Hybrid Model to Simulate Down Gradient Concentration Reduction Due to Contaminant Source Flux Reduction

Junqi Huang and Mark Goltz
Air Force Institute of Technology

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Problem

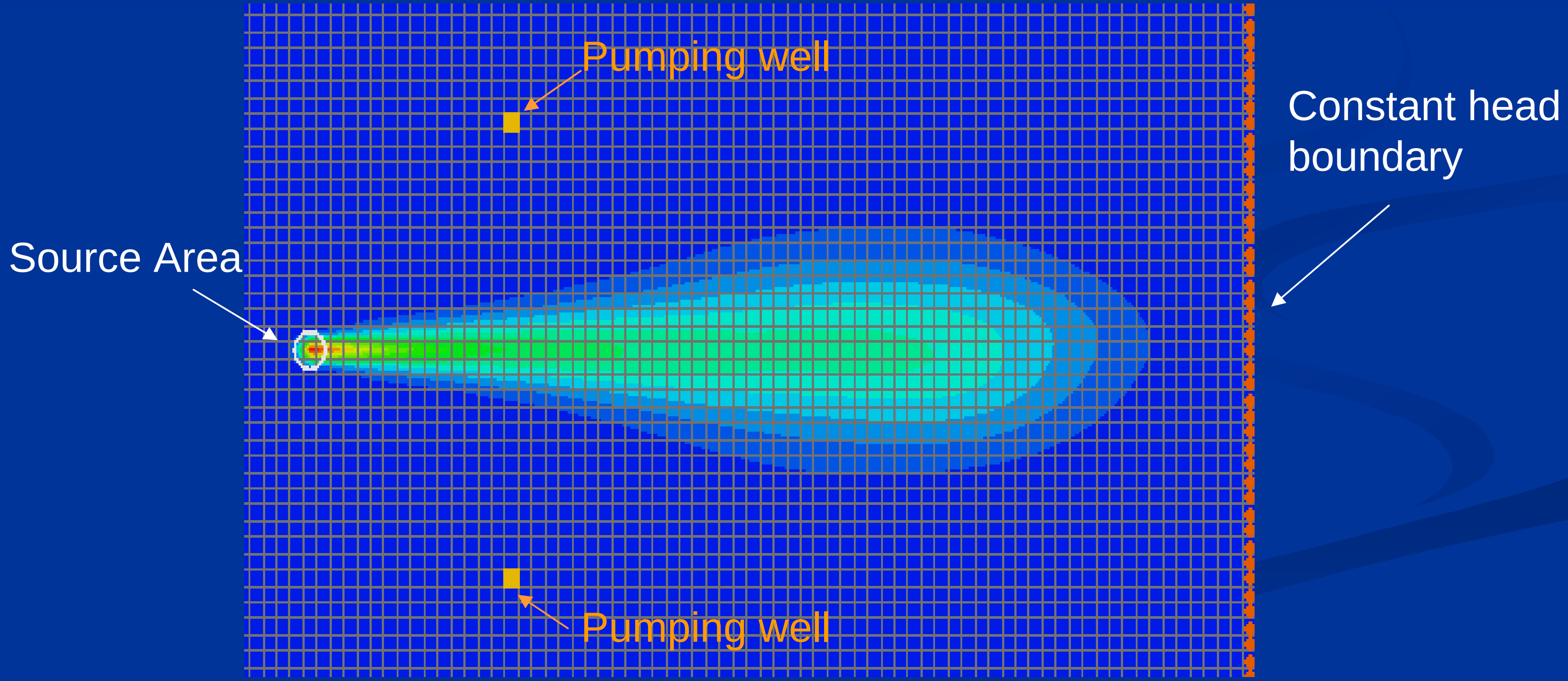
- The benefits of contaminant source flux reduction manifest themselves by reductions in contaminant plume concentrations
  - Relevant plume concentrations (in terms of impacts on health and the environment) may be far (in time and distance) from the source
  - Concentrations are affected by natural attenuation processes, that may be slow

Problem (cont.)

- To quantify these downgradient concentrations, a model is required
  - Model must be capable of accurately and rapidly simulating the small time and space scales associated with the contaminant source, as well as the large scales associated with the plume

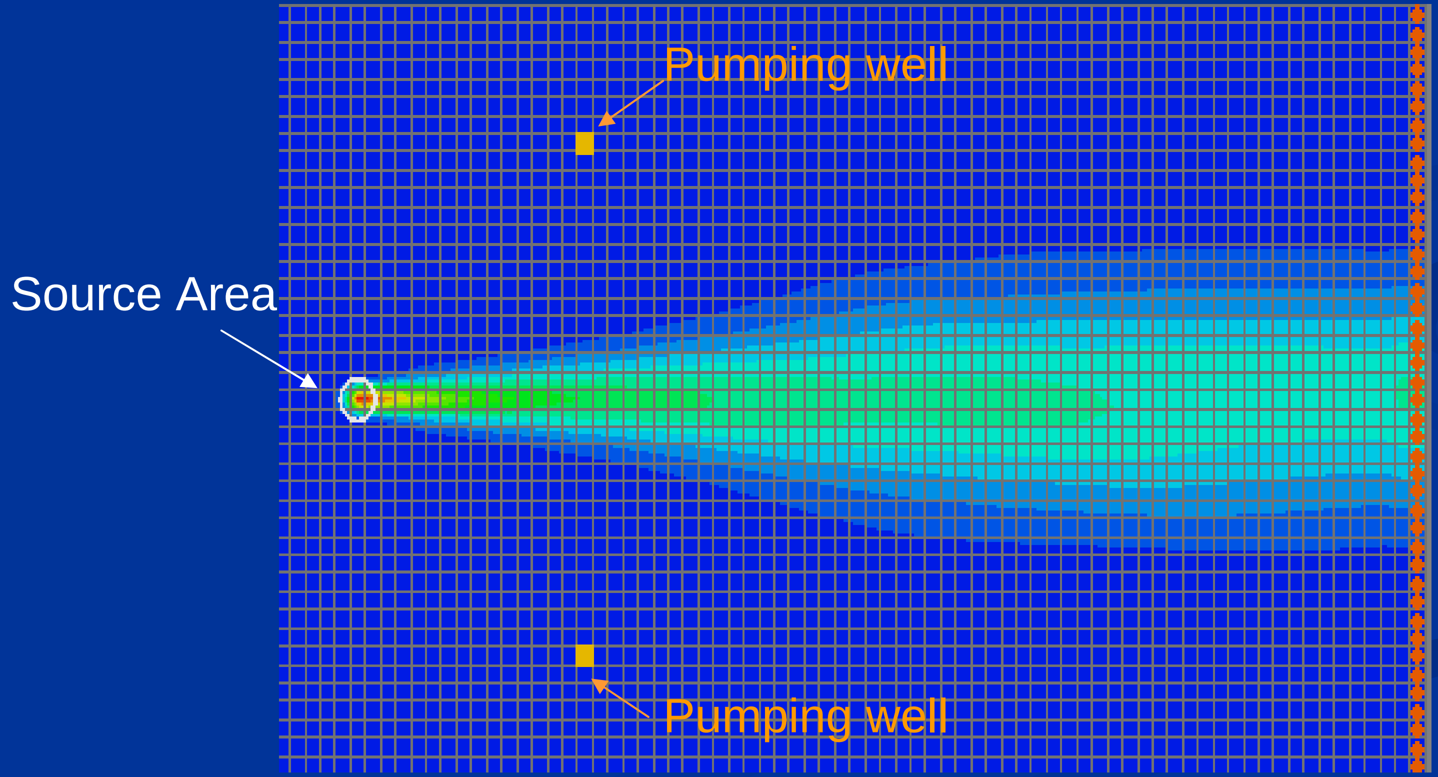
Problem (cont.)

So long as plume is far from downgradient boundary, conventional modeling approach is useful



Problem (cont.)

However, to simulate very large space and time scales, plume may travel to boundary and boundary assumptions may be violated

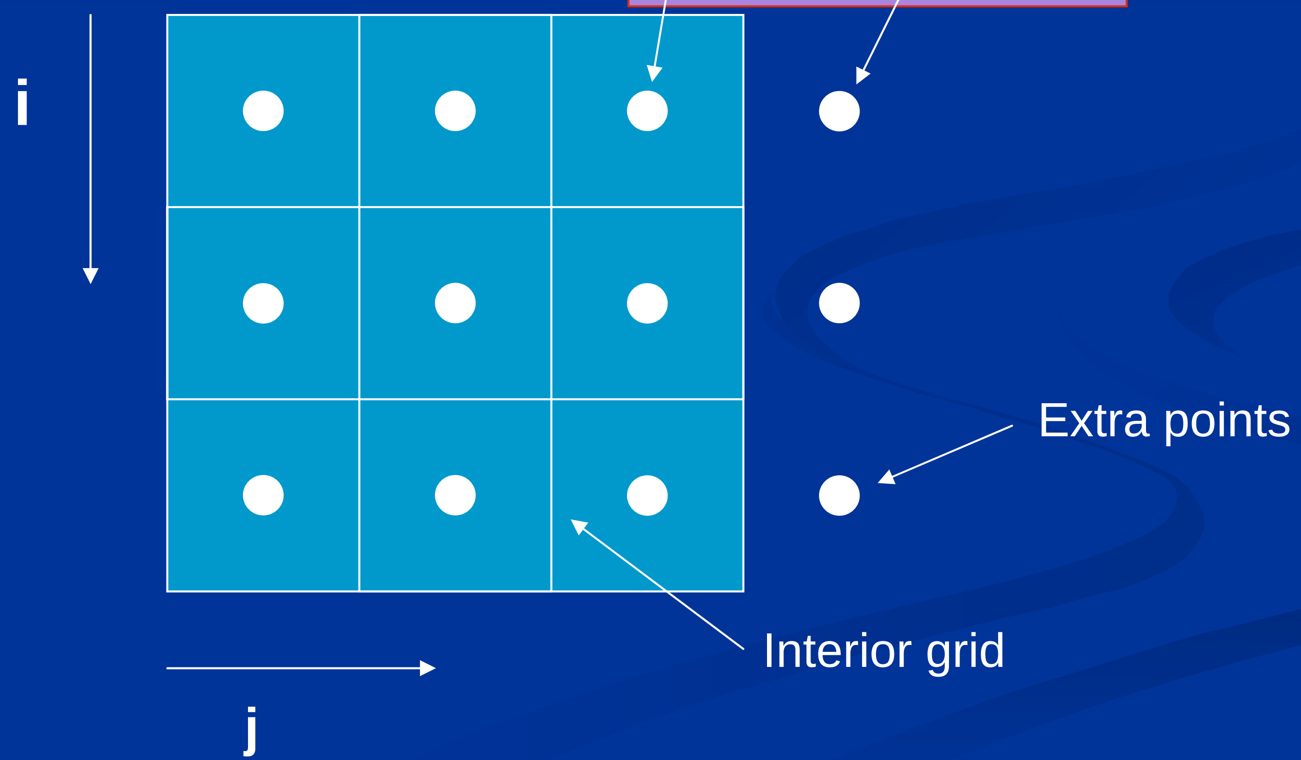


Constant head boundary, assumption of zero concentration gradient at boundary violated.

Problem (cont.)

If there is no natural boundary, conventional numerical model assumes a zero concentration gradient at the boundary and sets exterior and interior points at the same value

$$C_{j,i,k} = C_{j+1,i,k}$$



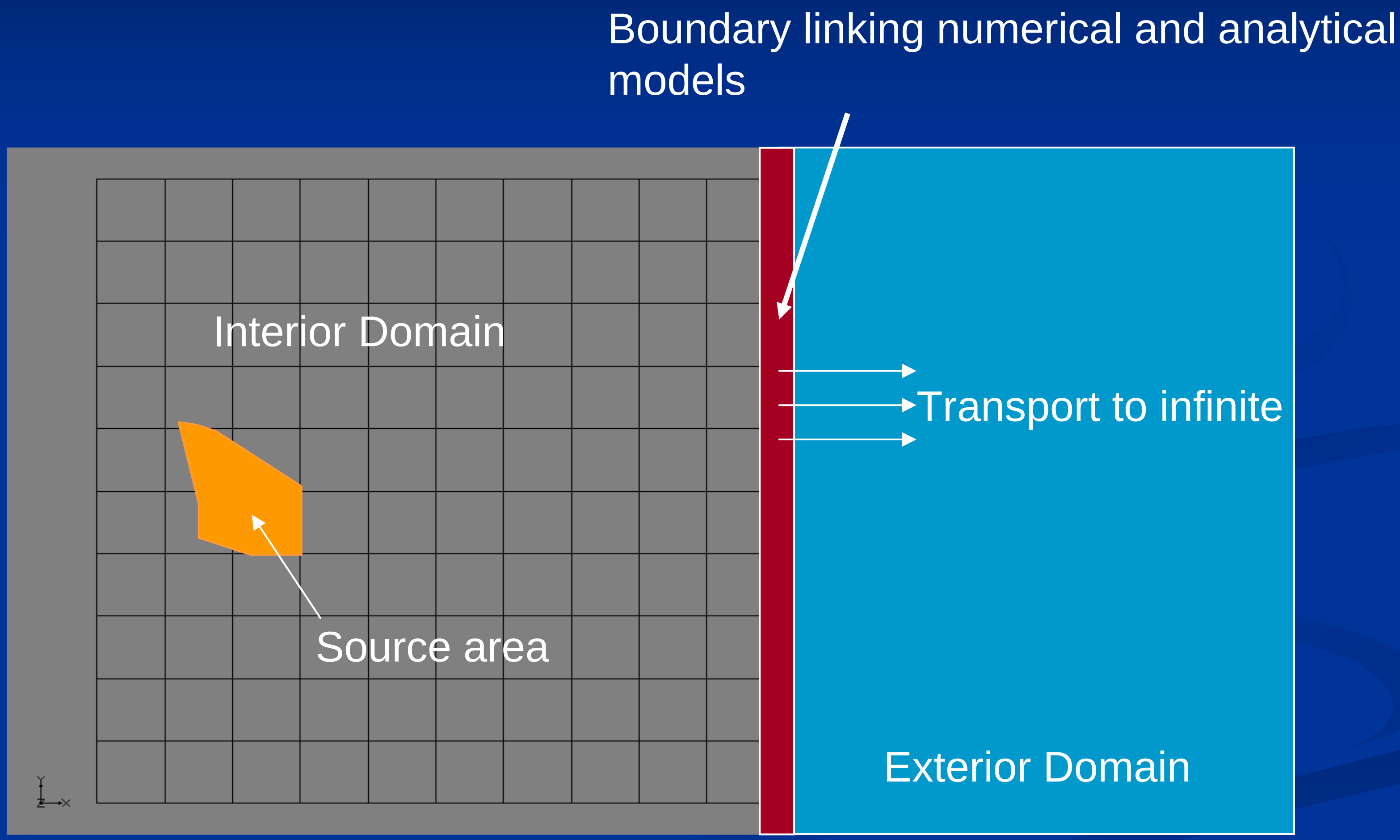
Problem (cont.)

- Assumption of a zero concentration gradient at a virtual boundary results in:
  - Neglect of dispersive flux at the boundary
  - Over prediction of boundary concentrations
  - Accumulation of error over time—particularly problematic over long time scales

Approach

- Hybrid model
  - Link a numerical model to simulate small scales near the source with an analytical model to rapidly simulate plume concentrations far downgradient
  - Linkage is at a boundary that serves as the downgradient boundary of the numerical model and the upgradient boundary of the analytical model

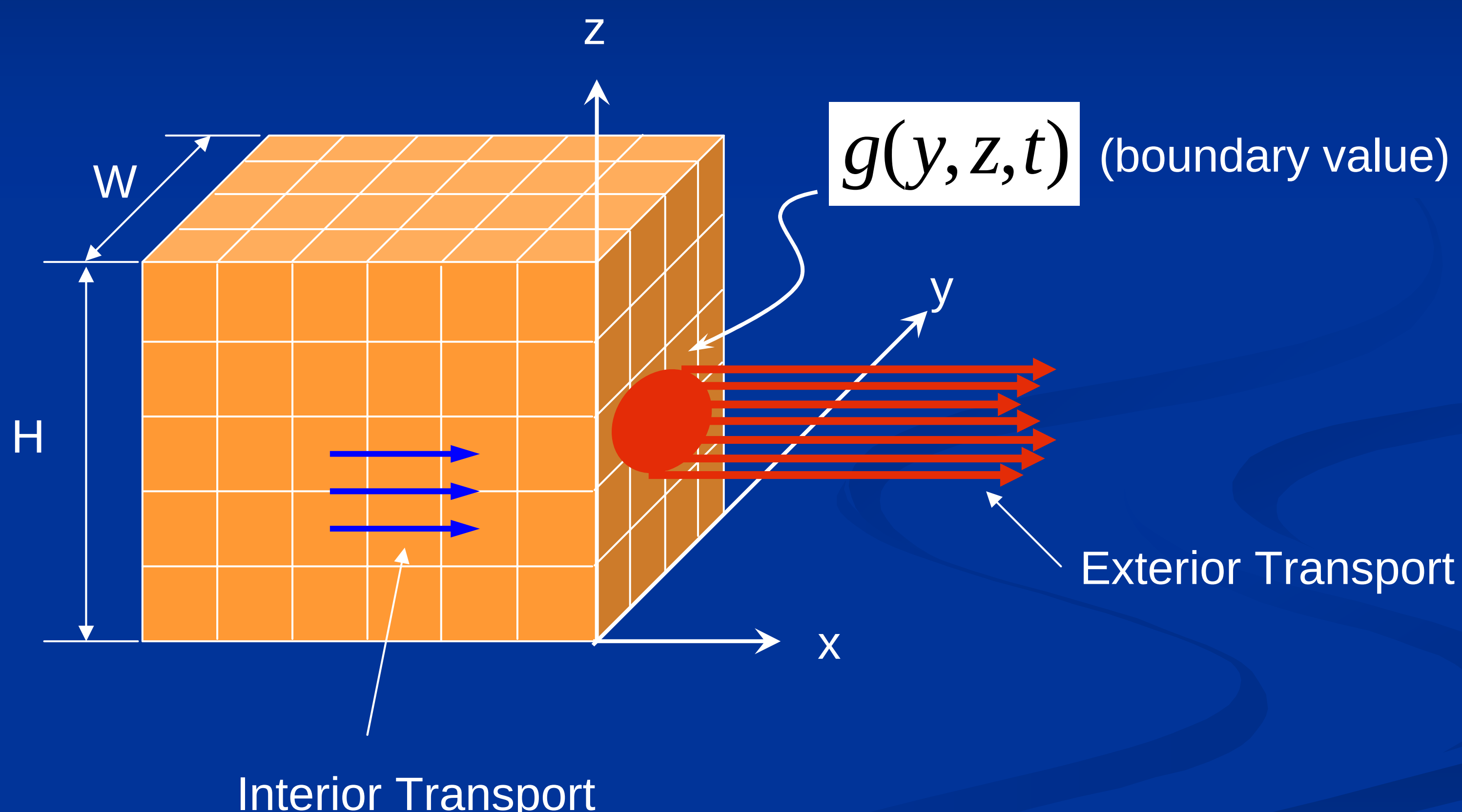
Approach


Boundary linking numerical and analytical models
Interior Domain
Transport to infinite
Source area
Exterior Domain

Basic Assumptions of the Hybrid Model

- Interior Domain
  1. "Standard" assumptions associated with conventional numerical model
- Exterior Domain
  1. One-dimensional flow in semi-infinite domain
  2. First-order decay chain reaction kinetics
  3. Dispersivity is constant
  4. No sources or sinks

Transport Geometry



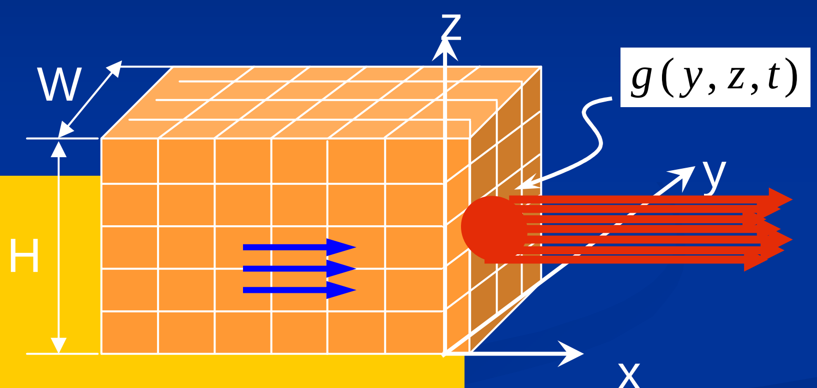
Analytical Model Equations in Exterior Domain

$$\theta R_i \frac{\partial C_i}{\partial t} = D_x \frac{\partial^2 C_i}{\partial x^2} - v_x \frac{\partial C_i}{\partial x} + D_y \frac{\partial^2 C_i}{\partial y^2} + D_z \frac{\partial^2 C_i}{\partial z^2} - \theta \lambda_i C_i + \theta \lambda_{i-1} C_{i-1}$$

$i = 1,2,3,4$ (PCE, TCE, DCE, VC)

$\lambda_0 = 0$

Analytical Model
Initial and Boundary Conditions



$$C_i(x,y,z,0)=0$$

$$C_i(0,y,z,t)=g_i(y,z,t)$$

$$C_i(\infty,y,z,t)=0$$

$$C_i(x,0,z,t)=C_i(x,W,z,t)=0$$

$$\partial C_i(x,y,0,t)/\partial z=\partial C_i(x,y,H,t)/\partial z=0$$

Link Between Interior and Exterior Solutions

$$C^{n}_{j+1,i,k} = C(\Delta x, y_i, z_k, t_n)$$

- n = time step
- j = the column index of interior grid system
- i = the row index of interior grid system
- k = the layer index of interior grid system
- 👎x = last delta-x in interior grid system

Analytical Model Solution using Laplace and Fourier Transforms

$$C_i(x,y,z,t) = \frac{2}{WH}\sum_{m=1}^{\infty}\sum_{n=0}^{\infty}\tilde{\hat{C}}_i(x,m,n,t)\sin\left(\frac{m\pi y}{W}\right)\cos\left(\frac{n\pi z}{H}\right)$$

$$\tilde{\hat{C}}_i(x,m,n,t) = \sum_{j=i}^{1}\Lambda_{i,j}\Omega_{i,j}(m,n,t)$$

$$\Omega_{i,j}(m,n,p) = \tilde{\hat{g}}_i e^{\gamma - k_j\sqrt{p+\beta_j(m,n)}}$$

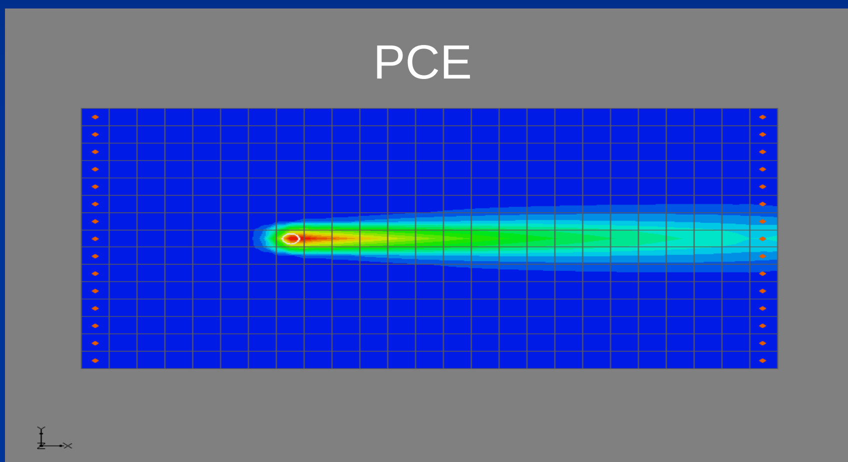
Model Implementation

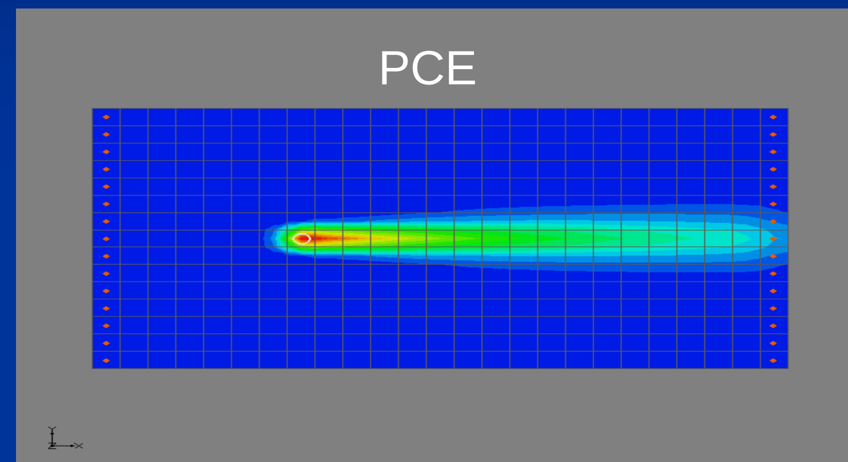
- RT3D used for the numerical model in the interior domain
- Grid system oriented so the x-axis of the analytical model coincides with the direction of background flow
- Boundary between interior and exterior domains must be far enough downgradient from flow source/sinks in the interior domain to assure a uniform one-dimensional flow field in the exterior domain
- Both the numerical and analytical models incorporate first-order decay chain kinetics to simulate natural attenuation via reductive dehalogenation of PCE
  - PCE->TCE->DCE->VC

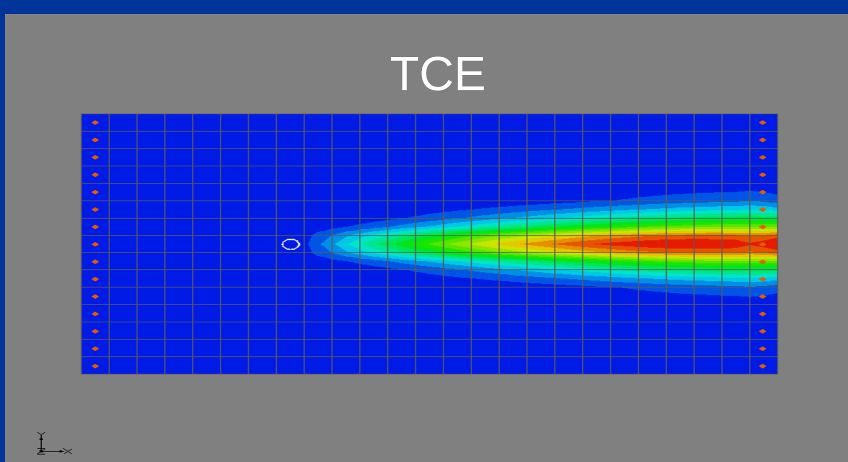
Concentration Contours after 200-day Simulation with a Continuous PCE Source Term Conventional Model (RT3D) and Hybrid Model

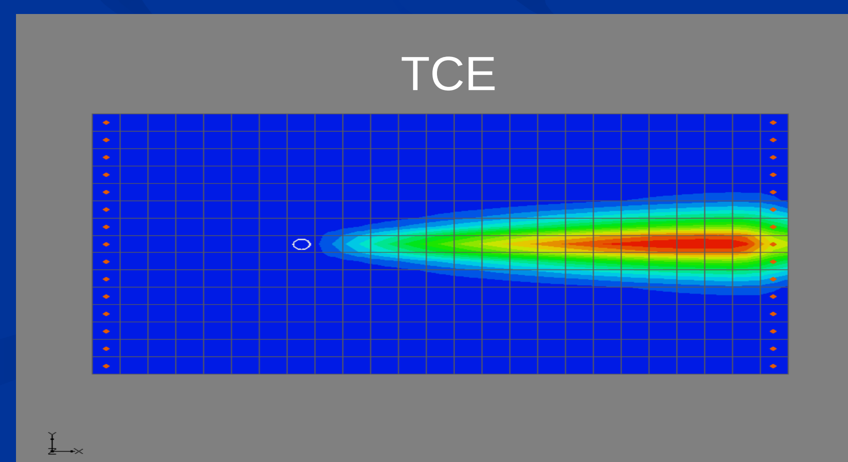
Conventional

Hybrid





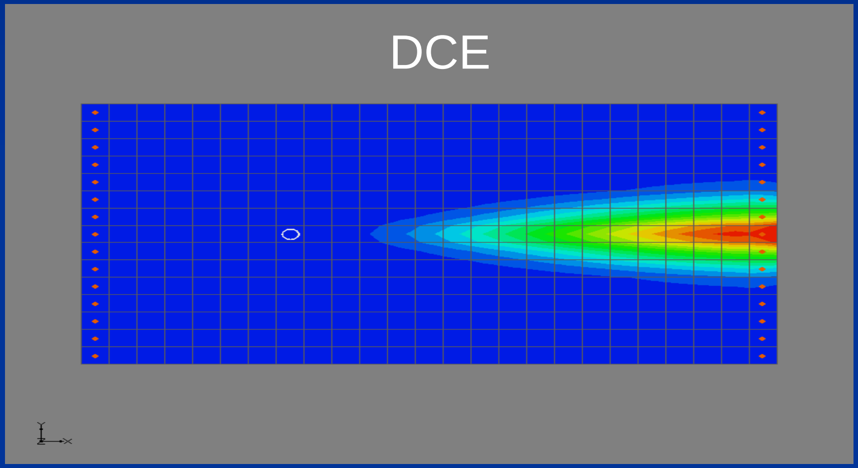


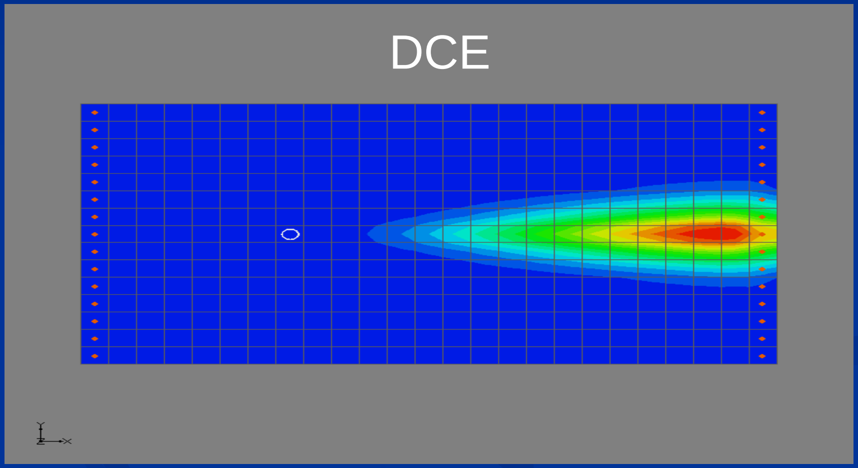


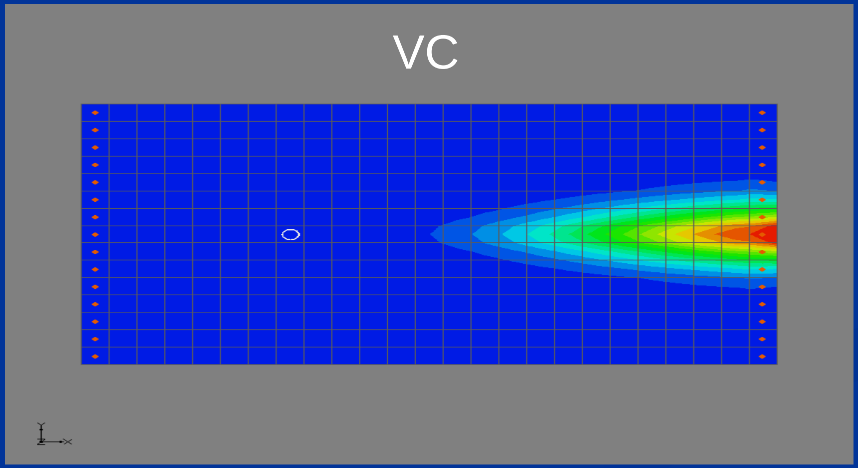
Concentration Contours after 200-day Simulation with a Continuous PCE Source Term

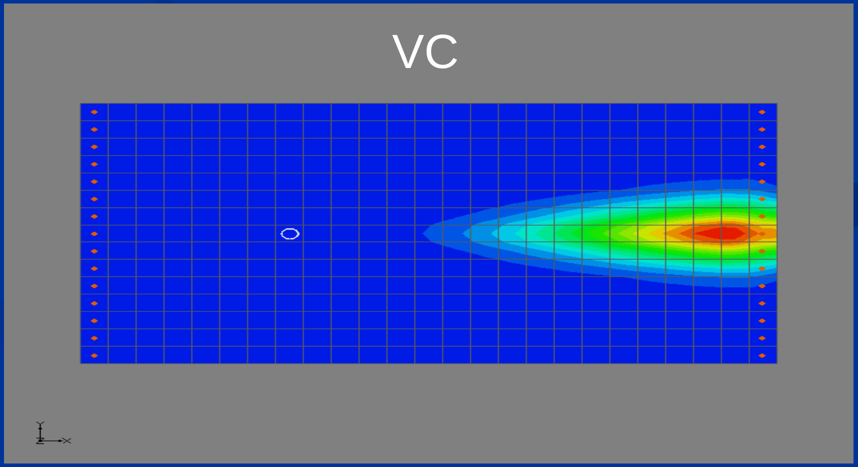
Conventional Model (RT3D) and Hybrid Model

Conventional | Hybrid

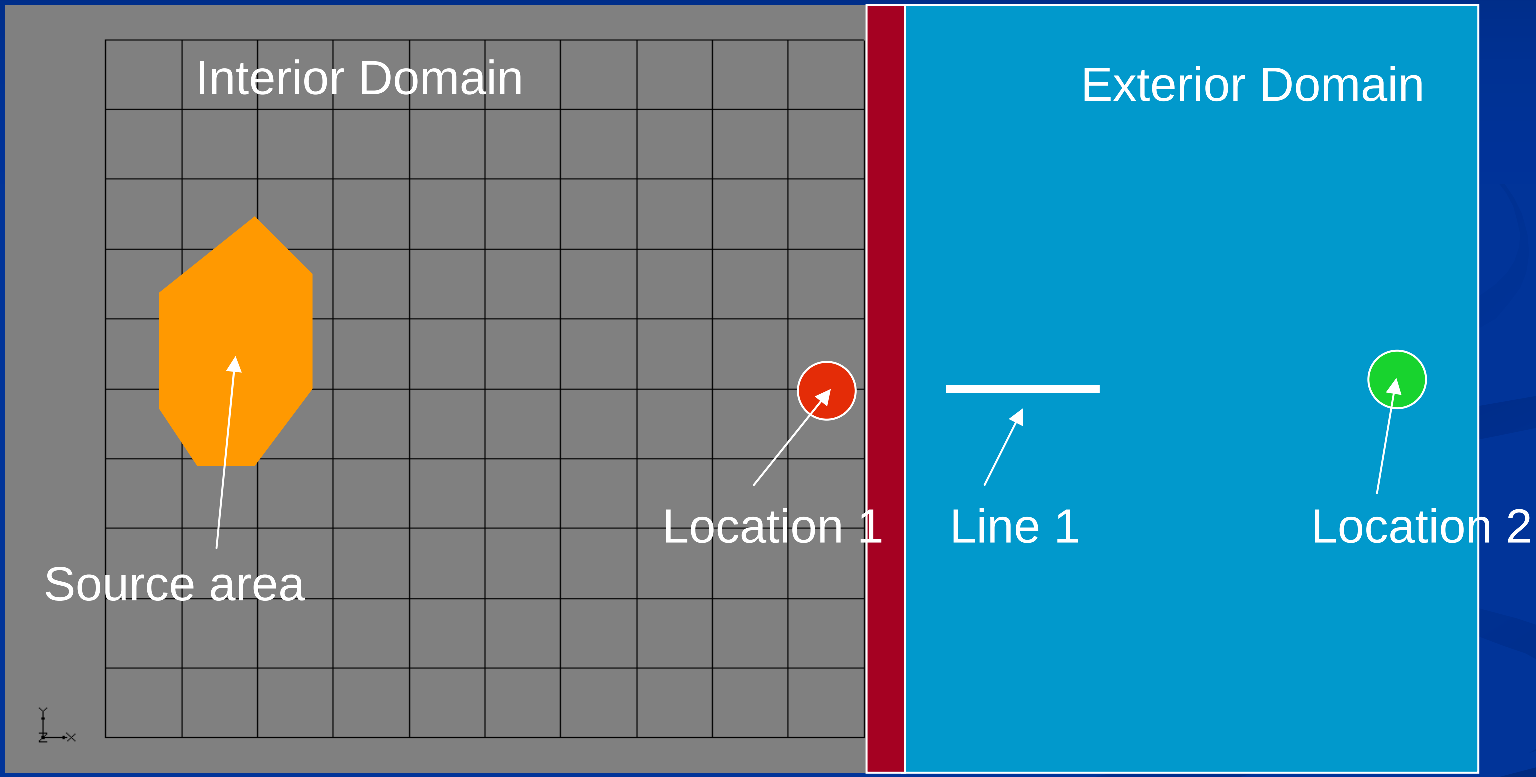




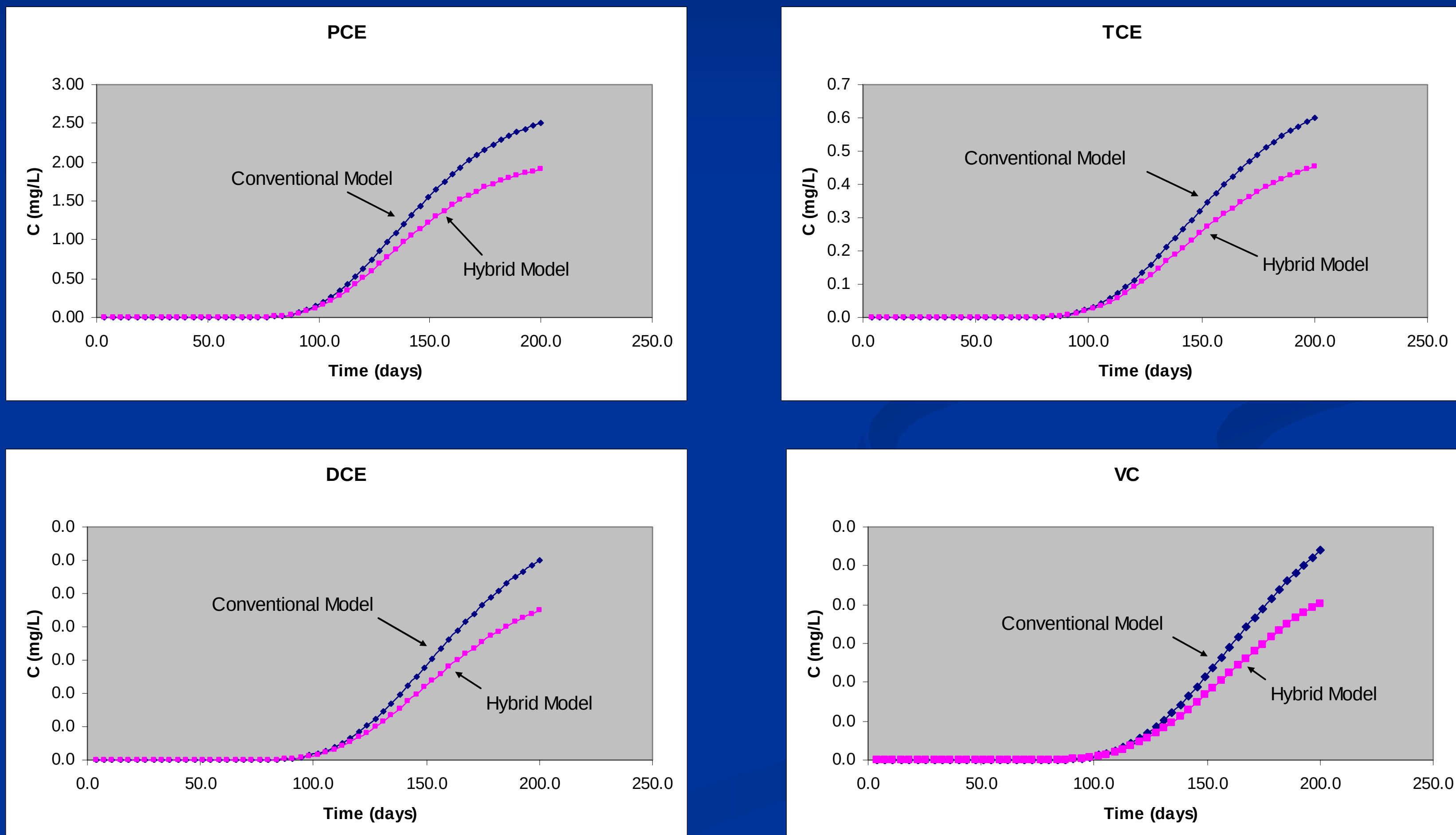




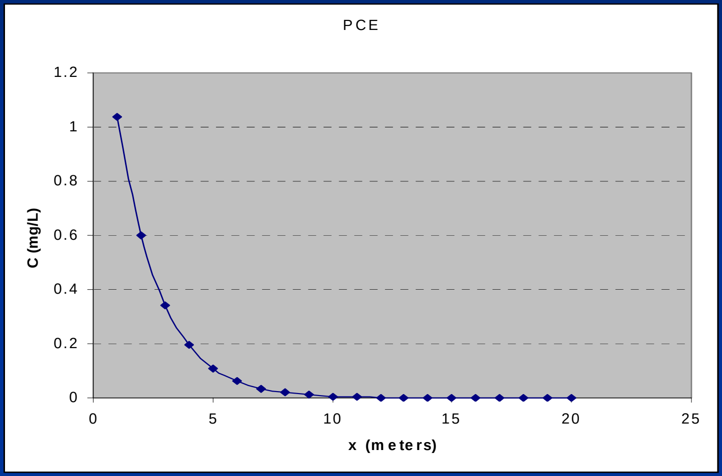
Reference Locations for Hybrid Model Simulations Depicted in the Following Slides

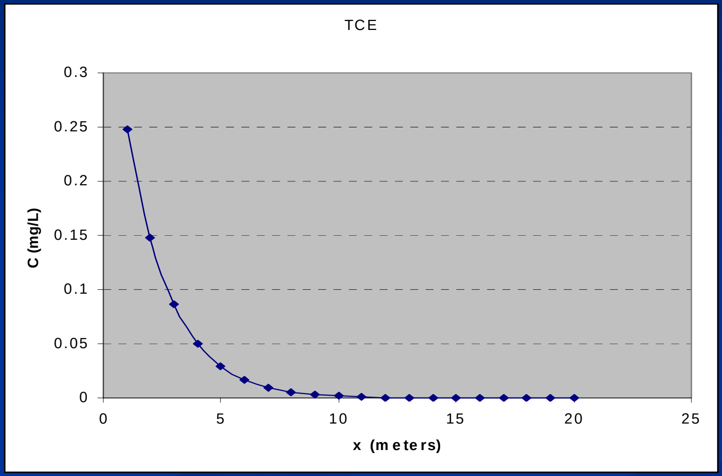


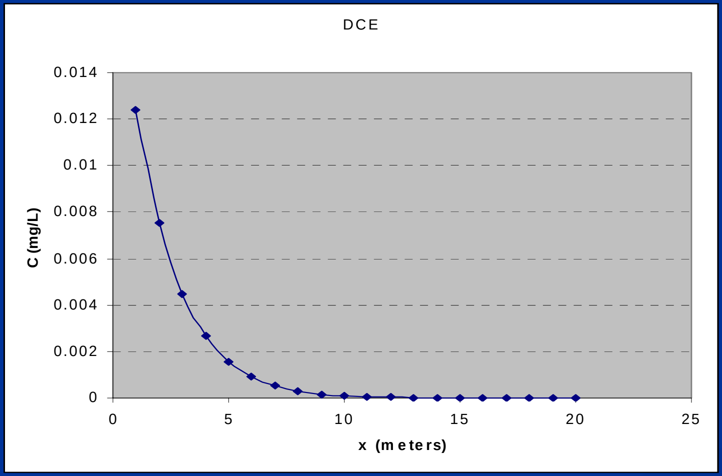
Breakthrough at Location 1 (interior domain near the downgradient boundary) for a Continuous PCE Source (comparison between conventional and hybrid models)

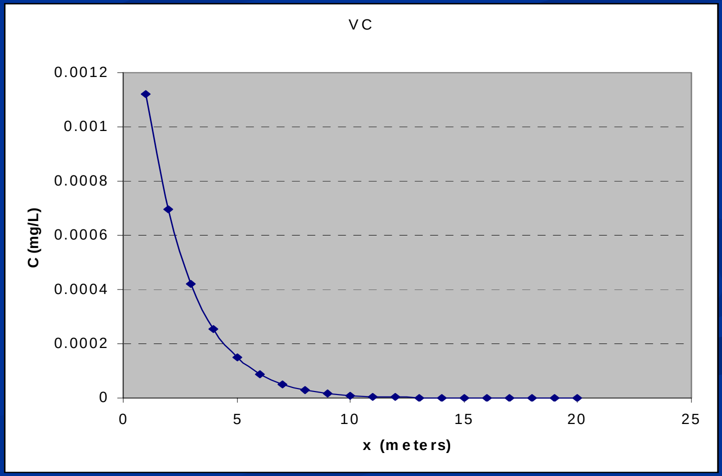


Concentration Distribution at Day 200 Along a Central Line in the Exterior Domain (Line 1) for a Continuous PCE Source

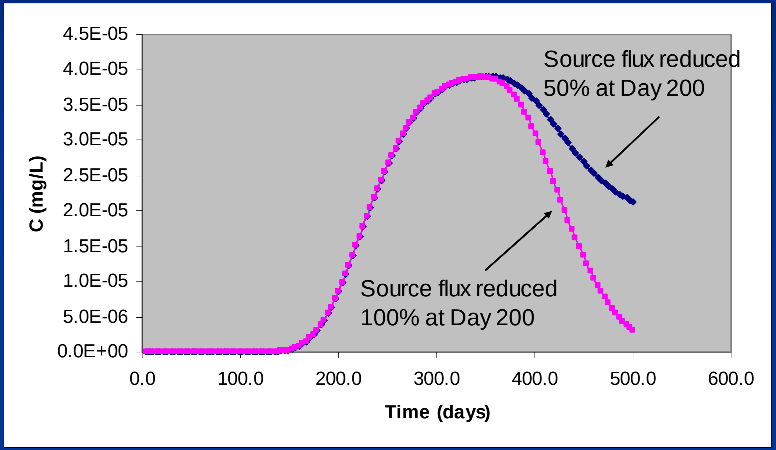


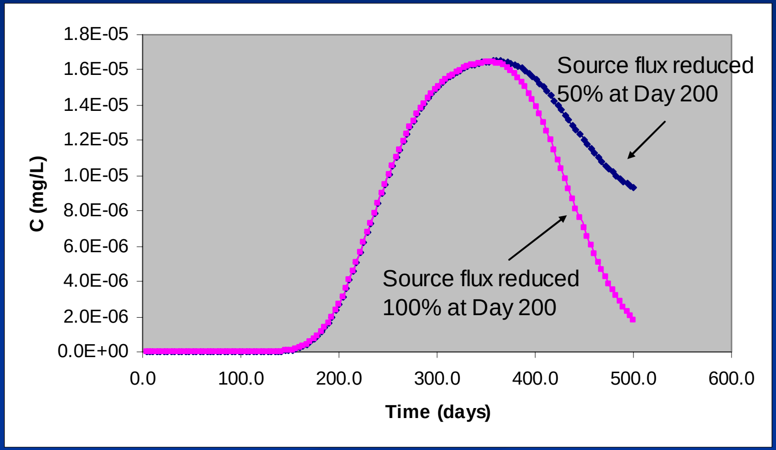


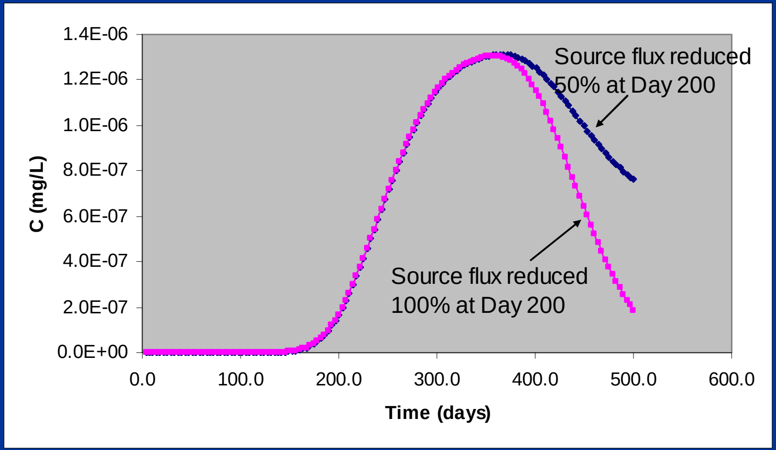


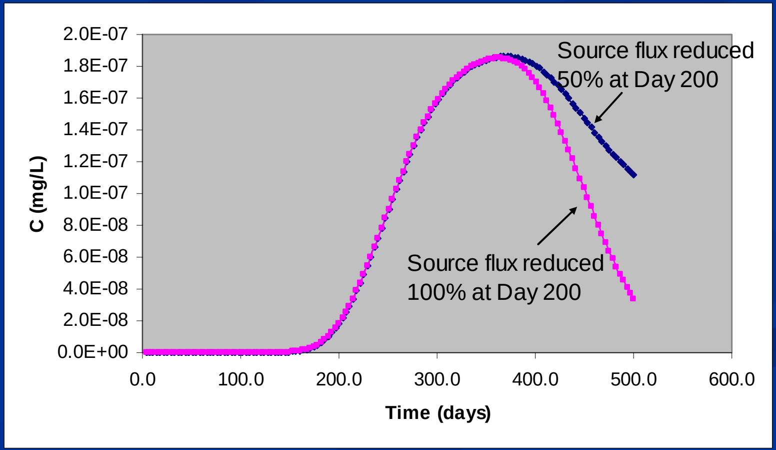


Breakthrough at Location 2 (exterior domain far downgradient) for a Pulse PCE Source, comparison for fully and half source removal









Conclusions

- A hybrid model was developed that combined the numerical RT3D code with an analytical model to simulate contaminant plume concentrations at large time and space scales
  - The model incorporates reductive dehalogenation of PCE assuming first-order decay chain kinetics
  - The model was used to simulate the impact of a reduction in source flux on contaminant concentrations at a downgradient well

Conclusion (cont.)

- By ignoring dispersive flux at the boundary, conventional numerical models overpredict boundary concentrations
  - The hybrid model improves concentration simulations near downgradient boundaries far from the contamination source
  - Such improvements are important if we hope to demonstrate the impact of source flux reductions on receptors which may be distant in both time and space from the source zone

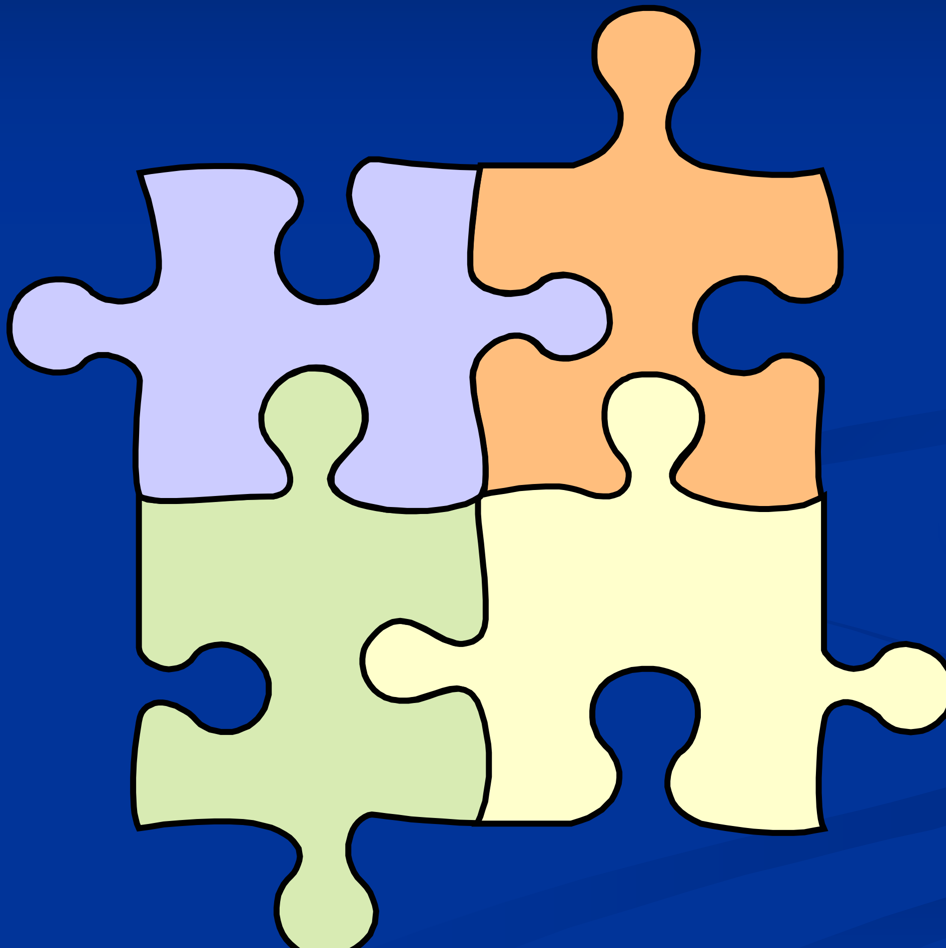
Limitations of Hybrid Model

- Requires extensive computational effort
- Because of the analytical solution in the exterior domain, flow field must be uniform and only simple, linear reactions can be simulated

Future work

- Improve speed
  - Since the concentration at each downgradient boundary node can be calculated independently, parallel computation may be conveniently implemented

Questions? Comments?



Intermediate Variables in the solutions (convolution)

$\Lambda_{i,j}$ Is only depends decay constants

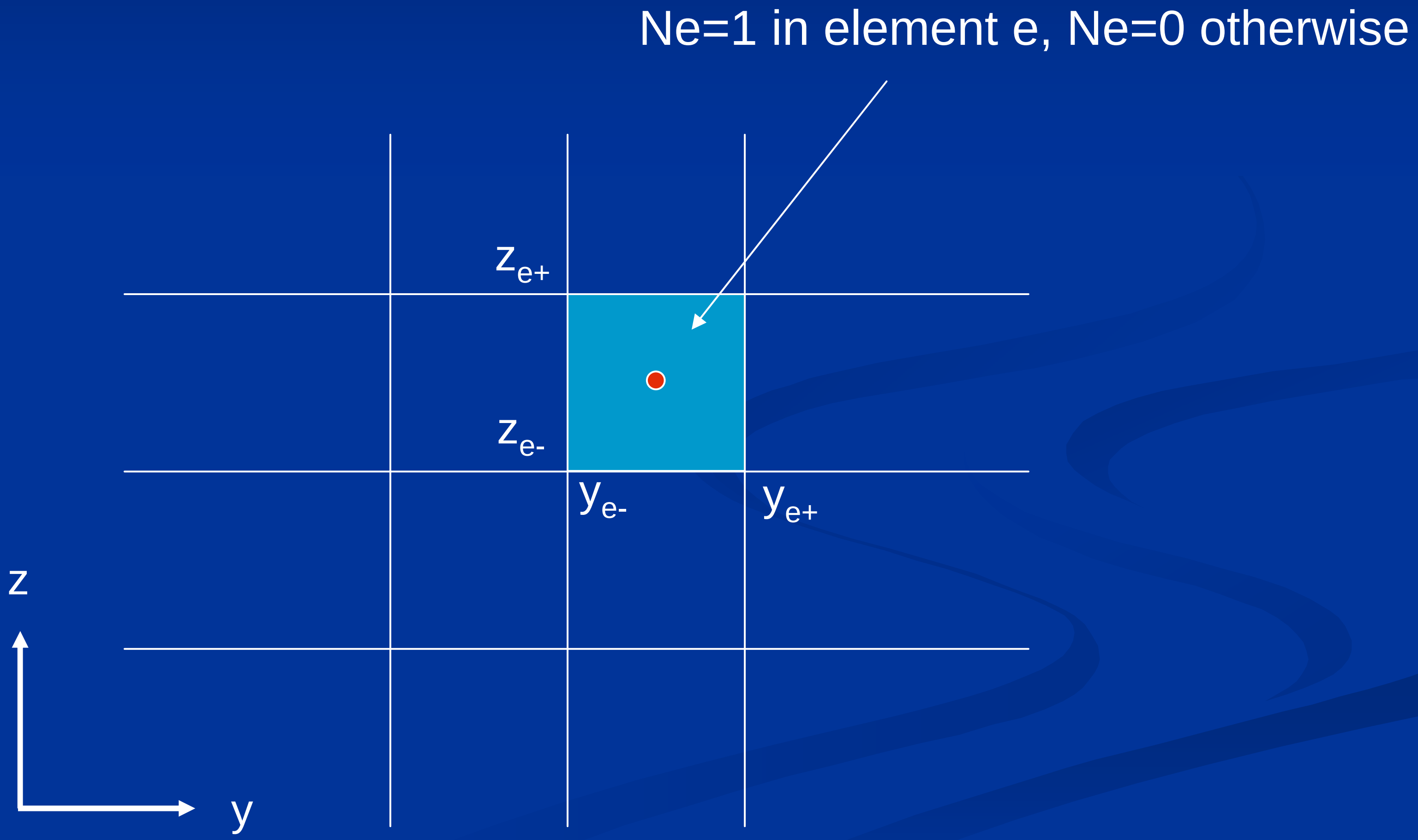
$$\Omega_{i,j}(m,n,t) = \frac{k_j e^{\gamma x}}{2\sqrt{\pi}} \int_0^t \tilde{\hat{g}}_i(m,n,t-\tau)\tau^{-\frac{3}{2}} e^{-\frac{k_j^2}{4\tau}-\beta_j(m,n)\tau} d\tau$$

Interpolation of function $\{g_i(y,z,t)\}$ in (y,z) domain—boundary area of model

$$g_i(y,z,t) = \sum_e N_e g_i(y_e, z_e, t)$$

e is the element number, N*e* is the base function

Bases function defined as:



Computing Effort for each component at each time step

- Nrow × Nlay × 2 Fourier transform operation (Nrow: grid row number, Nlay: grid layer number).
- 20×20 × (Nc+1) × Nt convolution, (Nc: component number, Nt: accumulated time step number).