Problems with the Domenico Solution for Contaminant Transport in Groundwater and Regulatory Implications on Risk Assessments

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RPIC 2008, Vancouver

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Outline

- What is the Domenico solution?
- What are the issues?
- Regulatory advice
- Next steps

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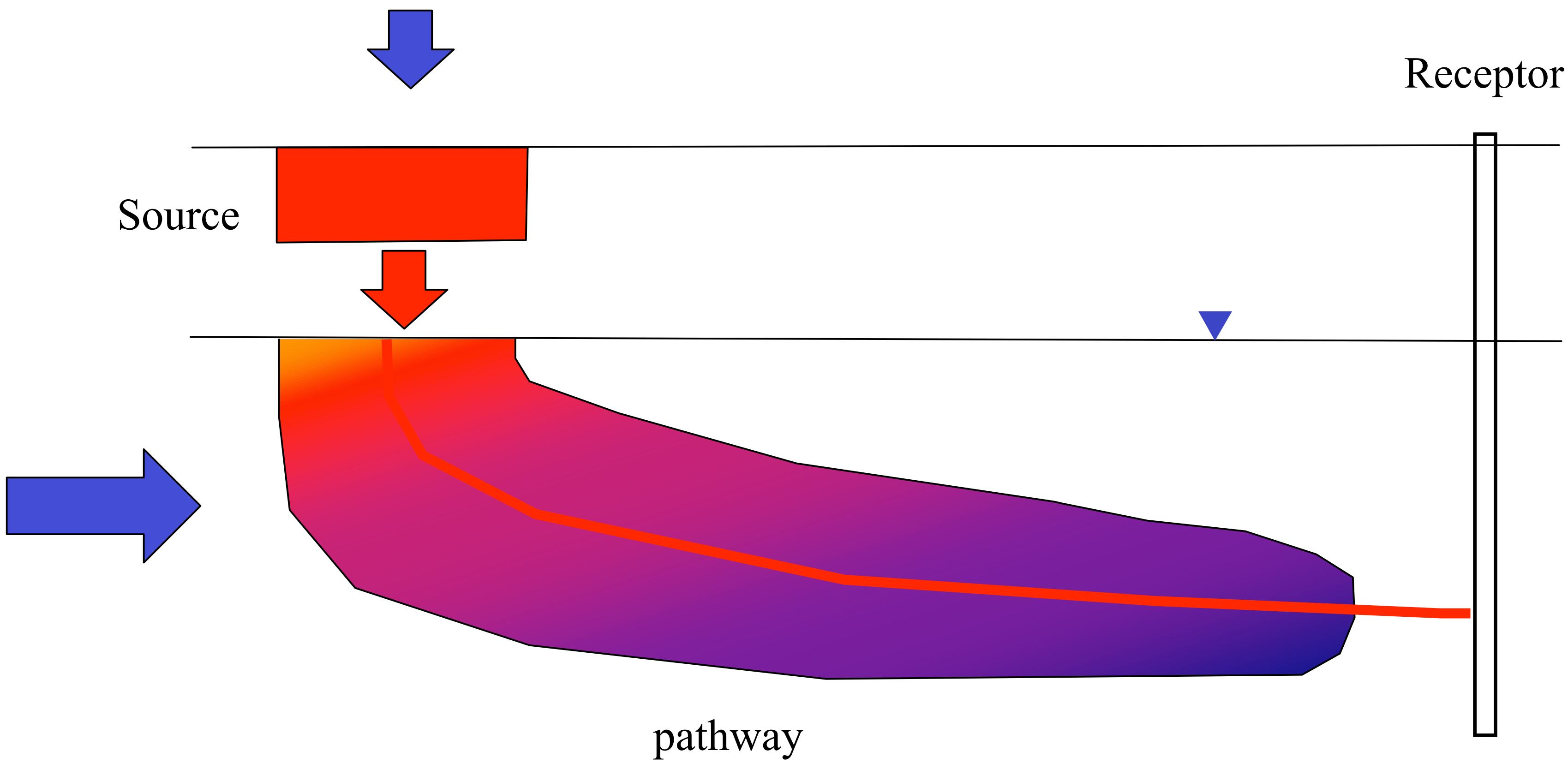
Let me be clear…

- This presentation will show that the Domenico solution does not solve the solute transport equation exactly
- This was understood and acknowledged by Dr. Domenico
- The Domenico solution has been and remains an important tool for our work
- My intent is to provide a better understanding of its limitations

Model Applications in Risk Assessment

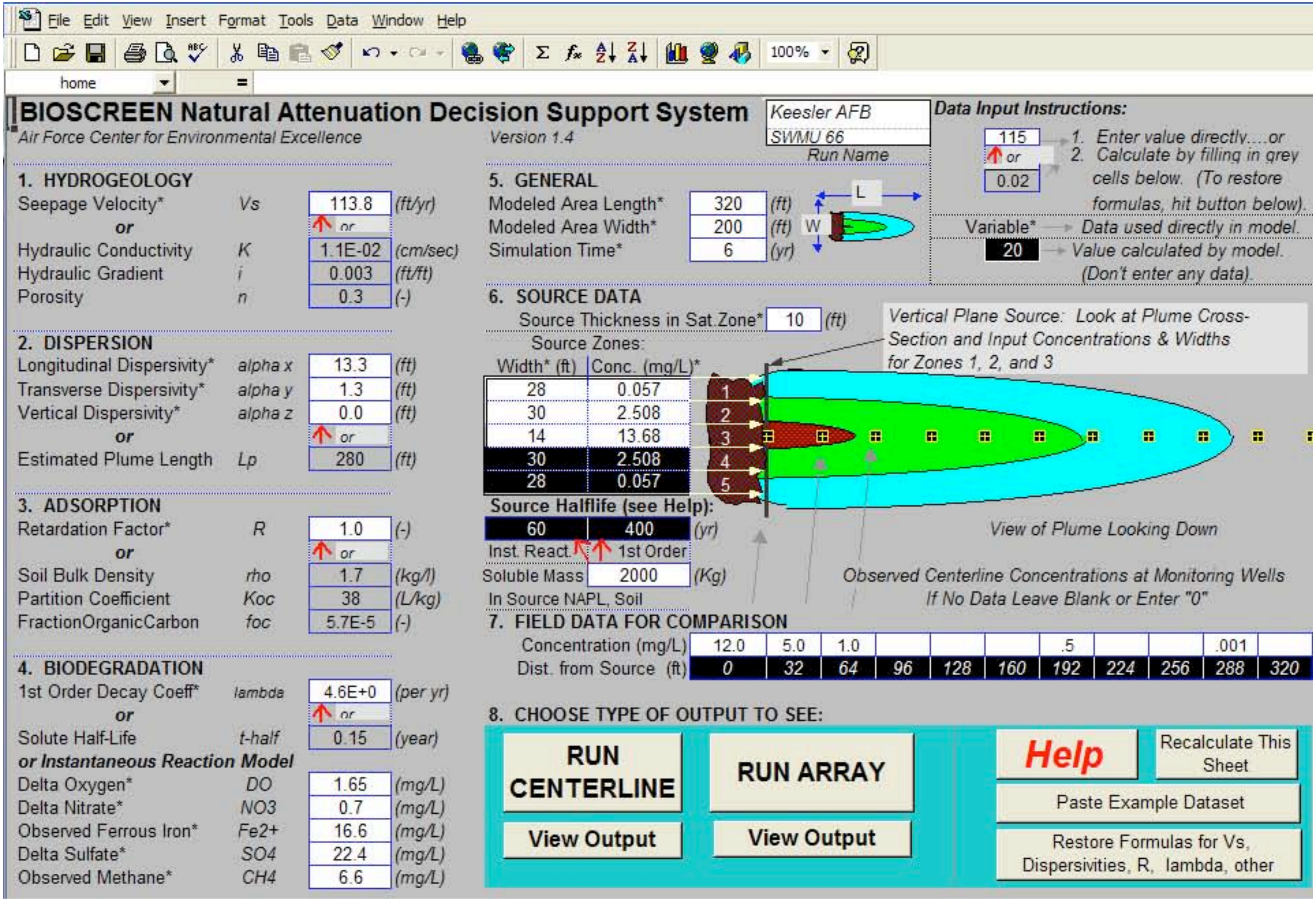


Domenico Solution

- Approximate solution of transport equation for a dissolved contaminant
  - Advection
  - Dispersion
  - Linear isothermal adsorption
  - First order biodegradation
- Extensions of the Domenico solution allow
  - Finite source
  - Instantaneous decay
  - Sequential decay reactions (e.g. chlorinated solvents)

Common applications of the Domenico solution

- BIOSCREEN
- BIOCHLOR
- RBCA Toolkit
- ASTM standards
- CCME, Ontario, Alberta, BC – used for setting regulatory criteria & standards
- It is in almost all risk assessment software packages

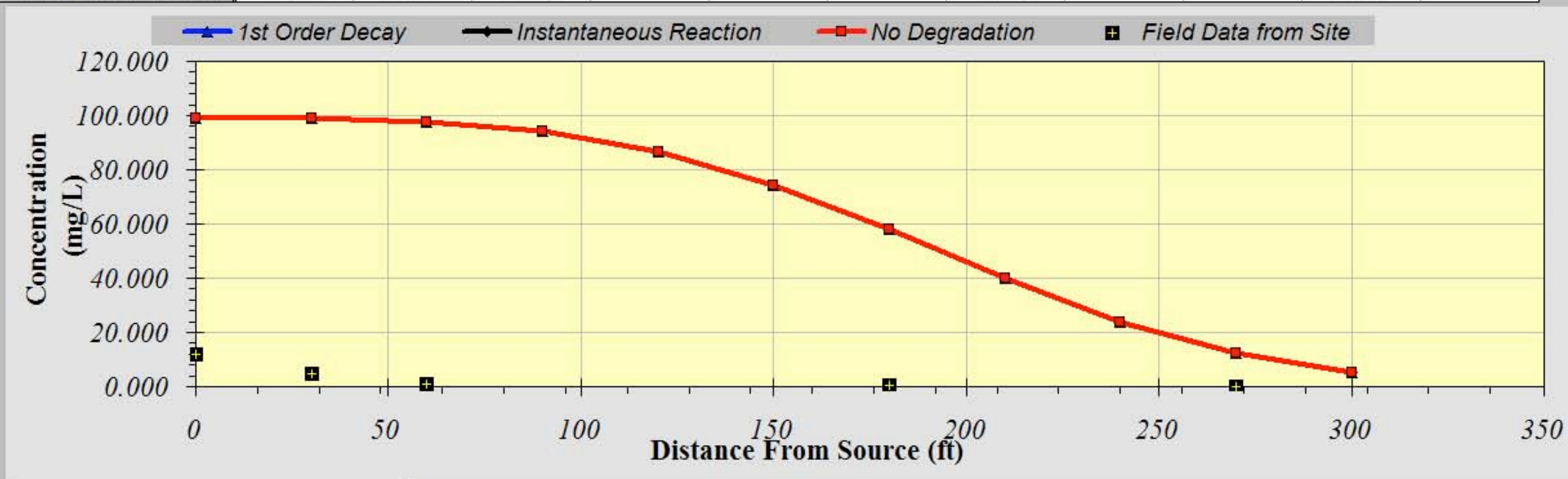


File Edit View Insert Format Tools Data Window Help
home
BIOSCREEN Natural Attenuation Decision Support System
Air Force Center for Environmental Excellence
Version 1.4
Keesler AFB
SWMU 66
Run Name
Data Input Instructions:
115
or
0.02
1. Enter value directly....or
2. Calculate by filling in grey cells below. (To restore formulas, hit button below).
Variable* → Data used directly in model.
20 → Value calculated by model. (Don't enter any data).
1. HYDROGEOLOGY
Seepage Velocity* Vs 113.8 (ft/yr)
or
Hydraulic Conductivity K 1.1E-02 (cm/sec)
Hydraulic Gradient i 0.003 (ft/ft)
Porosity n 0.3 (-)
2. DISPERSION
Longitudinal Dispersivity* alpha x 13.3 (ft)
Transverse Dispersivity* alpha y 1.3 (ft)
Vertical Dispersivity* alpha z 0.0 (ft)
or
Estimated Plume Length Lp 280 (ft)
3. ADSORPTION
Retardation Factor* R 1.0 (-)
or
Soil Bulk Density rho 1.7 (kg/l)
Partition Coefficient Koc 38 (L/kg)
FractionOrganicCarbon foc 5.7E-5 (-)
4. BIODEGRADATION
1st Order Decay Coeff* lambda 4.6E+0 (per yr)
or
Solute Half-Life t-half 0.15 (year)
or Instantaneous Reaction Model
Delta Oxygen* DO 1.65 (mg/L)
Delta Nitrate* NO3 0.7 (mg/L)
Observed Ferrous Iron* Fe2+ 16.6 (mg/L)
Delta Sulfate* SO4 22.4 (mg/L)
Observed Methane* CH4 6.6 (mg/L)
5. GENERAL
Modeled Area Length* 320 (ft)
Modeled Area Width* 200 (ft)
Simulation Time* 6 (yr)
L
W
6. SOURCE DATA
Source Thickness in Sat.Zone* 10 (ft)
Source Zones:
Width* (ft) Conc. (mg/L)*
28 0.057
30 2.508
14 13.68
30 2.508
28 0.057
1
2
3
4
5
Vertical Plane Source: Look at Plume Cross-Section and Input Concentrations & Widths for Zones 1, 2, and 3
Source Halflife (see Help):
60 400 (yr)
Inst. React. 1st Order
Soluble Mass 2000 (Kg)
In Source NAPL, Soil
View of Plume Looking Down
Observed Centerline Concentrations at Monitoring Wells
If No Data Leave Blank or Enter "0"
7. FIELD DATA FOR COMPARISON
Concentration (mg/L) 12.0 5.0 1.0 .5 .001
Dist. from Source (ft) 0 32 64 96 128 160 192 224 256 288 320
8. CHOOSE TYPE OF OUTPUT TO SEE:
RUN CENTERLINE
View Output
RUN ARRAY
View Output
Help
Recalculate This Sheet
Paste Example Dataset
Restore Formulas for Vs, Dispersivities, R, lambda, other

DISSOLVED HYDROCARBON CONCENTRATION ALONG PLUME CENTERLINE (mg/L at Z=0)

Distance from Source (ft)

TYPE OF MODEL	0	30	60	90	120	150	180	210	240	270	300
No Degradation	99.125	98.933	97.811	94.067	86.502	74.350	58.119	40.209	24.039	12.210	5.197
1st Order Decay	99.125	98.933	97.811	94.067	86.502	74.350	58.119	40.209	24.039	12.210	5.197
Inst. Reaction	99.125	98.933	97.811	94.067	86.502	74.350	58.119	40.209	24.039	12.210	5.197
Field Data from Site	12.000	5.000	1.000				0.500			0.001	



Calculate Animation

Time: 20 Years

Return to Input

Recalculate This Sheet

Why is it so widespread?

- It is much simpler than the exact solution
- It could be programmed directly within EXCEL (EXCEL 5)
- This is no longer a restriction
  - EXCEL can now run external programs and return results
  - Exact solution can now be programmed

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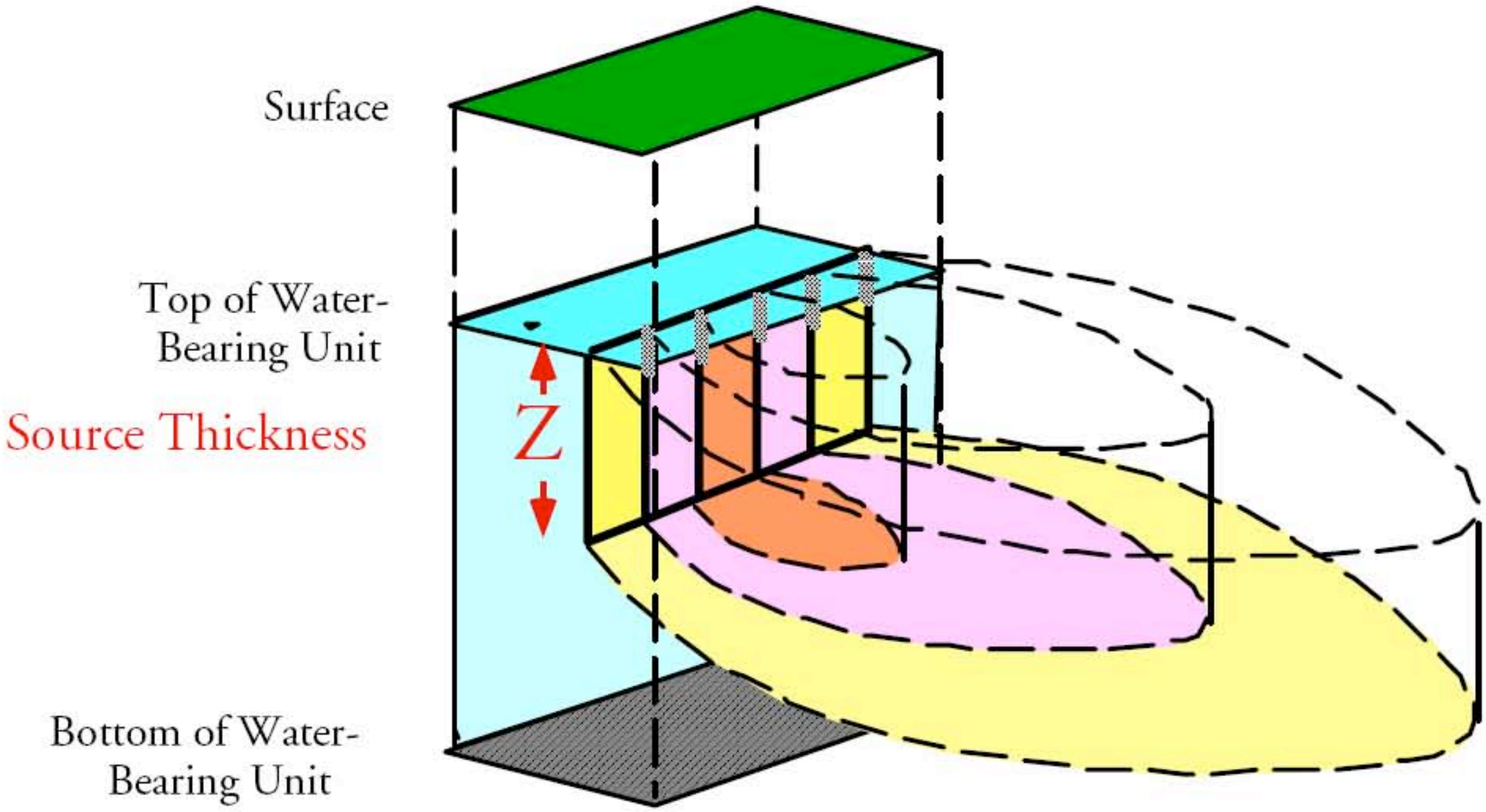
3-D Solute Transport Equation

$$R\frac{\partial c}{\partial t} = -v\frac{\partial c}{\partial x} + D_x\frac{\partial^2 c}{\partial x^2} + D_y\frac{\partial^2 c}{\partial y^2} + D_z\frac{\partial^2 c}{\partial z^2} - \lambda_{\mathrm{EFF}}c$$

Sorption Advection Dispersion Degradation

BIOSCREEN Conceptual Model



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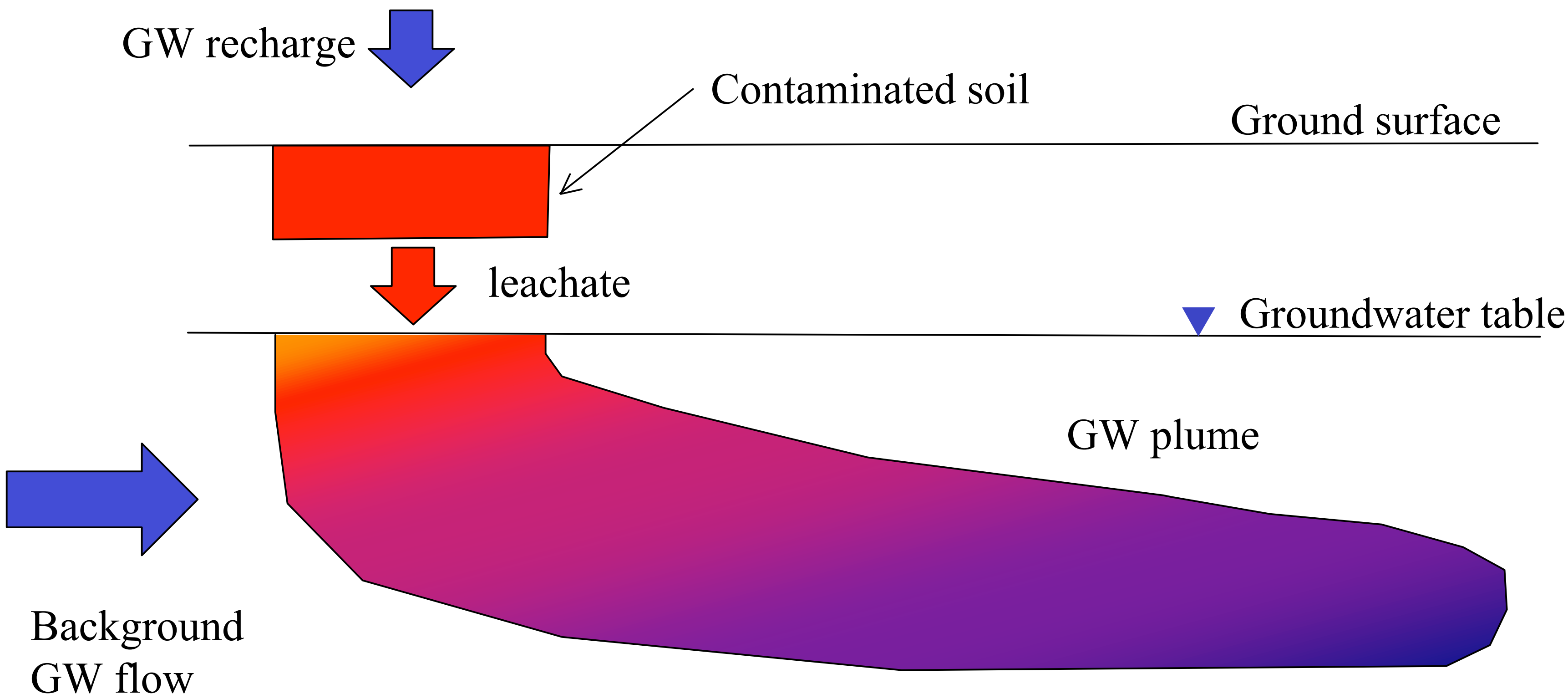
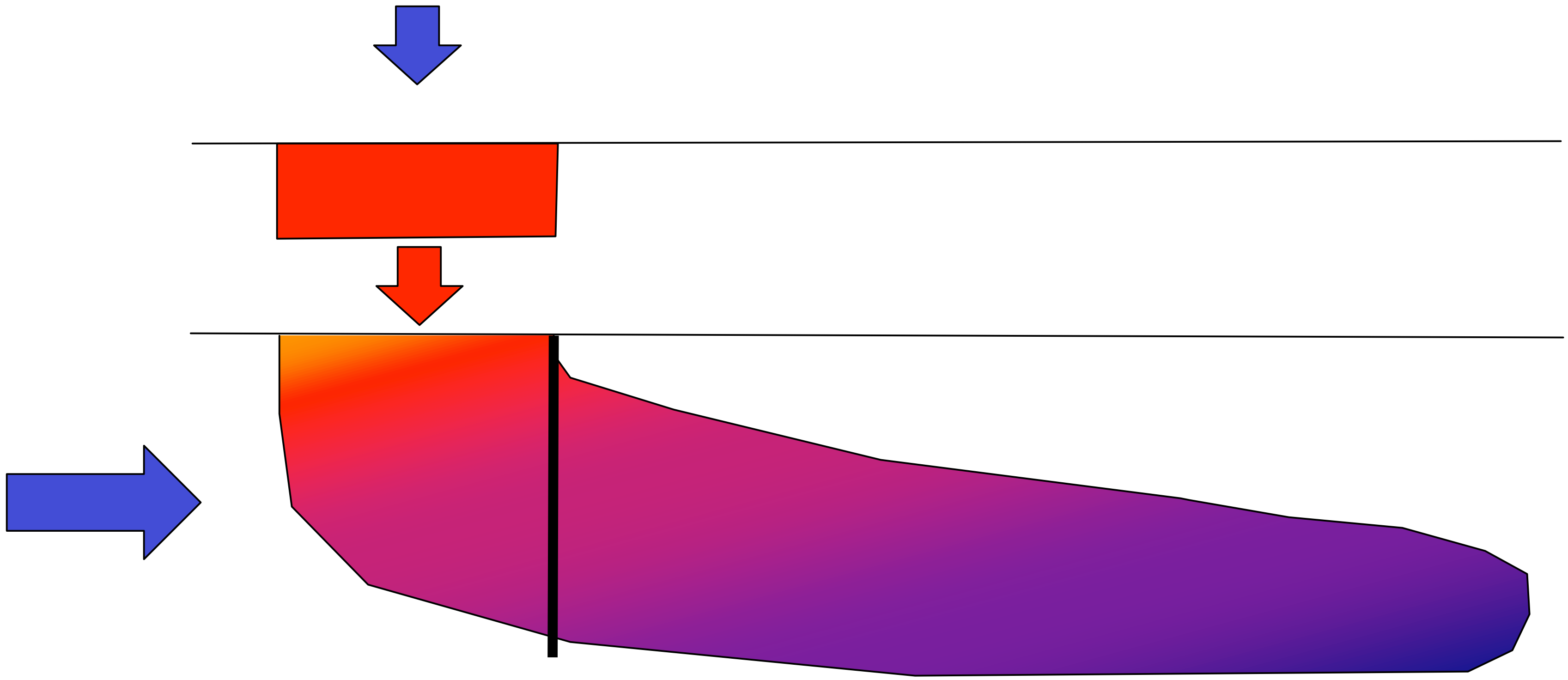
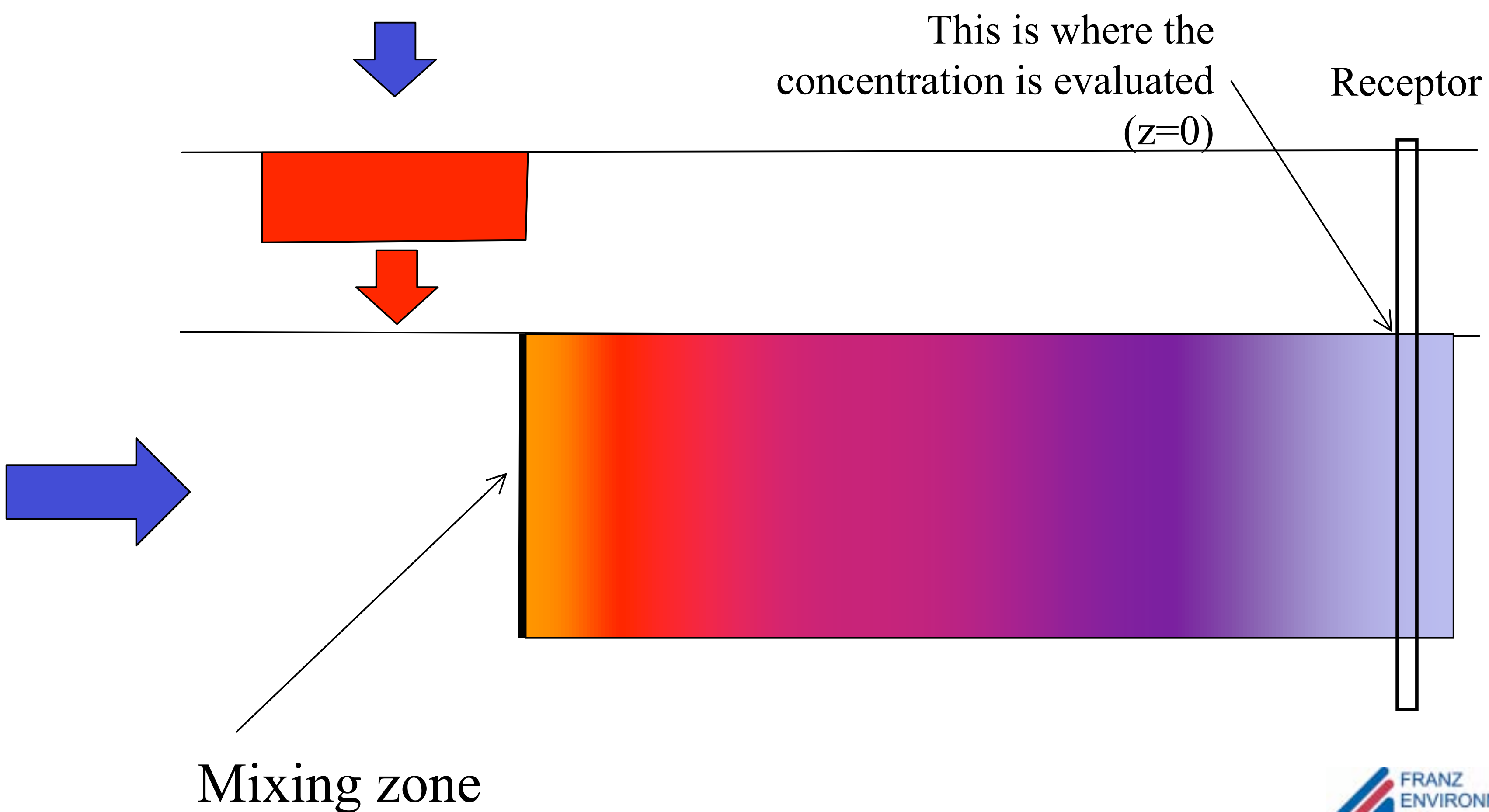
Conceptual Model



Actual BIOSCREEN Conceptual Model



Actual BIOSCREEN Conceptual Model



Exact Solution (Cleary & Ungs, 1978)

$$c(x,y,z,t) = \frac{c_o}{8}\int_{\tau=0}^{\tau=t} f_x'(x,\tau) f_y'(y,\tau) f_z'(z,\tau)\,\mathrm{d}\tau,$$

$$\text{where } f_x'(x,\tau) = \frac{x}{\sqrt{\pi D_x}}\exp\left(\frac{vx}{2D_x}\right) \times \frac{\exp\left(\frac{-v^2}{4D_x}\tau - k\tau + \frac{-x^2}{4D_x\tau}\right)}{\tau^{3/2}}$$

$$f_y'(y,\tau) = \left[\operatorname{erf}\left\{\frac{y+\frac{Y}{2}}{2(D_y\tau)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{y-\frac{Y}{2}}{2(D_y\tau)^{1/2}}\right\}\right]$$

$$f_z'(z,\tau) = \left[\operatorname{erf}\left\{\frac{z+\frac{Z}{2}}{2(D_z\tau)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{z-\frac{Z}{2}}{2(D_z\tau)^{1/2}}\right\}\right]$$

Domenico (1987)

$$c(x,y,z,t) = \frac{c_o}{8} f_x(x,t) f_y(y,x) f_z(z,x),$$

$$\text{where } f_x(x,t) = \left(\exp\left\{ \frac{x}{2\alpha_x} \left[1 - \left(1 + \frac{4k\alpha_x}{v} \right)^{1/2} \right] \right\} \right.$$

$$\left. \times \operatorname{erfc}\left\{ \frac{x - vt\left(1 + \frac{4k\alpha_x}{v} \right)^{1/2}}{2(\alpha_x vt)^{1/2}} \right\} \right)$$

$$f_y(y,x) = \left[\operatorname{erf}\left\{ \frac{y + \frac{Y}{2}}{2(\alpha_y x)^{1/2}} \right\} - \operatorname{erf}\left\{ \frac{y - \frac{Y}{2}}{2(\alpha_y x)^{1/2}} \right\} \right]$$

$$f_z(z,x) = \left[\operatorname{erf}\left\{ \frac{z + \frac{Z}{2}}{2(\alpha_z x)^{1/2}} \right\} - \operatorname{erf}\left\{ \frac{z - \frac{Z}{2}}{2(\alpha_z x)^{1/2}} \right\} \right]$$

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Exact Solution (Cleary & Ungs, 1978)

$$c(x,y,z,t) = \frac{c_o}{8}\int_{\tau=0}^{\tau=t} f_x'(x,\tau) f_y'(y,\tau) f_z'(z,\tau)\,\mathrm{d}\tau,$$

$$\text{where } f_x'(x,\tau) = \frac{x}{\sqrt{\pi D_x}} \exp\left(\frac{vx}{2D_x}\right) \times \frac{\exp\left(\frac{-v^2}{4D_x}\tau - k\tau + \frac{-x^2}{4D_x\tau}\right)}{\tau^{3/2}}$$

$$f_y'(y,\tau) = \left[\operatorname{erf}\left\{\frac{y+\frac{Y}{2}}{2(D_y\tau)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{y-\frac{Y}{2}}{2(D_y\tau)^{1/2}}\right\}\right]$$

$$f_z'(z,\tau) = \left[\operatorname{erf}\left\{\frac{z+\frac{Z}{2}}{2(D_z\tau)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{z-\frac{Z}{2}}{2(D_z\tau)^{1/2}}\right\}\right]$$

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Test Run 1

- v = 10 ft/yr
- a_L = 10 ft
- a_T=1 ft
- a_V=0.1 ft
- No sorption
- No degradation

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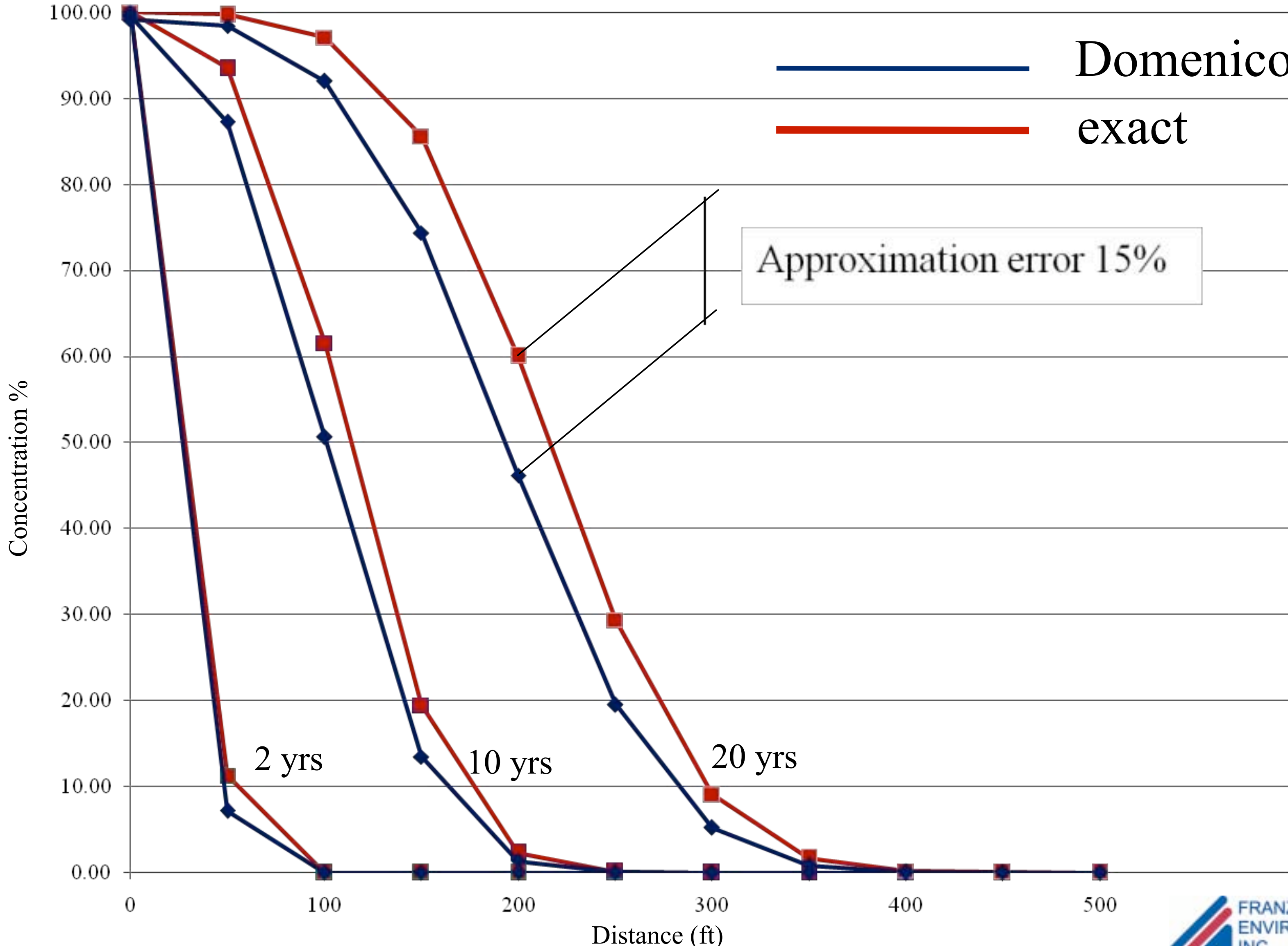

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Test Run 2

- v = 1 ft/yr
- $a_L = 20$ ft
- $a_T=2$ ft
- $a_V=0.2$ ft
- No sorption
- No degradation

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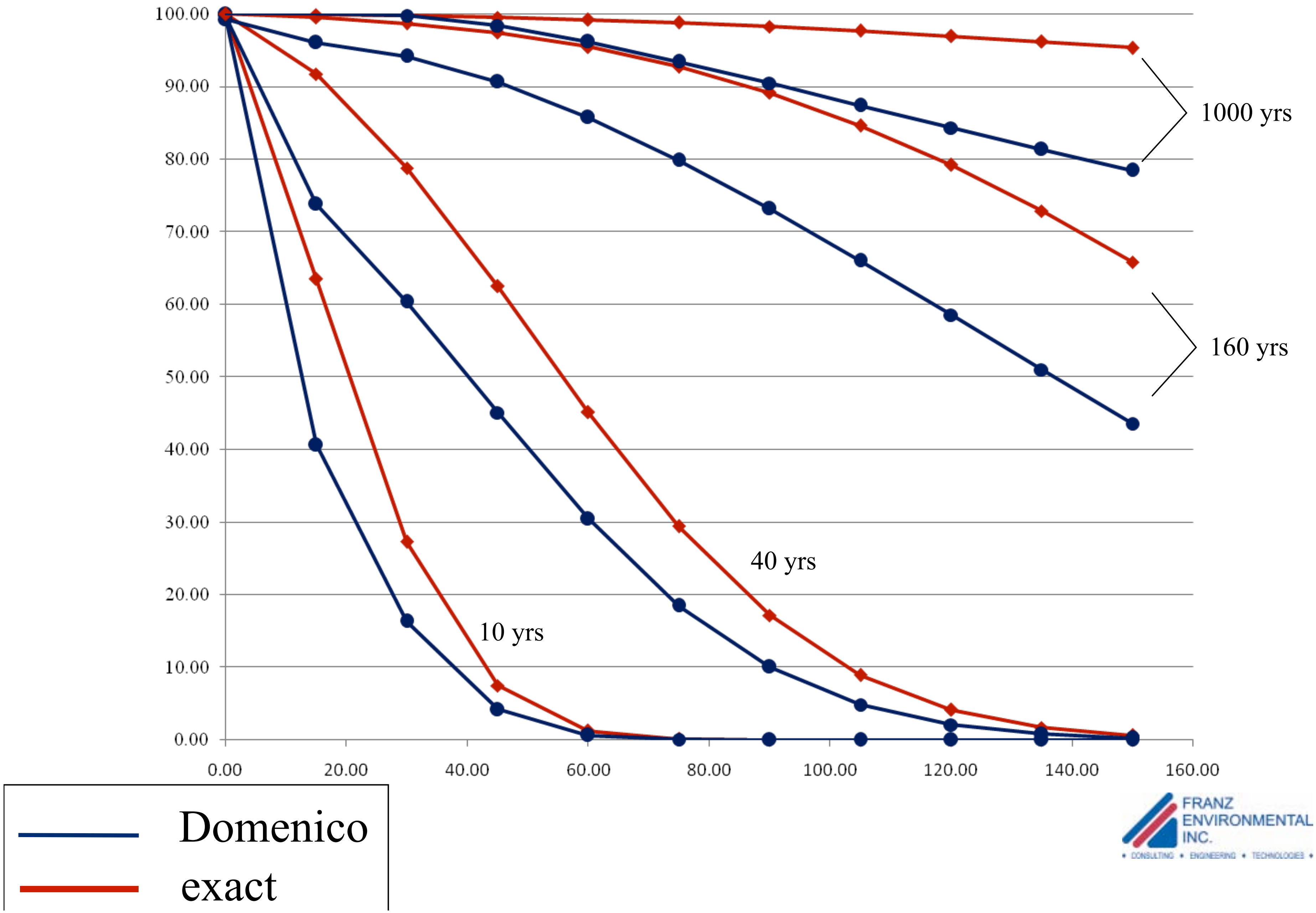

100.00
90.00
80.00
70.00
60.00
50.00
40.00
30.00
20.00
10.00
0.00
0.00
20.00
40.00
60.00
80.00
100.00
120.00
140.00
160.00
1000 yrs
160 yrs
40 yrs
10 yrs
Domenico
exact

Regulatory Response

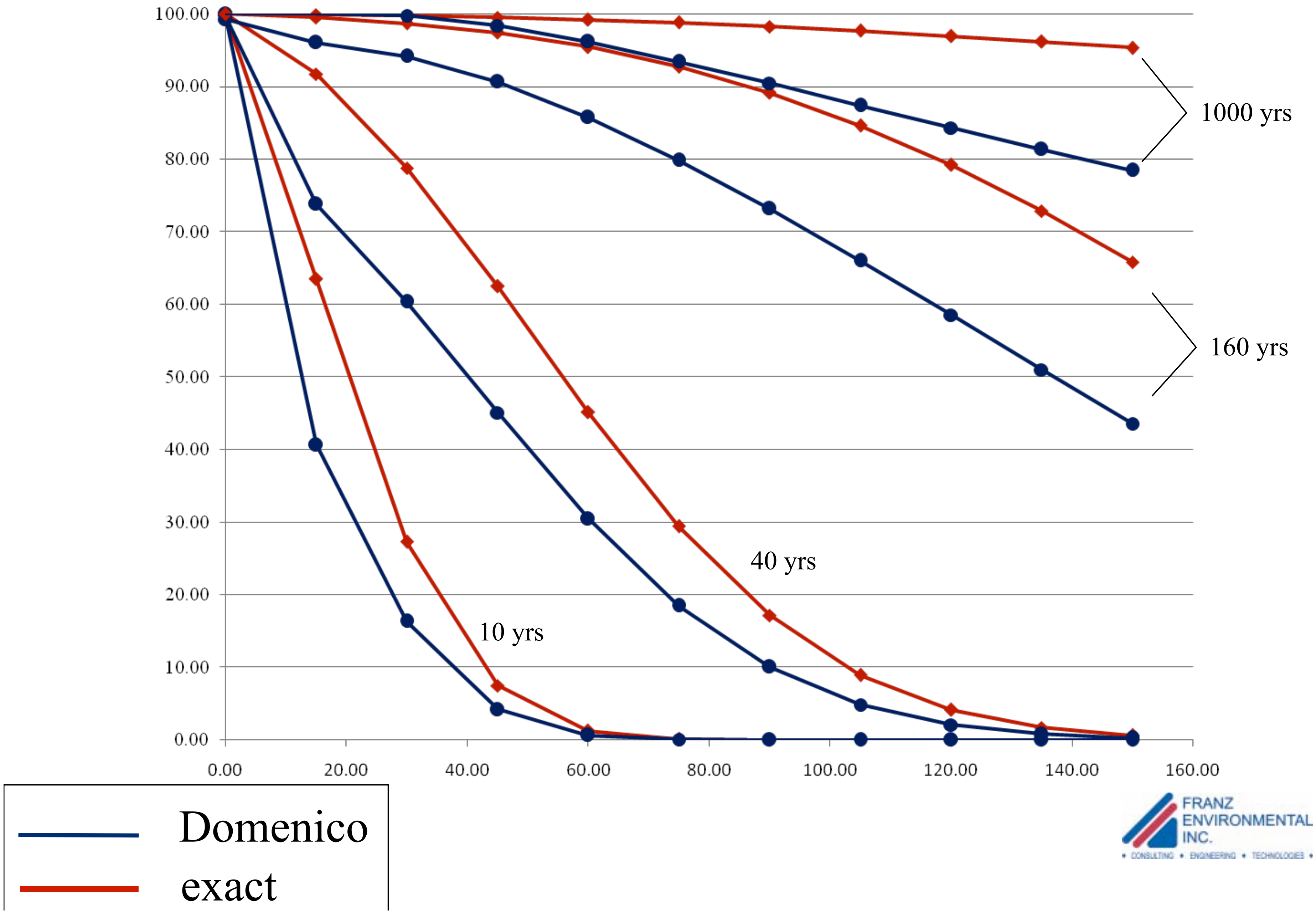
- In 2007, a series of papers were published pointing out the approximate nature of the Domenico solution
- Regulatory response was varied and does not appear to be settled yet

Regulatory Response

- Michigan was first to respond
  - Does not accept risk assessments that contain modeling with Domenico solution

Regulatory Response

- US EPA
  - Center for Subsurface Modeling Support (CSMOS) recommends to use caution when dispersion is a dominant process
  - Domenico can be used "safely" when the observation point (i.e. receptor) is greater than 10 x a_L
    - Peclet number must be greater than 10
    - This means that Domenico should be o.k. at greater distances from the source


100.00
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0.00
20.00
40.00
60.00
80.00
100.00
120.00
140.00
160.00
1000 yrs
160 yrs
40 yrs
10 yrs
Domenico
exact

Regulatory Response

- EPA Region 9
  - Issued newsletter in summer 2007
  - The developer of BIOSCREEN and BIOCHLOR (Dr. Charles Newell) "…recommended against the use of the BIOSCREEN model at this time…"

Next Steps

- Ontario MOE
  - Requested development of Domenico replacement
  - Motivated by elimination of approximation AND other issues:
    - Elimination of artificial mixing zone
    - Find peak concentration at receptor for a finite source (finite in time)
    - Provide Tier 2 (risk assessment) modeling tool within full EXCEL spreadsheet
  - Development by Franz Environmental, Papadopulos, U of Waterloo and BRGM

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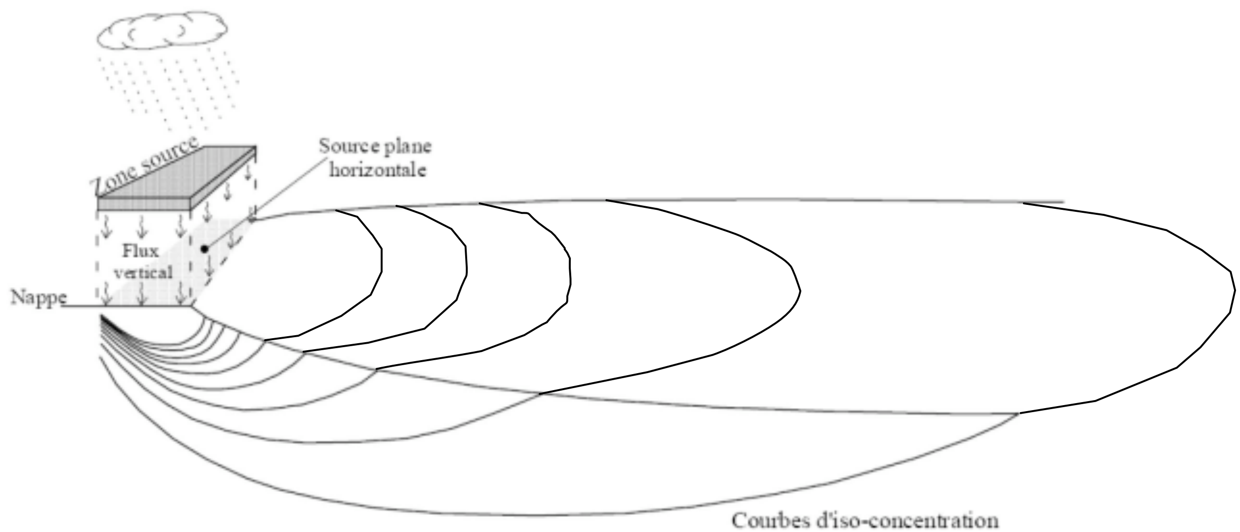
MISP (BRGM France)



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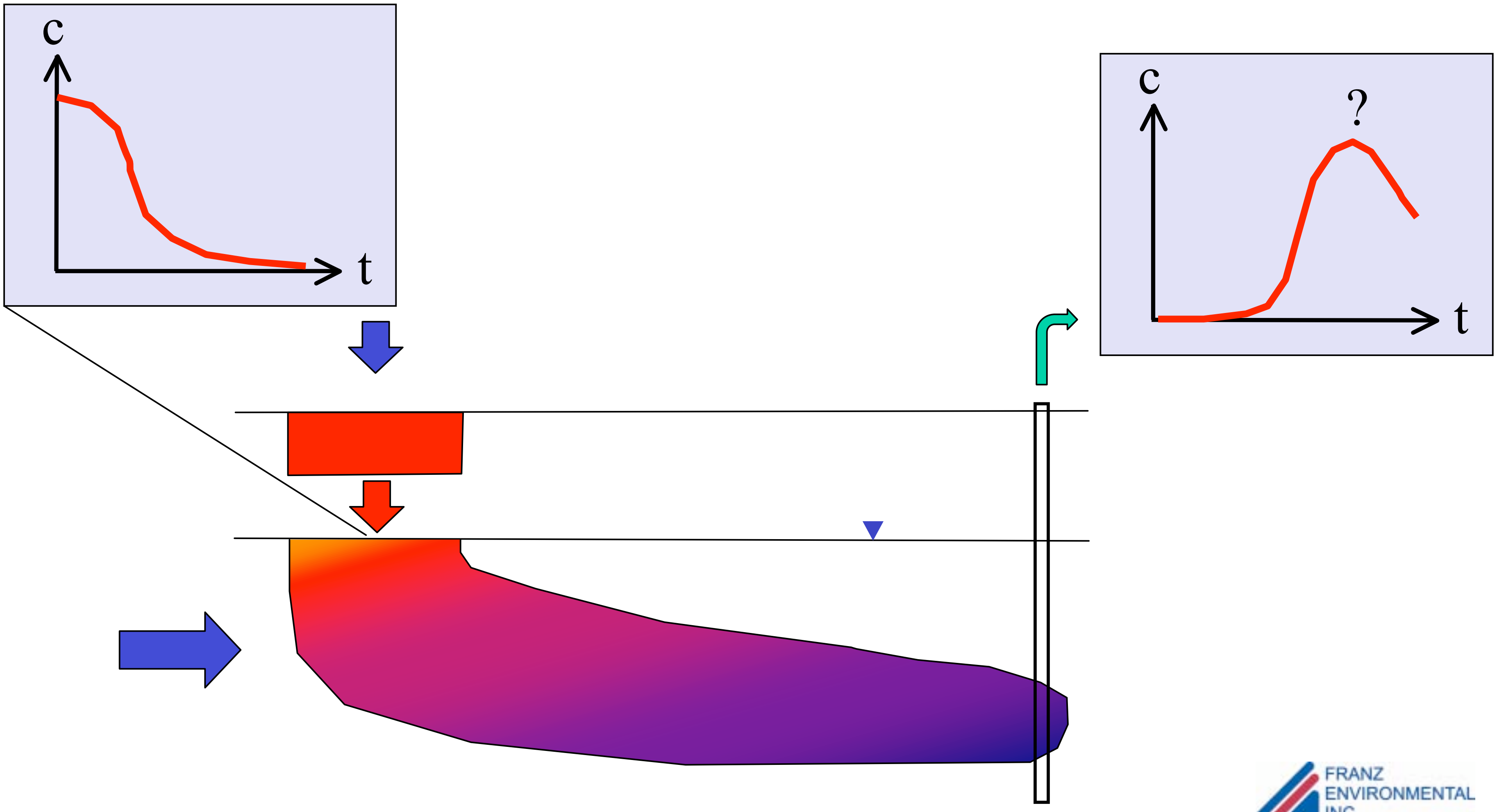
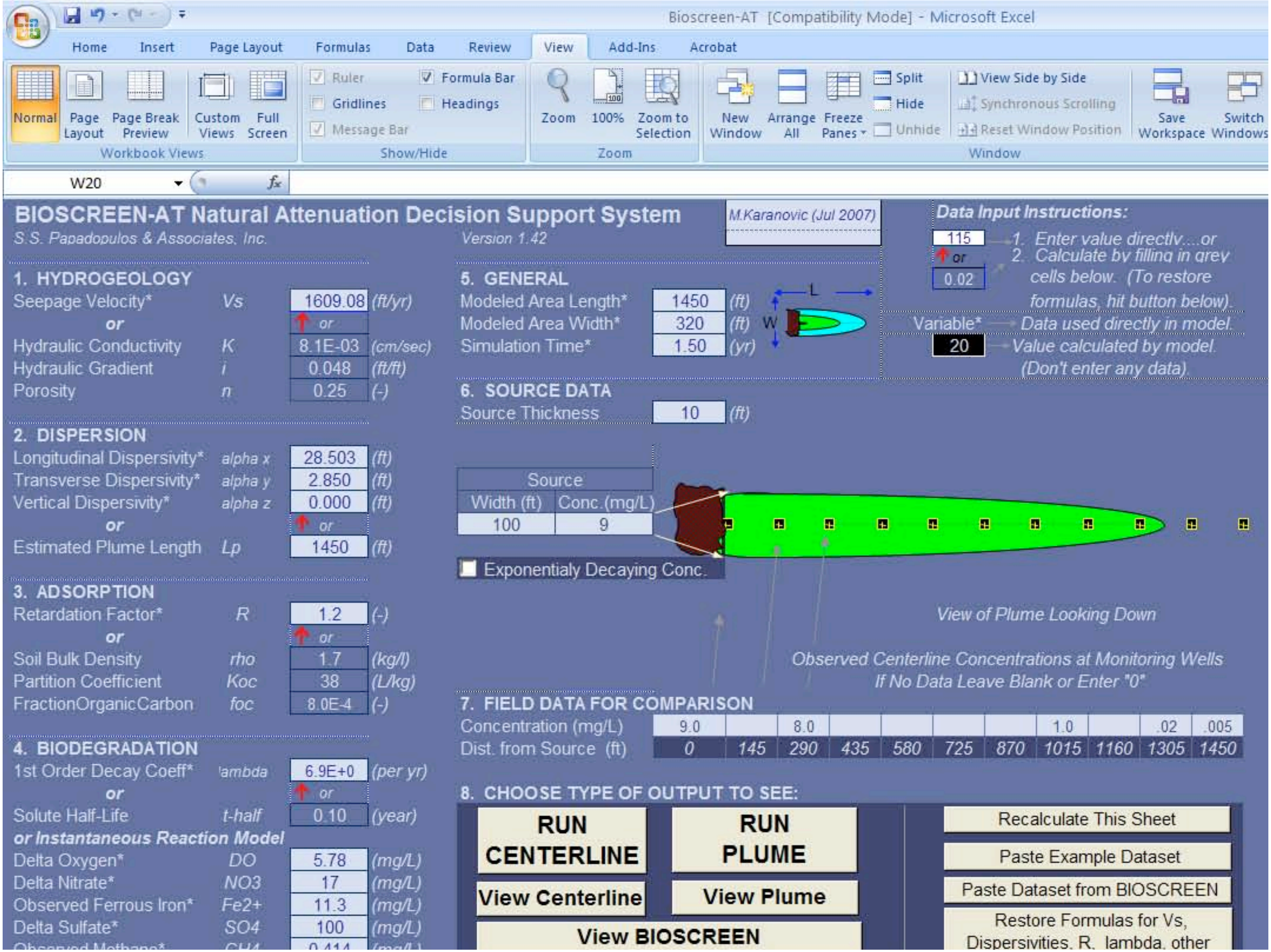
Finding peak receptor concentration



Karanovic, Neville & Andrews, 2007

- Developed BIOSCREEN-AT
- Available for free from
  - http://www.sspa.com/Software/bioscreen.shtml
  - S.S. Papadopulos & Associates, Inc.


Bioscreen-AT [Compatibility Mode] - Microsoft Excel
Home Insert Page Layout Formulas Data Review View Add-Ins Acrobat
Normal Page Layout Page Break Preview Custom Views Full Screen
Workbook Views
Ruler Formula Bar Gridlines Headings Message Bar
Show/Hide
Zoom 100% Zoom to Selection
Zoom
New Window Arrange All Freeze Panes Split Hide Unhide
View Side by Side Synchronous Scrolling Reset Window Position
Save Workspace Switch Windows
Window
W20
BIOSCREEN-AT Natural Attenuation Decision Support System
S.S. Papadopulos & Associates, Inc.
Version 1.42
M.Karanovic (Jul 2007)
Data Input Instructions:
115
or
0.02
1. Enter value directly....or
2. Calculate by filling in grey cells below. (To restore formulas, hit button below).
Variable* Data used directly in model.
20 Value calculated by model. (Don't enter any data).
1. HYDROGEOLOGY
Seepage Velocity* Vs 1609.08 (ft/yr)
or
Hydraulic Conductivity K 8.1E-03 (cm/sec)
Hydraulic Gradient i 0.048 (ft/ft)
Porosity n 0.25 (-)
2. DISPERSION
Longitudinal Dispersivity* alpha x 28.503 (ft)
Transverse Dispersivity* alpha y 2.850 (ft)
Vertical Dispersivity* alpha z 0.000 (ft)
or
Estimated Plume Length Lp 1450 (ft)
3. ADSORPTION
Retardation Factor* R 1.2 (-)
or
Soil Bulk Density rho 1.7 (kg/l)
Partition Coefficient Koc 38 (L/kg)
FractionOrganicCarbon foc 8.0E-4 (-)
4. BIODEGRADATION
1st Order Decay Coeff* lambda 6.9E+0 (per yr)
or
Solute Half-Life t-half 0.10 (year)
or Instantaneous Reaction Model
Delta Oxygen* DO 5.78 (mg/L)
Delta Nitrate* NO3 17 (mg/L)
Observed Ferrous Iron* Fe2+ 11.3 (mg/L)
Delta Sulfate* SO4 100 (mg/L)
5. GENERAL
Modeled Area Length* 1450 (ft)
Modeled Area Width* 320 (ft)
Simulation Time* 1.50 (yr)
L
W
6. SOURCE DATA
Source Thickness 10 (ft)
Source
Width (ft) Conc. (mg/L)
100 9
Exponentialy Decaying Conc.
View of Plume Looking Down
Observed Centerline Concentrations at Monitoring Wells
If No Data Leave Blank or Enter "0"
7. FIELD DATA FOR COMPARISON
Concentration (mg/L) 9.0 8.0 1.0 .02 .005
Dist. from Source (ft) 0 145 290 435 580 725 870 1015 1160 1305 1450
8. CHOOSE TYPE OF OUTPUT TO SEE:
RUN CENTERLINE
RUN PLUME
View Centerline
View Plume
View BIOSCREEN
Recalculate This Sheet
Paste Example Dataset
Paste Dataset from BIOSCREEN
Restore Formulas for Vs, Dispersivities, R, lambda, other

Conclusions

- Domenico solution is an approximation
- Concentrations calculated with Domenico appear to be always lower than exact solution
- Errors of up to 70% have been reported in the recent literature
- Use cautiously, or use alternative models

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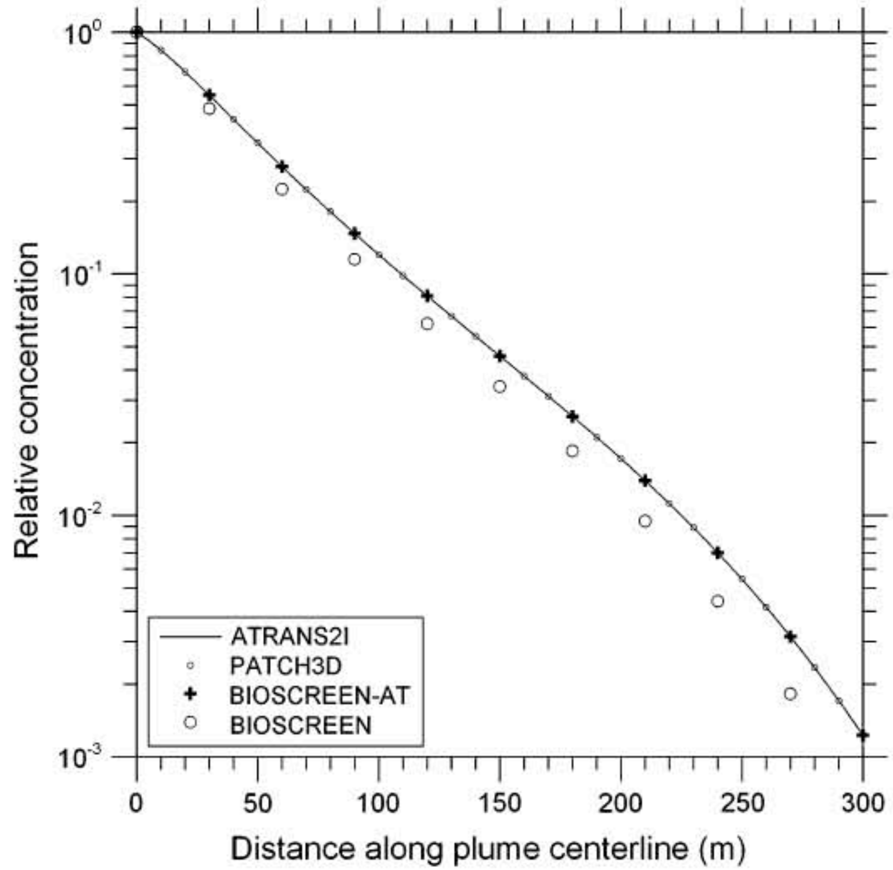
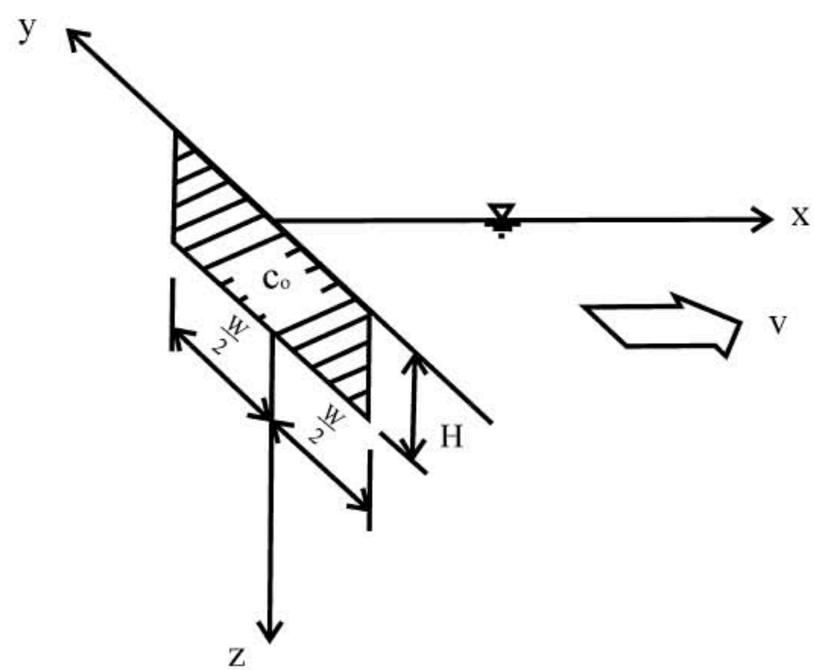
Karanovic, Neville & Andrews, 2007

Table 1
Input Parameters for the Example Calculations

Parameter	Value
Average linear ground water velocity, v	10.0 m/yr
Longitudinal dispersivity, α_L	10.0 m
Horizontal transverse dispersivity, α_{TH}	0.5 m
Vertical transverse dispersivity, α_{TV}	0.05
Effective diffusion coefficient, $D*$	0.0
Retardation factor, R	1.0
Effective first-order decay coefficient, λ_{EFF}	0.1386/year
Initial source concentration, c_0	1.0
Source decay coefficient, γ	0.0
Depth of source, H	2.0 m
Width of source, $2y_0$	20.0 m





y
x
c_o
W/2
W/2
H
v
z

Conceptual Model