



# Development of human health risk assessment software for a chlorinated solvent contaminated groundwater site

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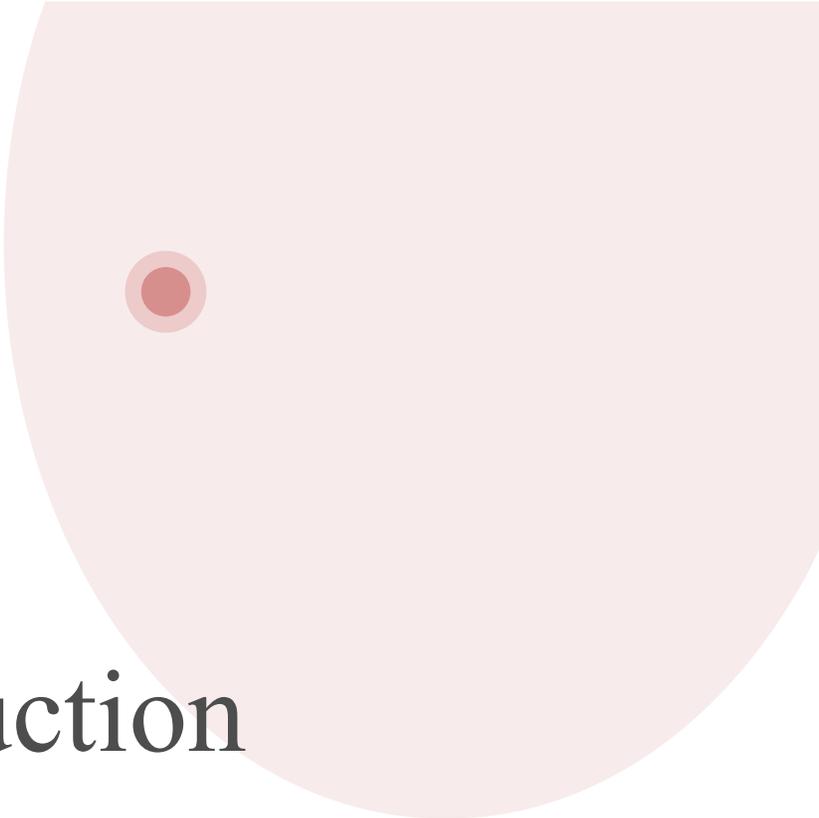
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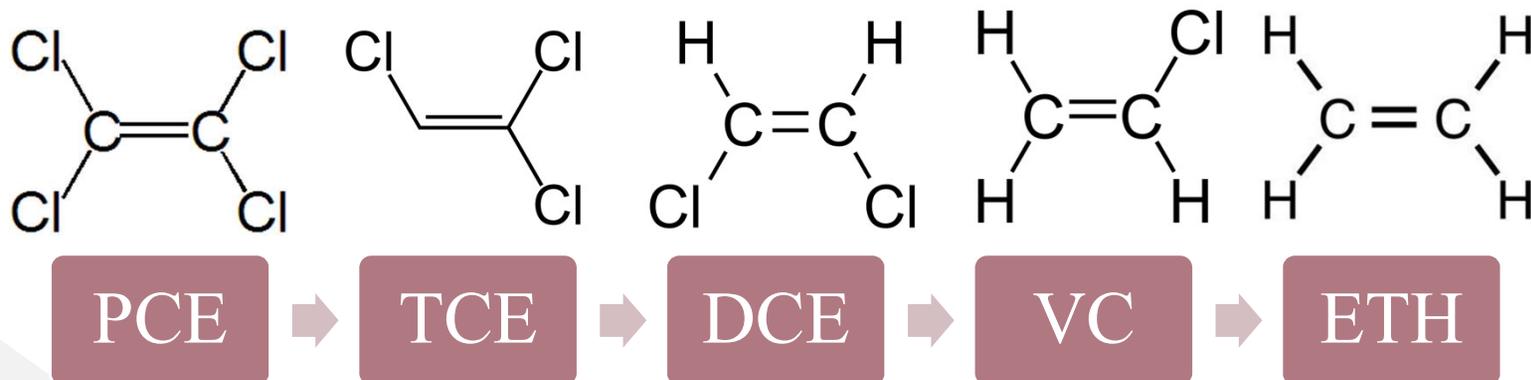
**1**



# Introduction

# Groundwater contaminant

- Chlorinated solvents are common contaminants in groundwater.



USEPA

Group A

Group A

Group A

USEPA: US Environmental Protection Agency  
Group A: Human carcinogen

PCE: Tetrachloroethene  
TCE: Trichloroethylene  
DCE: Dichloroethylene  
VC: Vinyl chloride  
ETH: Ethene

# Health risk assessment

- A process that estimates human health and environmental risks associated with chemicals of concern present in the environment.
- We can set the remediation goals and improvement methods of contaminated sites through the health risk assessment.



# Health risk assessment



Hazard  
Identification



Dose Response  
Assessment



Exposure  
Assessment



Risk  
Characterization

# Target Risk (Cancer Risk)

## Fate and Transport Model



$C_w$ : Contaminant Concentration (mg/L)

CSF: Cancer Slope Factor  
(mg/kg-day)

$$\text{Risk} = C_w \times \frac{\text{IR} \times \text{EF} \times \text{ED}}{\text{BW} \times \text{AT} \times 365 \text{ day/year}} \times \text{CSF}$$

Exposure Factor

IR: Water ingestion rate (L/day)

EF: Exposure frequency (days/year)

ED: Exposure duration (years)

BW: Body weight (kg)

AT: Average lifetime (years)

# RBCA Tool Kit

Environmental site managers, regulatory authorities, and consultants around the world have increasingly turned to Risk-Based Corrective Action (RBCA) for the management of contaminated soil and groundwater. RBCA is a practical management approach that focuses explicitly on the protection of human health and the environment while promoting energy and cost-efficient remedies to allow limited resources to be targeted to the most hazardous sites. A keystone of the RBCA framework is the development of site-specific environmental cleanup criteria following a tiered risk evaluation approach. This approach is broadly applicable to chemical release sites located in different geographical settings and managed under various regulatory authorities.

# BIOCHLOR

**BIOCHLOR Natural Attenuation Decision Support System** Cape Canaveral Data Input Instructions:

TYPE OF CHLORINATED SOLVENT: Ethanes

**1. ADVECTION**  
 Seepage Velocity\*  $V_s$  111.7  
 Hydraulic Conductivity  $K$  1E-02  
 Hydraulic Gradient  $i$  0.0012  
 Effective Porosity 0.2

**2. DISPERSION**  
 Alpha x\* 40 (ft)  
 (Alpha y) / (Alpha x)\* 0.1 (-)

**3. ADSORPTION**  
 Retardation Factor\*  $R$  2.87  
 Soil Bulk Density, rho 1.6 (kg/L)  
 Fraction Organic Carbon,  $f_{oc}$  1.85E-2  
 Partition Coefficient  $K_{oc}$

PCE	426 (L/kg)	7.13
TCE	130 (L/kg)	2.87
DCE	125 (L/kg)	2.80
VC	30 (L/kg)	1.43
ETH	302 (L/kg)	5.35

Common R (used in model)\* = 2.87

**4. BIOTRANSFORMATION** -1st Order Decay Coefficient\*

**Zone 1**

Contaminant	Reaction	$\lambda$ (1/yr)	half-life (yrs)	Yield
PCE	→ TCE	2.000		0.79
TCE	→ DCE	1.000		0.74
DCE	→ VC	0.700		0.64
VC	→ ETH	0.400		0.45

**Zone 2**

Contaminant	Reaction	$\lambda$ (1/yr)	half-life (yrs)	Yield
PCE	→ TCE	0.000		
TCE	→ DCE	0.000		
DCE	→ VC	0.000		
VC	→ ETH	0.000		

**5. MONITORING DATA**

Contaminant	Conc. (mg/L)	Distance from Source (ft)	Date Data Collected
PCE	98.5	3.48	1998
TCE	3.1	3.08	1998
DCE	0.0	1.88	1998
VC	0.0	0.0	1998
ETH	0.0	0.0	1998

CHOOSE TYPE OF OUTPUT TO SEE:  
 RUN CENTERLINE    RUN ARRAY    Help    Restore    RESET  
 SEE OUTPUT    Paste    Unprotect

The most popular analytical screening model is the public domain BIOCHLOR model by Center for Subsurface Modeling Support of USEPA (Aziz et al., 2000)

It described aquifer remediation by simulating natural attenuation process

The limitation is that BIOCHLOR requires the use of identical retardation factors for all contaminants.

# MULTISPECIES TRANSPORT ANALYTICAL MODEL (MUST)

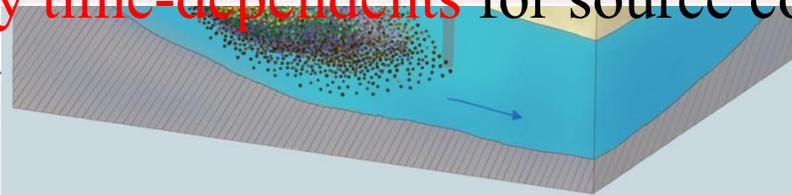
MUST can use different retardation factor values among individual species.



	(Chen et., 2016)	(Chen et., 2019b)	MUST
PCE	6.3	1.5	0.0005
TCE	20.1	7.6	0.001
DCE	87.2	25.1	0.003
VC	103.3	62.1	0.01
ETH	184.9	125.3	0.02

MUST can use different types of inlet source boundary conditions.

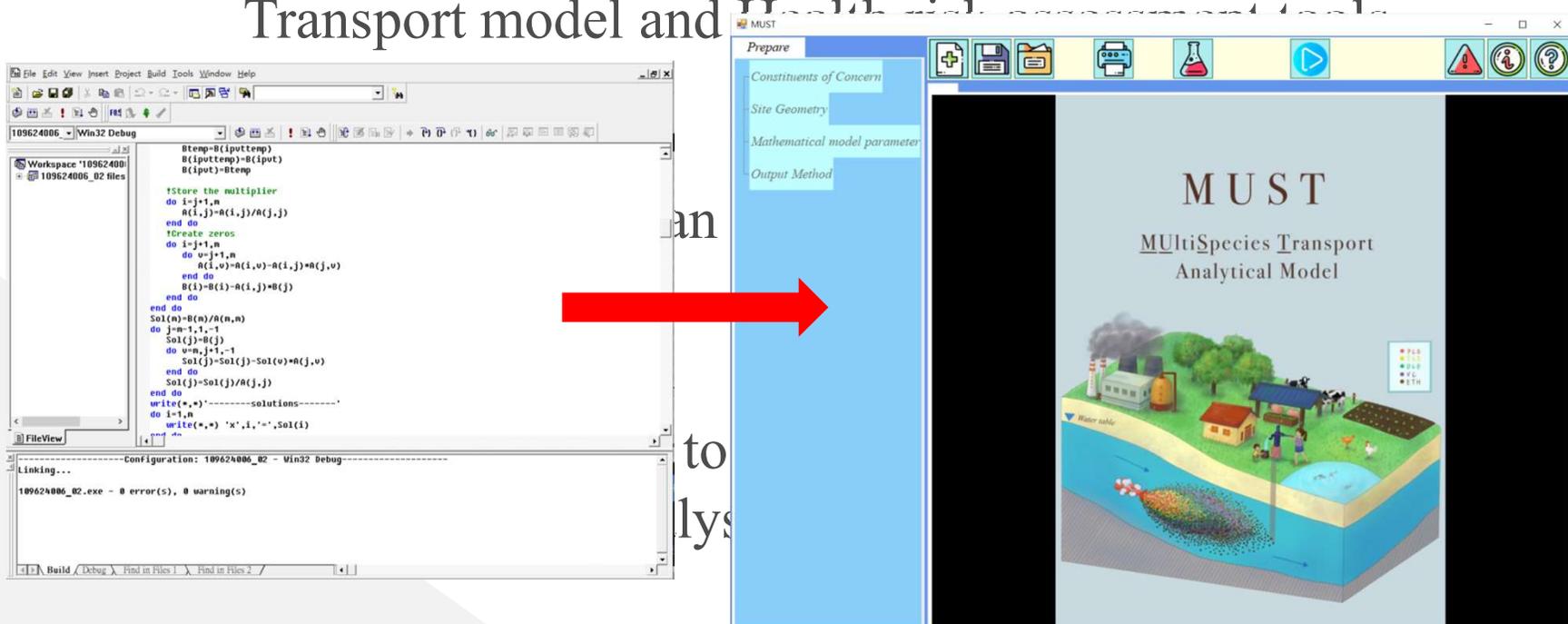
MUST can use constant, Exponential decay, and Arbitrary time-dependents for source conditions.



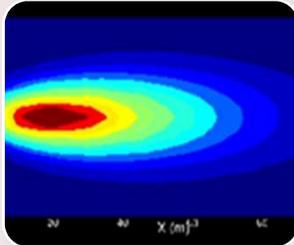
<sup>d</sup> Department of Nursing, Fooyin University, Daliao

# Graphical User Interface

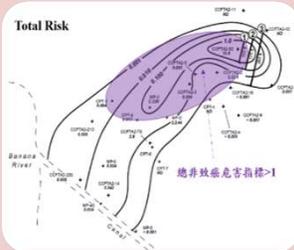
- Fortran programming language is often used to develop Transport model and Health risk assessment tools



# Objective



MUlti-Species Transport (MUST)



Development of Health risk assessment



Graphical User Interface

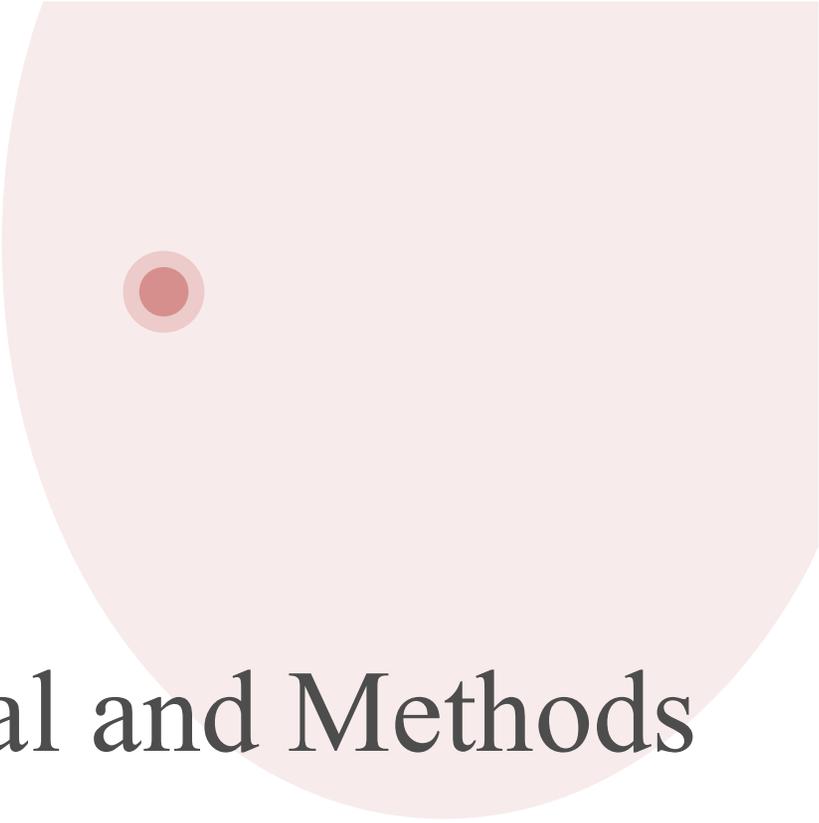
# Objective

- To develop a computer software for **human health risk assessment** of a chlorinated solvent contaminated groundwater site using **the most advanced multispecies transport analytical model (MUST)** equipped with a **user-friendly graphical interface**.



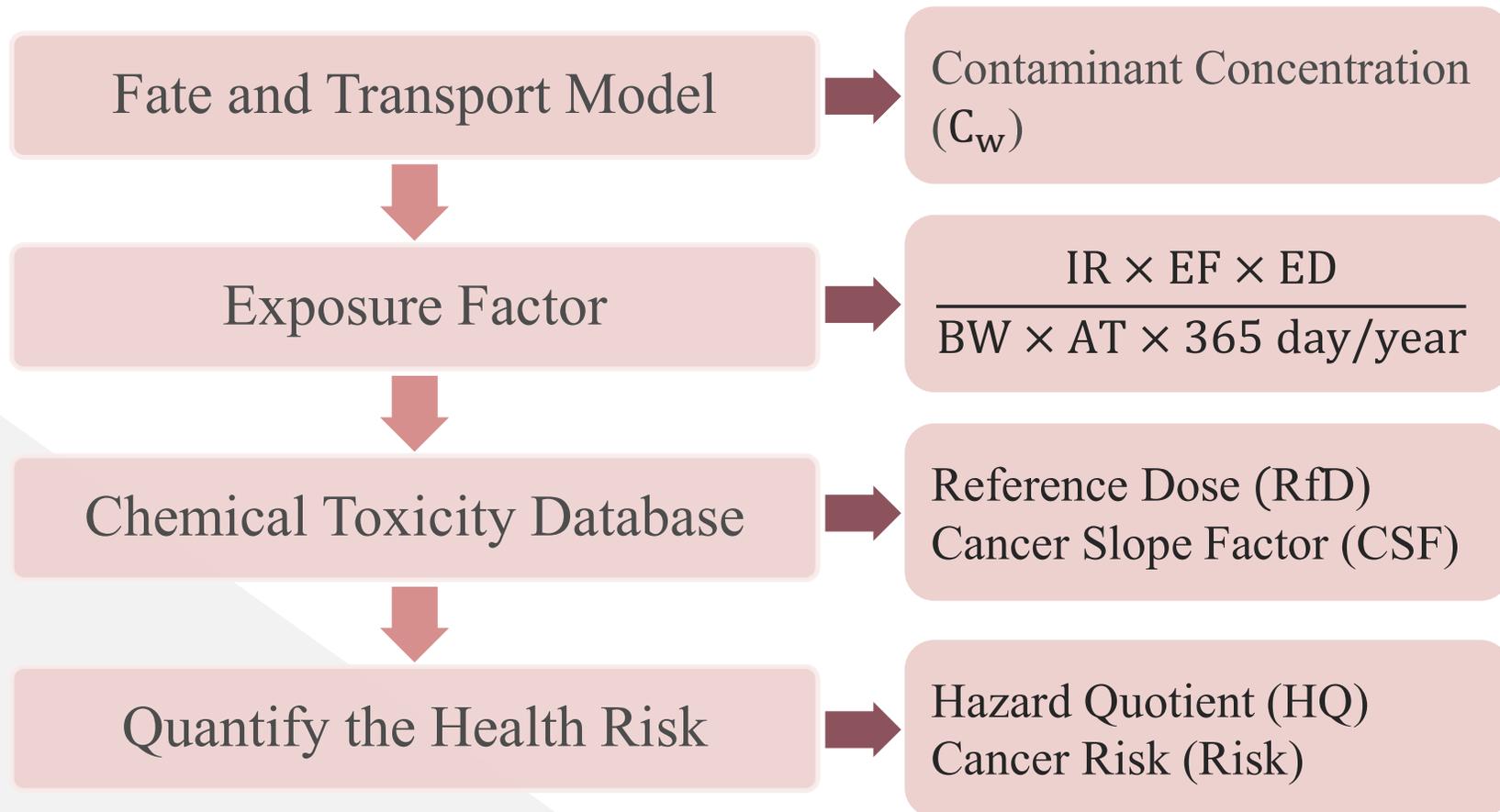


2



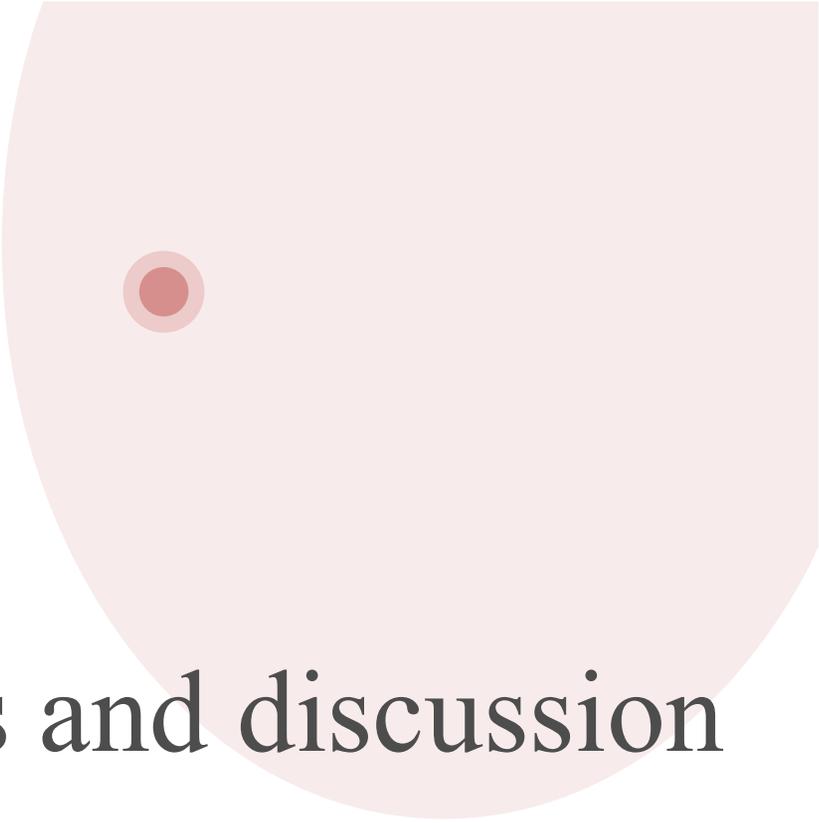
## Material and Methods

# Flow chart





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## Results and discussion

# Constituents of concern

1.  Example - Chlorinated Solvents

1.  Others

2. Number of Compounds

1  2  3  4  5

C1 → C2 → C3 → C4 → C5

Constituents of Concern

C1	<input type="text" value="C1"/>
C2	<input type="text" value="C2"/>
C3	<input type="text" value="C3"/>
C4	<input type="text" value="C4"/>
C5	<input type="text" value="C5"/>

After opening a new file, the workspace will appear. First, choose the Constituents of concern.

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# Mathematical model parameter - Source

1. Source

2. Dimensions

Input the dimension and Model size.

Mathematical model parameters are divided into Source and Plume. After clicking the button, the button will turn yellow, showing the position of this page.

Obs Well  
Dx = 100 (m) / 17

# Step 3. Mathematical model parameter - Source

1. Click Boundary.

2. Choose first - or third -type inlet source boundary conditions.

3.  $V = 0 \text{ (m/s)}$

18  
Dx = 0 (m/s) yd

# Step 3. Mathematical model parameter - Source

MUST

Prepare

- Constituents of Concern
- Site Geometry
- Mathematical model parameter
- Output Method

1. **Source** | Plume

Dimensions | Boundary | **Source** | Source Function | Source Concentration

2. Number of sources

1  2  3  4  5

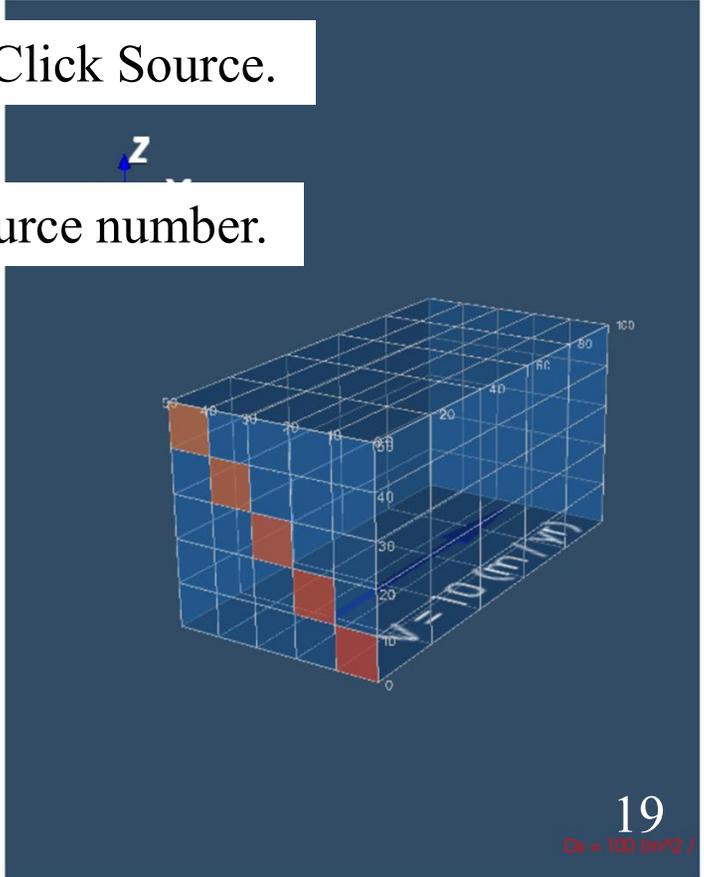
3. **Source 1** | Source 2 | Source 3 | Source 4 | Source 5

Y1 0 (m) Z1 0 (m)  
Y2 10 (m) Z2 10 (m)

Click Source.

Choose the Source number.

Input the Source dimension.



19  
Ck = 100 (m<sup>2</sup>)

# Step 3. Mathematical model parameter - Source

1. Click Source Function

2. If click Exponential decay, Choose the Source Function. of Source decay will appear.

3. Input the Source decay.

Source Condition

Constant

Exponential decay

Arbitrary time-dependents

Source decay

PCE

TCE

DCE

VC

ETH

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# Step 4. Mathematical model parameter - Plume

MUST

Prepare

Constituents of Concern

Site Geometry

Mathematical model parameter

Output Method

1.

2.

Source Plume

Transport parameter

Decay and Retardation

Click Decay and Retardation.

Decay Constant (Unit: (1/yr))

Occur in aqueous phase

Occur in both aqueous and sorbed phase

$K_{PCE}$

$K_{TCE}$

$K_{DCE}$

$K_{VC}$

$K_{ETH}$

Species-specific Retardation Factor (Unit: (-))

$R_{PCE}$

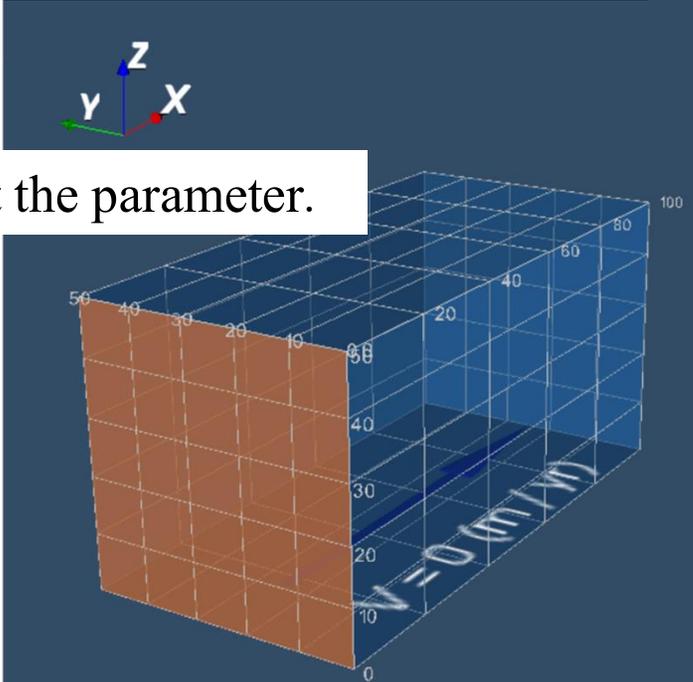
$R_{TCE}$

$R_{DCE}$

$R_{VC}$

$R_{ETH}$

Input the parameter.



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$D_x = 0 \text{ (m}^2/\text{yr)}$

The image shows a software interface for setting model parameters. A sidebar on the left lists 'Constituents of Concern', 'Site Geometry', 'Mathematical model parameter', and 'Output Method'. The 'Mathematical model parameter' section is active, showing 'Source' as 'Plume'. Two tabs are visible: 'Transport parameter' and 'Decay and Retardation'. A red box highlights the 'Decay and Retardation' tab, and a callout points to it with the text 'Click Decay and Retardation.' Below this, another red box highlights the input fields for 'Decay Constant' and 'Species-specific Retardation Factor'. A callout points to these fields with the text 'Input the parameter.' To the right, a 3D grid diagram shows a rectangular prism with axes X, Y, and Z. The Z-axis is vertical, X is horizontal, and Y is depth. A value of 0.001 yr<sup>-1</sup> is displayed on the grid. At the bottom right, the page number '21' and the text 'D<sub>x</sub> = 0 (m<sup>2</sup>/yr)' are visible.

# Step 5. Output Method

The screenshot displays the MUST software interface for configuring the output method. The sidebar on the left lists the following options: *Constituents of Concern*, *Site Geometry*, *Mathematical model parameter*, and *Output Method*. The main panel is divided into tabs: *Constituents of Concern*, *Site Geometry*, *Mathematical model parameter*, and *Output Method*. The *Output Method* tab is active, showing the following configuration options:

- Observation type:** Three radio button options: *Point*, *Concentration contour on plane*, and *Concentration profile along line*. The *Concentration profile along line* option is selected.
- Observation Location:** A section containing:
  - Simulation Time* (Unit: (yr)) with an input field.
  - Concentration profile along line* (Unit: (m)) with an input field.
  - Profile direction:** Three radio button options: *X-direction*, *Y-direction*, and *Z-direction*. The *X-direction* option is selected.
  - Input fields for *X0*, *Y*, *XL*, and *Z*.

On the right side of the interface, a 3D grid visualization is shown with axes labeled X, Y, and Z. A red line is drawn along the X-axis, and a blue line is drawn along the Z-axis. The grid is labeled with values from 0 to 100. A text box at the bottom right of the grid area contains the text "V = 10 (m/s)".

1. *Concentration profile along line*

2. *Simulation Time* (Unit: (yr))

*Concentration profile along line* (Unit: (m))

*Profile direction*

*X-direction* *Y-direction* *Z-direction*

*X0* *Y*

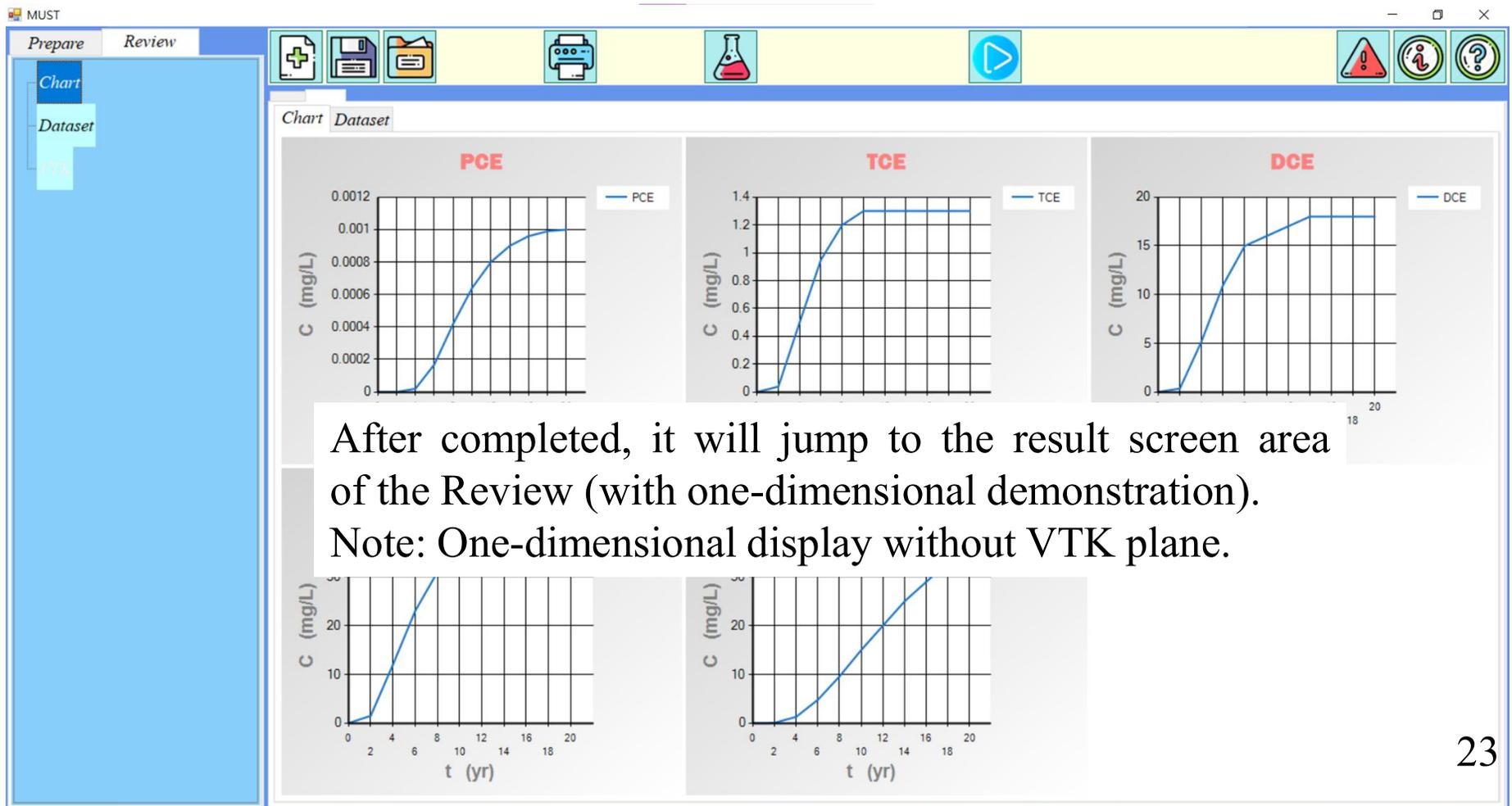
*XL* *Z*

If click *Concentration profile along line*, the lower input area will display the profile along line input area.

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Dx = 100 (m) /

# Step 6. Result - Chart



After completed, it will jump to the result screen area of the Review (with one-dimensional demonstration).

Note: One-dimensional display without VTK plane.

# Step 6. Result - Dataset

1.

Click Dataset to move to Dataset result.

PCE	
t (yr)	C (mg /L)
1E-10	0
2	2.1E-08
8	0.00042
10	0.00064
12	0.0008

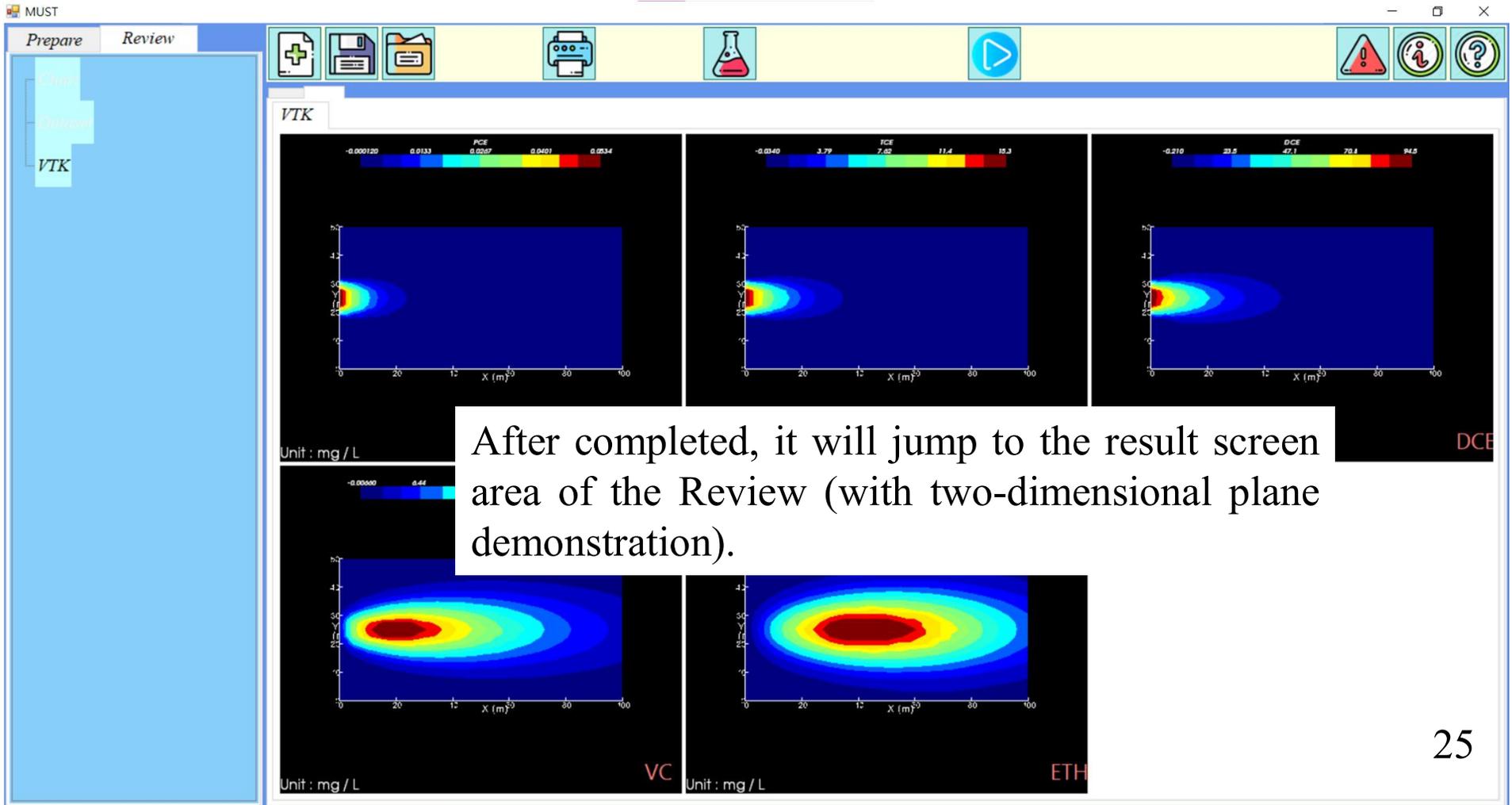
TCE	
t (yr)	C (mg /L)
1E-10	0
2	0.039
8	1.2
10	1.3
12	1.3

DCE	
t (yr)	C (mg /L)
1E-10	0
2	0.36
4	5.2
6	11
8	15
10	16
12	17

VC	
t (yr)	C (mg /L)
1E-10	0
2	1.5
4	12
6	23
8	31
10	35
12	37

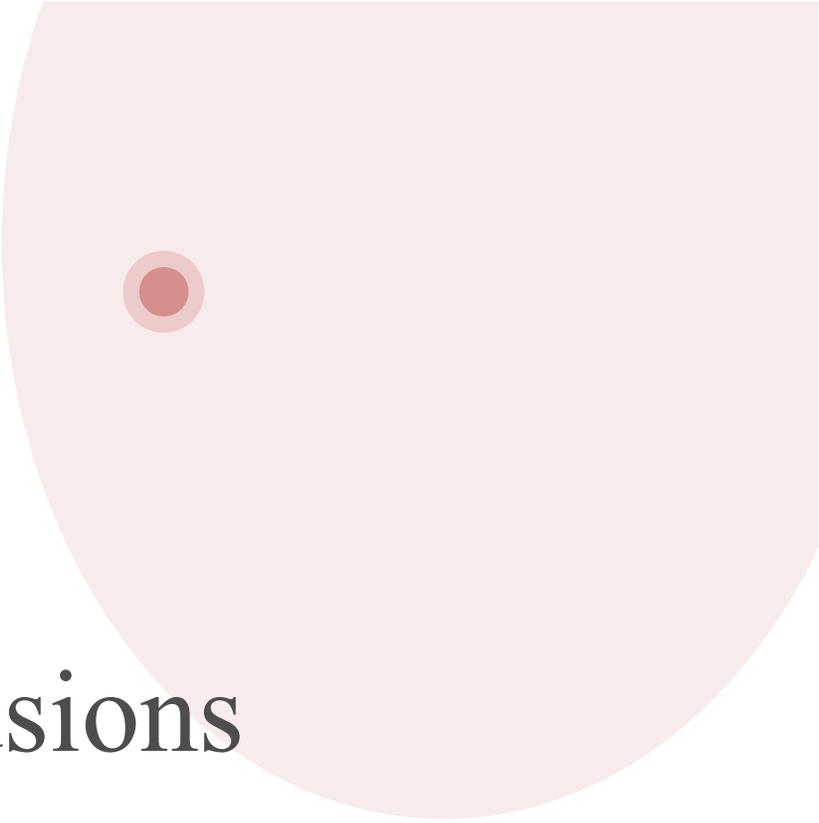
ETH	
t (yr)	C (mg /L)
1E-10	0
2	0.054
4	1.3
6	4.8
8	9.6
10	15
12	20

# Step 6. Result - VTK





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# Conclusions

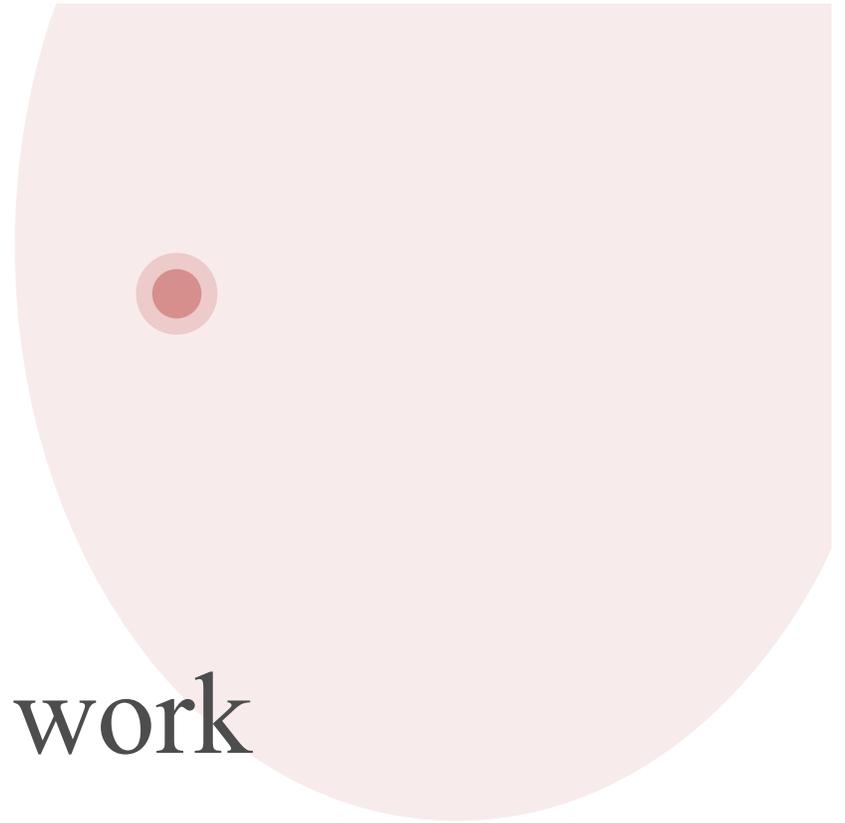


# Conclusions

- Now the Software is being tested and optimized.
- Establishing a friendly interactive interface and visual display module will be more conducive to risk communication and risk management.



## Future work



# Future work

- To make the software easier to use, compare the user interface with HYDROSCAPE and optimize the software interface.

## HYDROSCAPE

The screenshot shows the HYDROSCAPE software interface with the following configuration options:

- X-Length (m): 100
- Y-Length (m): 25
- Z-Height (m): 10
- Time (yr): 4
- Nodes: 64
- Discretization (X): 20
- Discretization (Y): 20
- Discretization (Z): 5
- Discretization (t): 10
- Preferred Units:  Years,  Days,  Seconds
- Preferred Concentration Units:  Relative (C/Cmax),  Absolute (mg/L)
- Background Noise Level (mg/L): 0.01

Buttons: Previous, Calculate, Estimate Time, Next

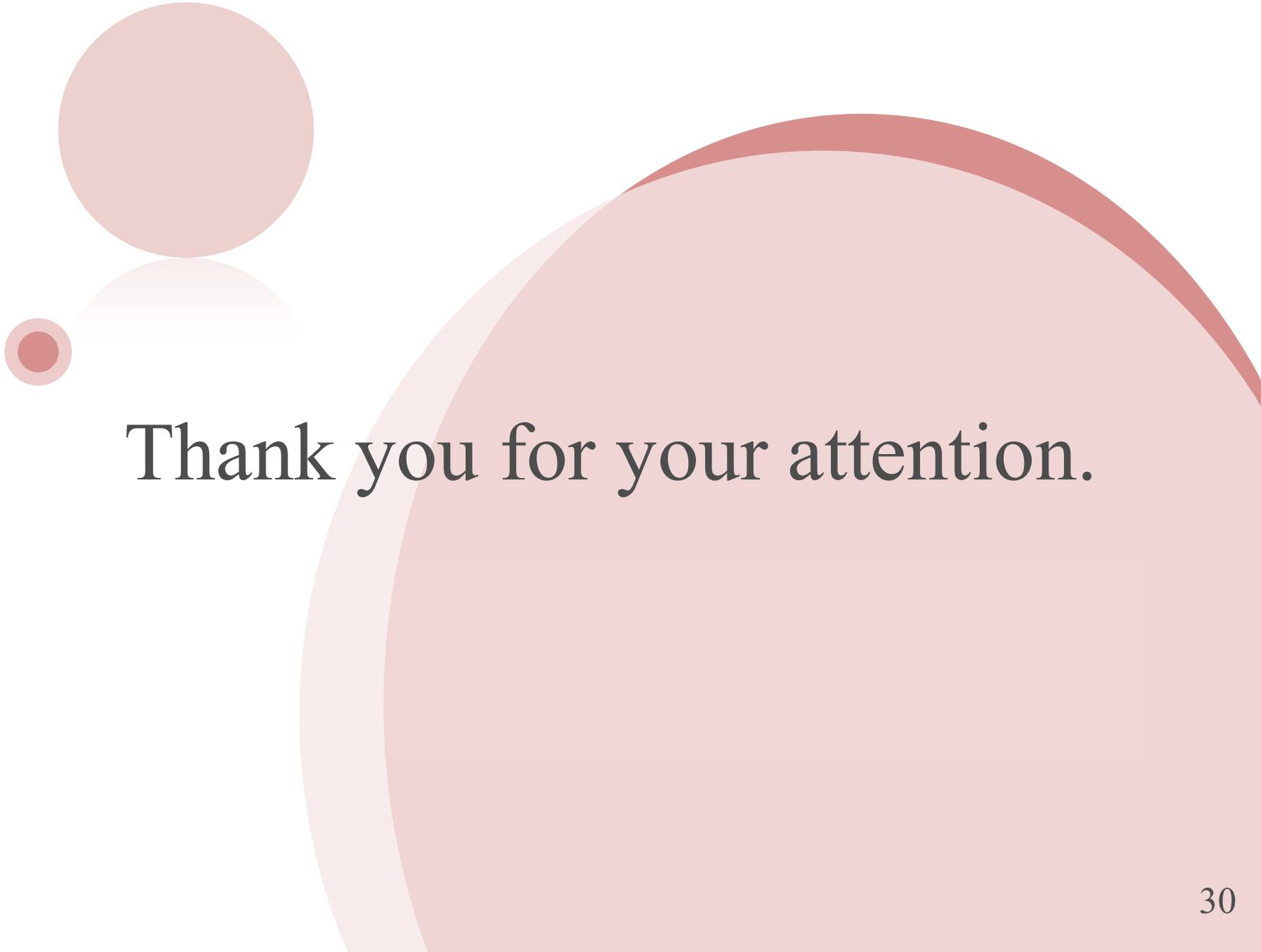
## Risk Assessment Software

The screenshot shows the MUST software interface with the following configuration options:

- Constituent of concerns
- Geometry
- Source
- Transport Properties
- Output Method
- Model Configuration

	Variable	Value	Unit
X-Length	L	100	m
Y-Length	W	80	m
Z-Height	H	80	m

3D visualization of the domain with dimensions: L=100(m), W=80(m), H=80(m).

A decorative graphic consisting of several overlapping circles and a large semi-circle. The circles are in shades of light red and pink. The semi-circle is a darker shade of red and is positioned on the right side of the slide, partially overlapping the text.

Thank you for your attention.