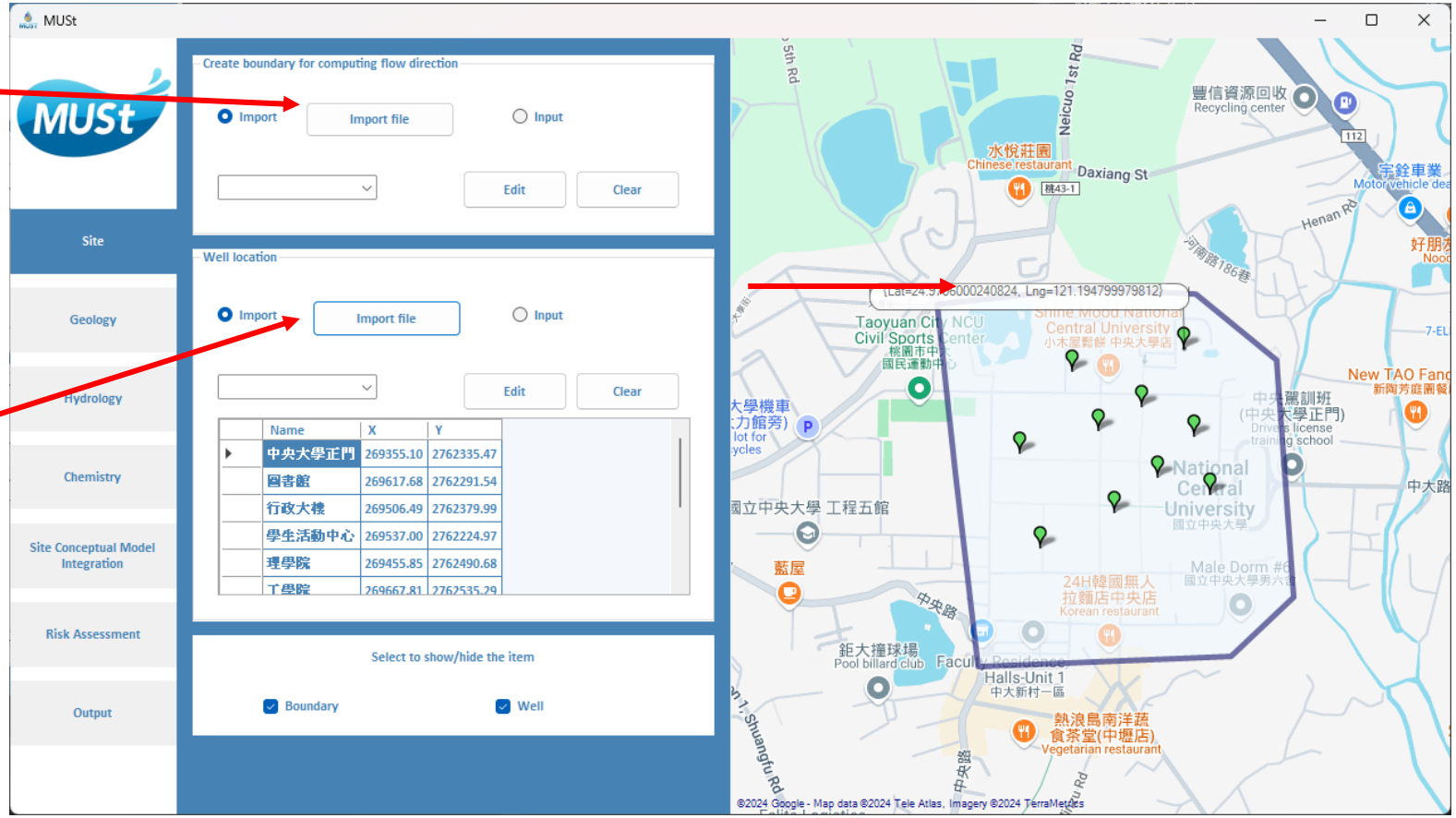
Shapefile create by QGIS

WellLocation3826.txt

檔案 編輯 檢視

Name	X	Y
中央大學正門	269355.10	2762335.47
圖書館	269617.68	2762291.54
行政大樓	269506.49	2762379.99
學生活動中心	269537.00	2762224.97
理學院	269455.85	2762490.68
工學院	269667.81	2762535.29
文學院	269587.20	2762424.41
商學院	269688.24	2762369.17
教育學院	269718.69	2762258.46
體育館	269395.74	2762158.31

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



User interface : Geology

borehole3826.txt

檔案 編輯 檢視

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BH_01	269355.10	2762335.47	125.1224518	9	Aquifuge_1
BH_01	269355.10	2762335.47	24.88004684	5	Aquifer_1
BH_01	269355.10	2762335.47	1.282514095	8	Aquifuge_2
BH_01	269355.10	2762335.47	-38.6497345	4	Aquifer_2
BH_01	269355.10	2762335.47	-48.87359619	7	Aquifuge_3
BH_01	269355.10	2762335.47	-105.6902161	3	Aquifer_3
BH_01	269355.10	2762335.47	-119.8641663	10	Aquifuge_4
BH_01	269355.10	2762335.47	-151.4880524	6	Aquifer_4
BH_01	269355.10	2762335.47	-163.753952	6	Aquifer_4
BH_02	269617.68	2762291.54	12.61678886	9	Aquifuge_1
BH_02	269617.68	2762291.54	-26.61739159	5	Aquifer_1
BH_02	269617.68	2762291.54	-36.5585289	8	Aquifuge_2
BH_02	269617.68	2762291.54	-85.4553299	4	Aquifer_2
BH_02	269617.68	2762291.54	-101.8764343	7	Aquifuge_3
BH_02	269617.68	2762291.54	-123.8853836	3	Aquifer_3
BH_02	269617.68	2762291.54	-150.0936279	10	Aquifuge_4
BH_02	269617.68	2762291.54	-189.2824707	6	Aquifer_4
BH_02	269617.68	2762291.54	-212.1426392	6	Aquifer_4
BH_03	269506.49	2762379.99	182.7165985	9	Aquifuge_1
BH_03	269506.49	2762379.99	70.55046082	5	Aquifer_1
BH_03	269506.49	2762379.99	45.55046463	8	Aquifuge_2
BH_03	269506.49	2762379.99	18.31370926	4	Aquifer_2
BH_03	269506.49	2762379.99	-4.4495368	7	Aquifuge_3
BH_03	269506.49	2762379.99	-29.44487572	3	Aquifer_3
BH_03	269506.49	2762379.99	-54.44953537	10	Aquifuge_4
BH_03	269506.49	2762379.99	-79.44461823	6	Aquifer_4
BH_03	269506.49	2762379.99	-104.4495392	6	Aquifer_4
BH_04	269537.00	2762224.97	89.02435303	9	Aquifuge_1
BH_04	269537.00	2762224.97	36.22627258	5	Aquifer_1
BH_04	269537.00	2762224.97	14.29684925	8	Aquifuge_2
BH_04	269537.00	2762224.97	-11.81618404	4	Aquifer_2
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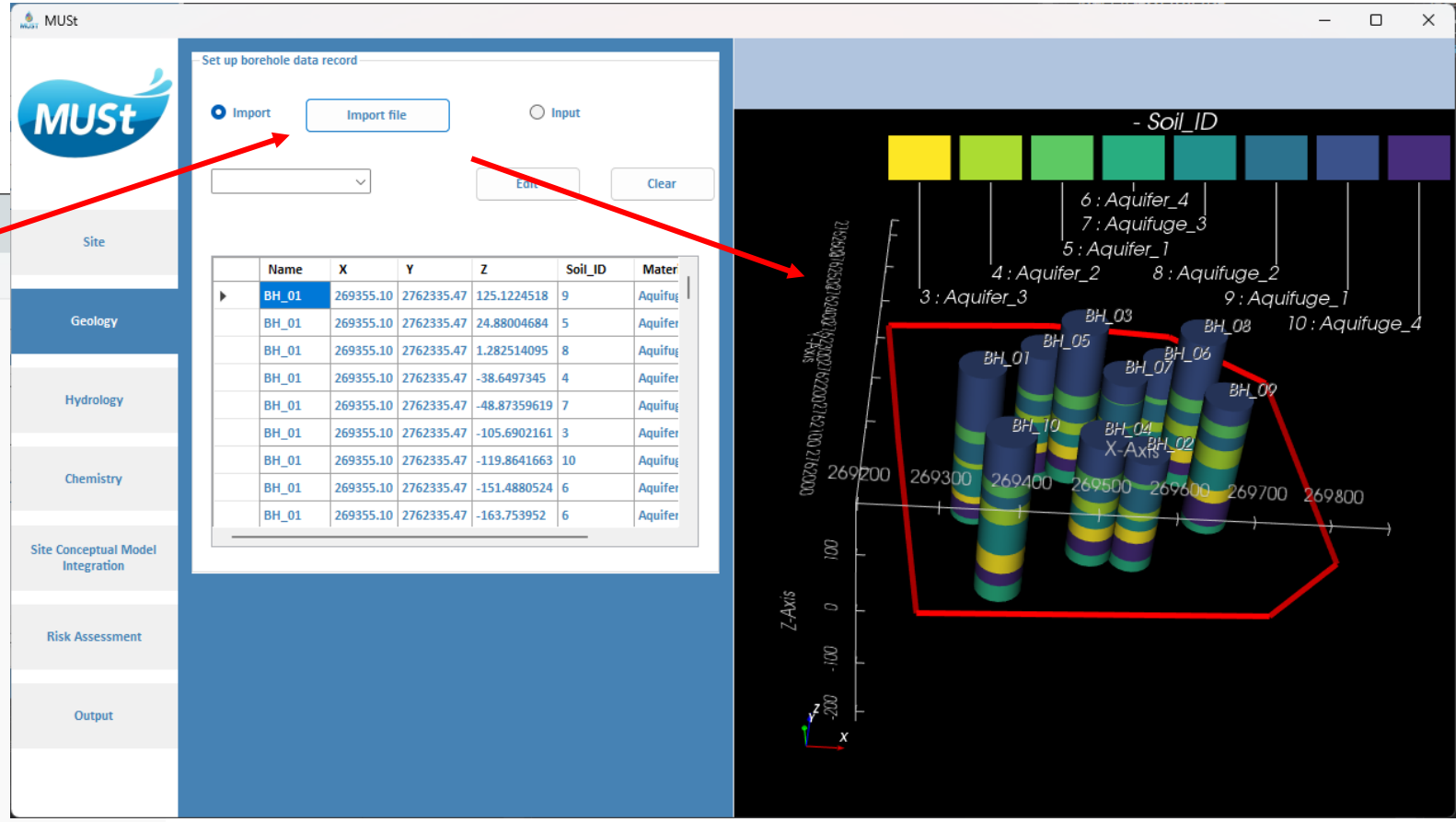
第 18 行，第 52 欄 4,723 個字元



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

User interface : Hydrology

elevation_ncu_3826.txt

檔案 編輯 檢視

```
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圖書館,269617.68,2762291.54,188
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學生活動中心,269537.00,2762224.97,86
理學院,269455.85,2762490.68,176
工學院,269667.81,2762535.29,134
文學院,269587.20,2762424.41,97
商學院,269688.24,2762369.17,104
教育學院,269718.69,2762258.46,80
體育館,269395.74,2762158.31,150
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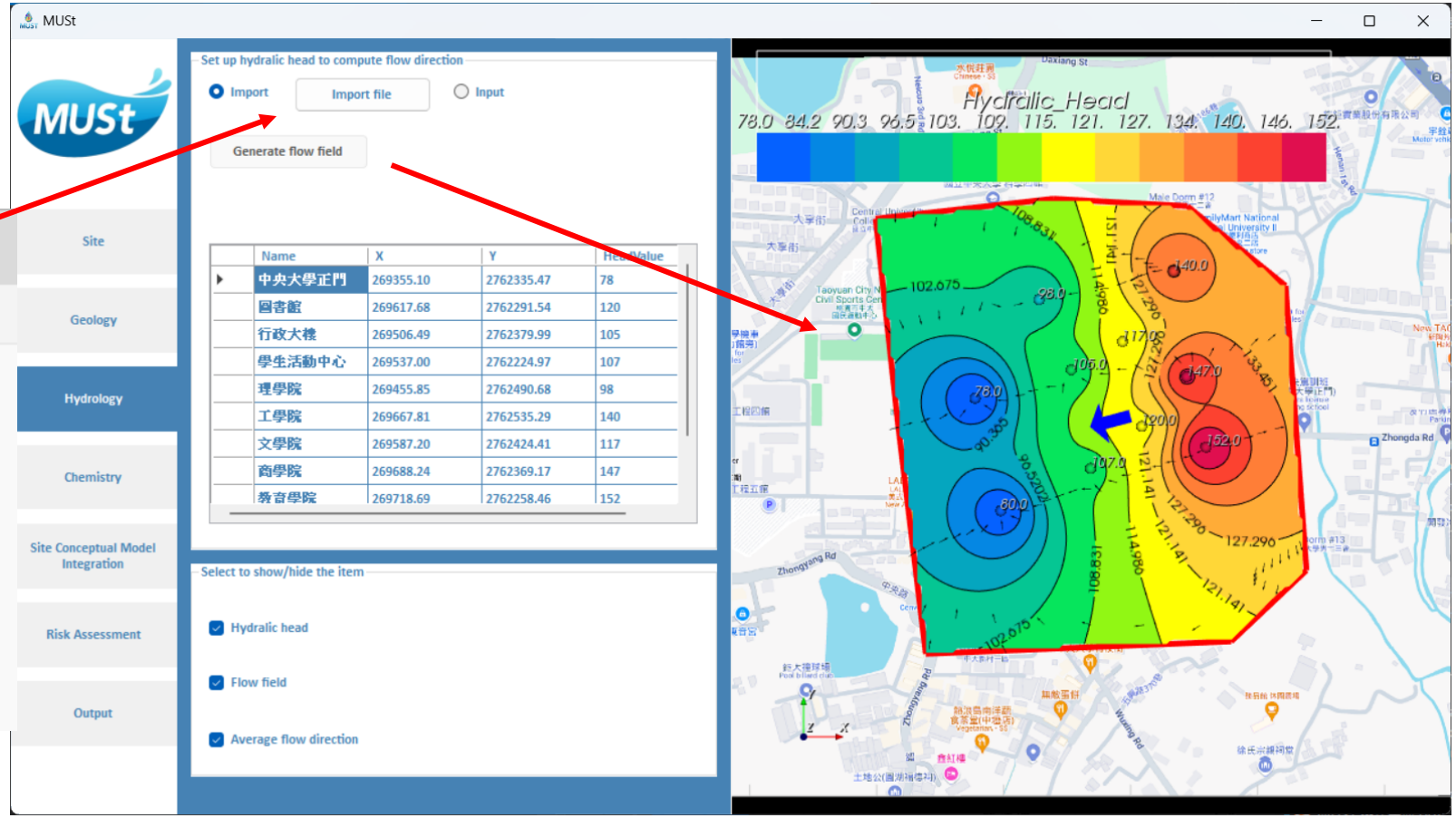
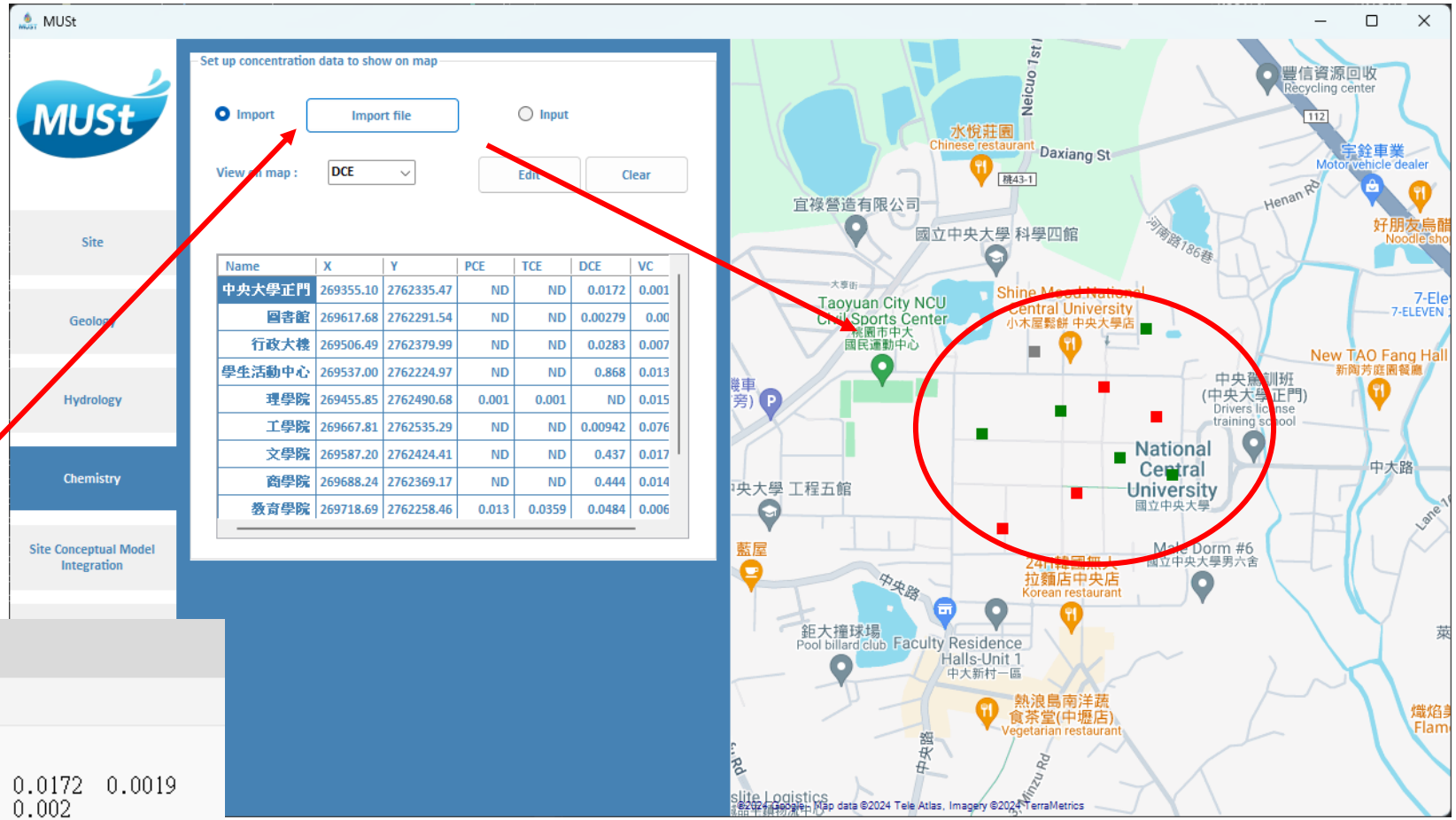


By importing text file,
the hydraulic head record can be shown on the map picture,
also to generate flow field and average flow direction.

User interface : Chemistry



concentration3826.txt

檔案 編輯 檢視

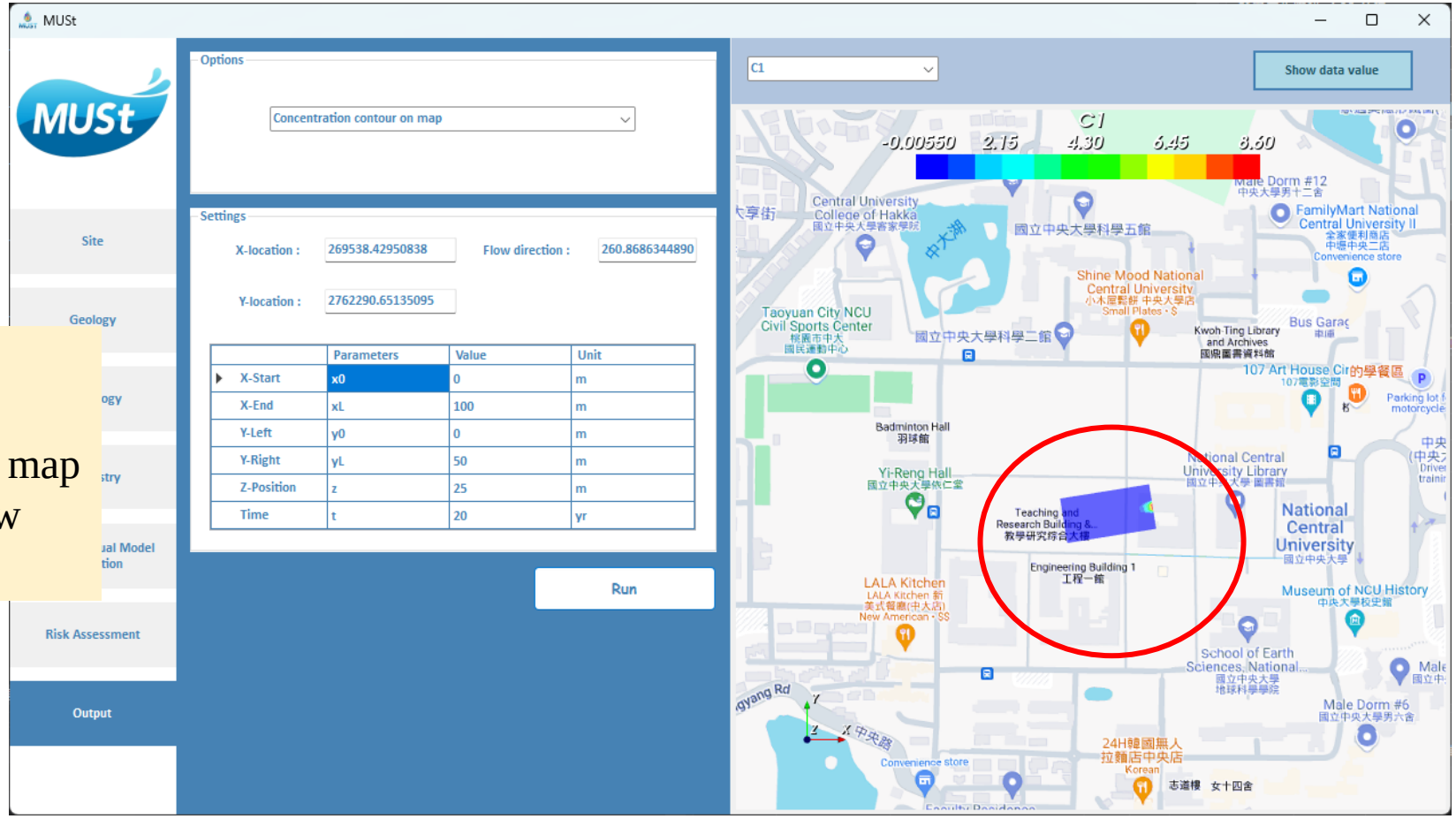
Name	X	Y	PCE	TCE	DCE	VC		
中央大學正門	269355.10	2762335.47	ND	ND	0.0172	0.0019		
圖書館	269617.68	2762291.54	ND	ND	0.00279	0.002		
行政大樓	269506.49	2762379.99	ND	ND	0.0283	0.0078		
學生活動中心	269537.00	2762224.97	ND	ND	0.868	0.0136		
理學院	269455.85	2762490.68	0.001	0.001	ND	0.0153		
工學院	269667.81	2762535.29	ND	ND	0.00942	0.0764		
文學院	269587.20	2762424.41	ND	ND	0.437	0.0173		
商學院	269688.24	2762369.17	ND	ND	0.444	0.0146		
教育學院	269718.69	2762258.46	0.013	0.0359	0.0484	0.0062		
體育館	269395.74	2762158.31	ND	ND	2.18	0.0241		

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.



Conclusions and future work

- The software is still under development, but after completion, it will provide users with a more comprehensive evaluation process and have better risk management and communication.

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

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

Thank you for your attention!

Development of site management module for multi-species transport analytical model software for chlorinated solvents contaminated site

MUSt 2 : A subsurface modeling software
for natural attenuation and health risk assessment
of groundwater chlorinated solvent contaminated sites,
integrating multispecies transport analytical solutions, a user-friendly graphical interface, and geographic information system

Smart GIS site management tool for decontamination of recalcitrant solvents in groundwater

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Advances in Water Resources

journal homepage: www.elsevier.com/locate/advwatres

Exact analytical solutions with great computational efficiency to three-dimensional multispecies advection-dispersion equations coupled with a sequential first-order reaction network

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[d] Department of Nursing, Fooyin University, Daliao Dist., Kaohsiung 83101, Taiwan

SoftwareX 6 (2017) 261–266

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Original software publication

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

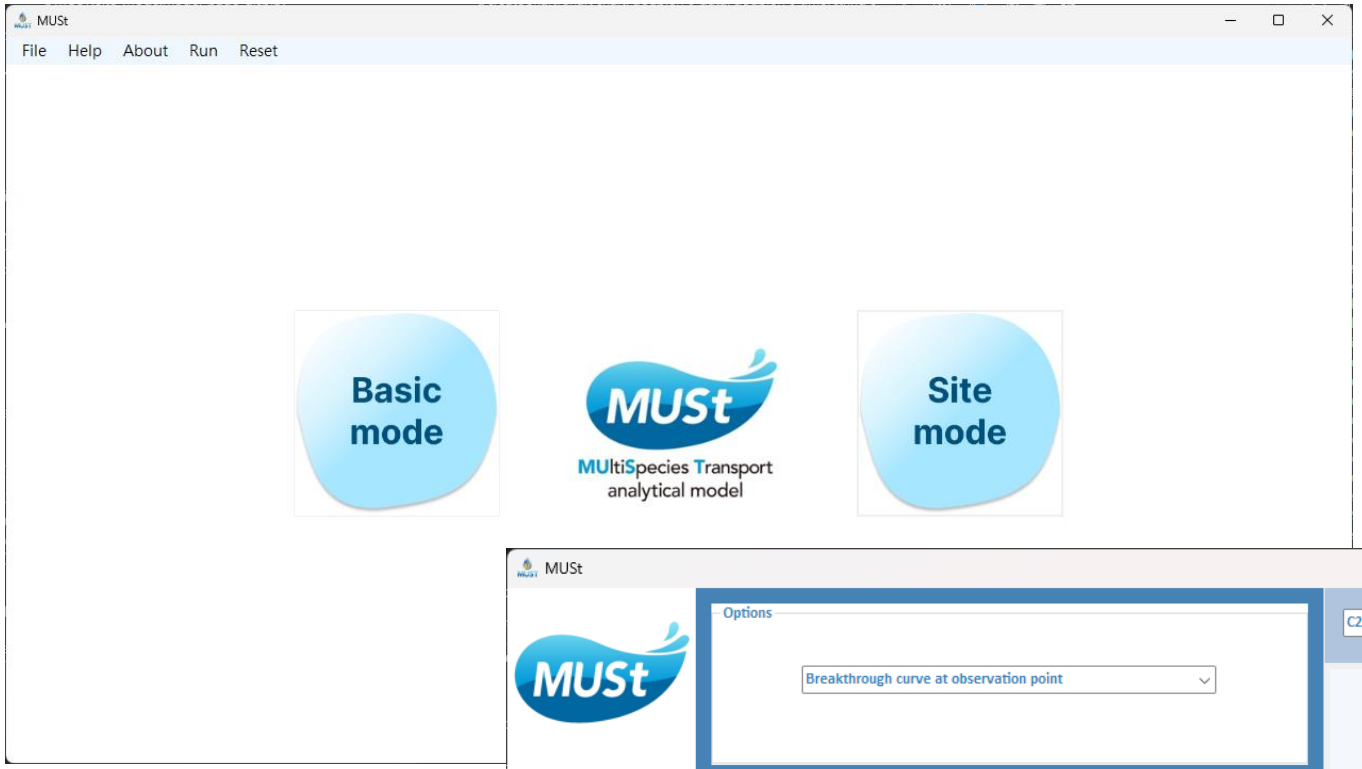
Sean P. Funk *, Danny Hnatyshin, Daniel S. Alessi

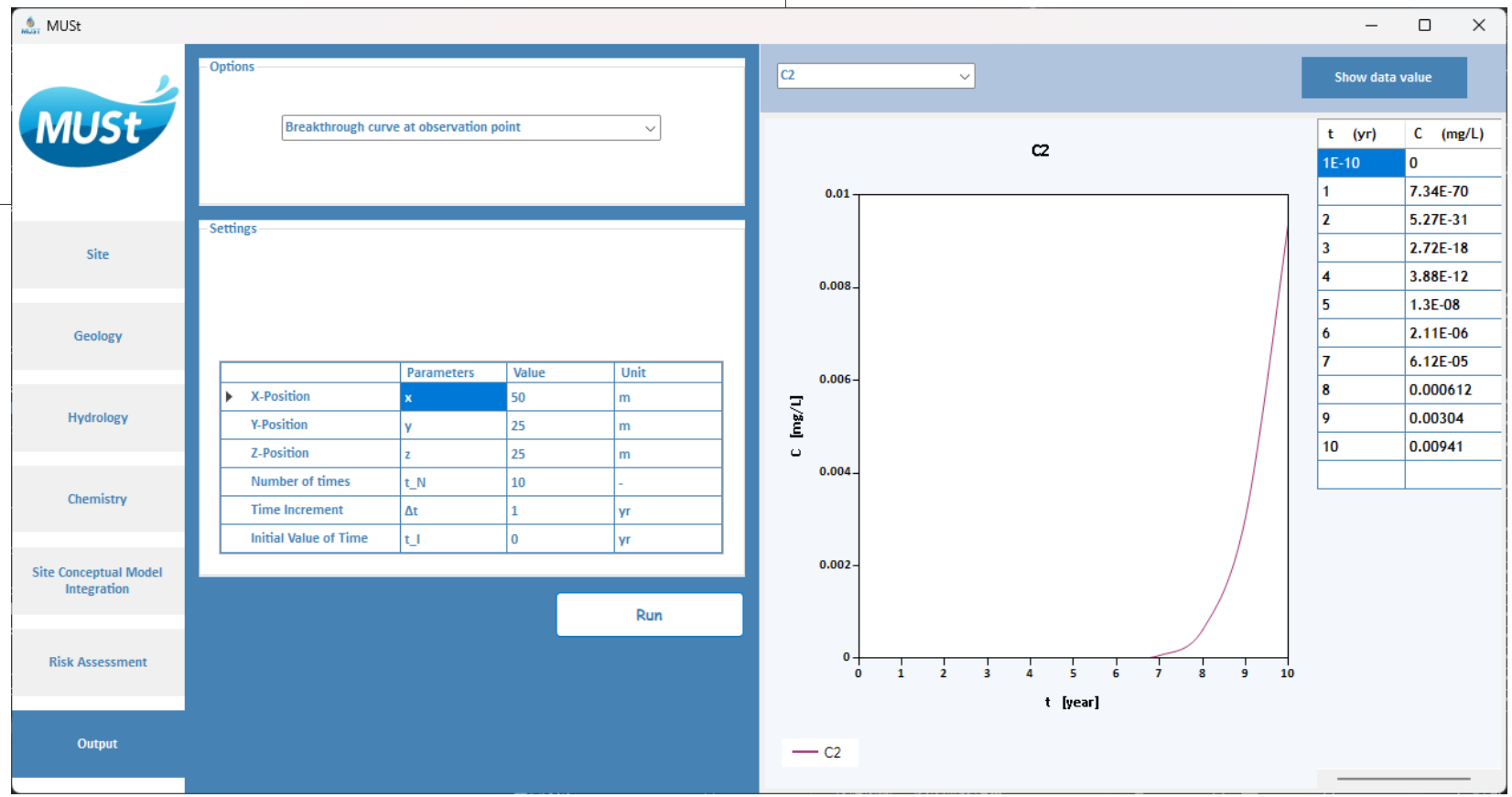
Department of Earth & Atmospheric Sciences, University of Alberta, Edmonton, AB, Canada, T6G 2E3

C: contaminant concentration (mg/L)
IR: water ingestion rate (L/day)
EF: exposure frequency (days/year)
ED: exposure duration (years)
BW: body weight (kg); AT : average time (days)
RfD: reference dose; SF: slope factor

- Exposure dose (average daily dose) is calculated as:
  - $ADD = C \times \frac{IR \times EF \times ED}{BW \times AT}$
- Non-carcinogenic and carcinogenic risk indexes are calculated as:
  - Non-carcinogenic: $R = \frac{ADD}{RfD}$
  - Carcinogenic: $R = ADD \times SF$

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


MUSt
File
Help
About
Run
Reset
Basic mode
MUSt
MUltiSpecies Transport analytical model
Site mode


MUSt
MUSt
Options
Breakthrough curve at observation point
Settings
Site
Geology
Hydrology
Chemistry
Site Conceptual Model Integration
Risk Assessment
Output
Parameters
Value
Unit
X-Position
x
50
m
Y-Position
y
25
m
Z-Position
z
25
m
Number of times
t_N
10
-
Time Increment
Δt
1
yr
Initial Value of Time
t_I
0
yr
Run
C2
Show data value
C2
C [mg/L]
t [year]
0.01
0.008
0.006
0.004
0.002
0
0
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2
3
4
5
6
7
8
9
10
C2
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C (mg/L)
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