Development and Verification of a Solute Transport Module for IWFM

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Overview

- Why solute transport modeling
- Governing equations
- Challenges of solving governing equations
- Approach
- Comparison of numerical solutions with analytical solutions
  - MT3D, SUTRA and other published solutions
- Application to a real world problem
  - Rocky Mountain Arsenal site, Colorado
- Next steps

Why solute transport modeling?

- **Water quality degradation** and **seawater intrusion** are two sustainable groundwater management indicators (Sustainable Groundwater Management Act-SGMA, 2014)
- Groundwater Sustainable Agencies (GSA) are required to identify and manage potential water quality and seawater intrusion issues
  - Groundwater contamination due to use of agricultural fertilizers is a common issue within the Central Valley, California
  - Coastal groundwater basins are vulnerable for seawater intrusion due to sea-level rise and climate change
- **Identifying and managing potential water quality and seawater intrusion** issues requires numerical tools that can simulate solute transport through groundwater
- Currently IWFM does not have the in-built capability to simulate solute transport and hence water quality or seawater intrusion

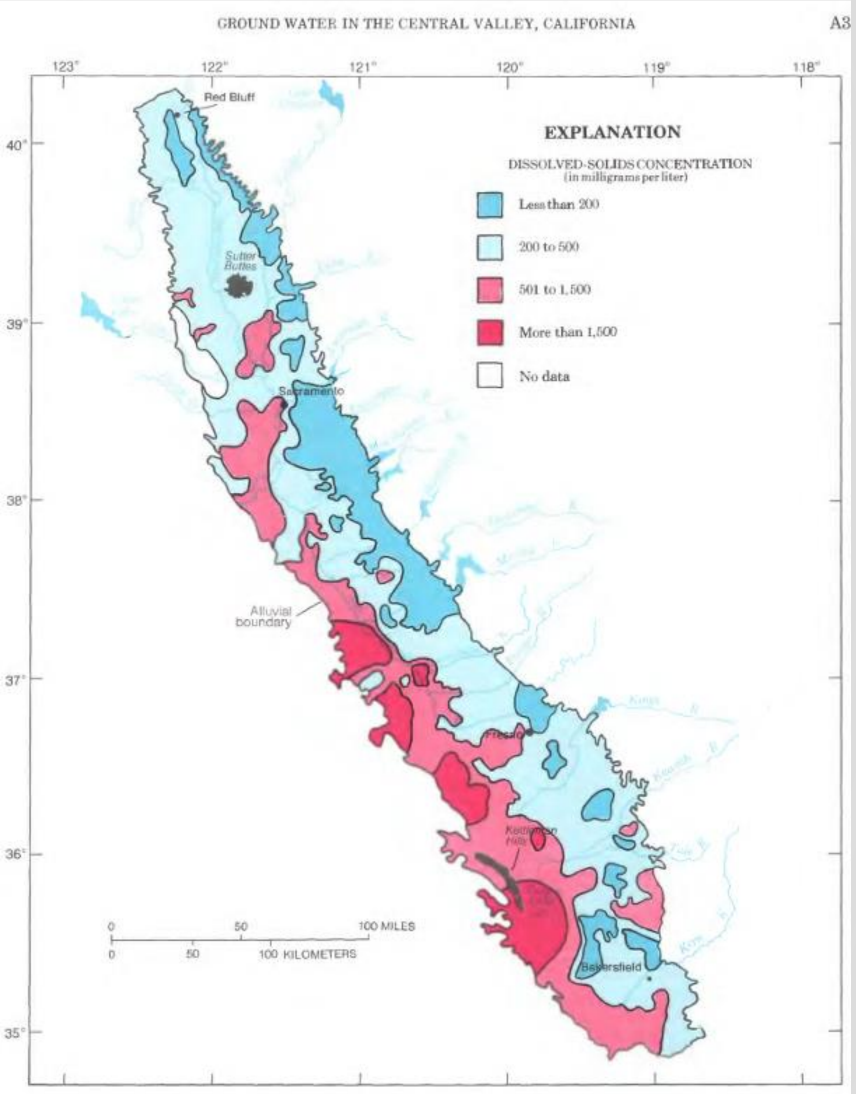


FIGURE 24.—Distribution of dissolved-solids concentrations in ground water of the Central Valley.

Bertoldi et al. 1991

Advection-Dispersion Equation for Porous Media

$$\theta \frac{\partial C^k}{\partial t} + \frac{\partial}{\partial x_i}\left(\theta v_i C^k\right) = \frac{\partial}{\partial x_i}\left(\theta D_{ij} \frac{\partial C^k}{\partial x_j}\right) + q_s C_s^k$$

Advection

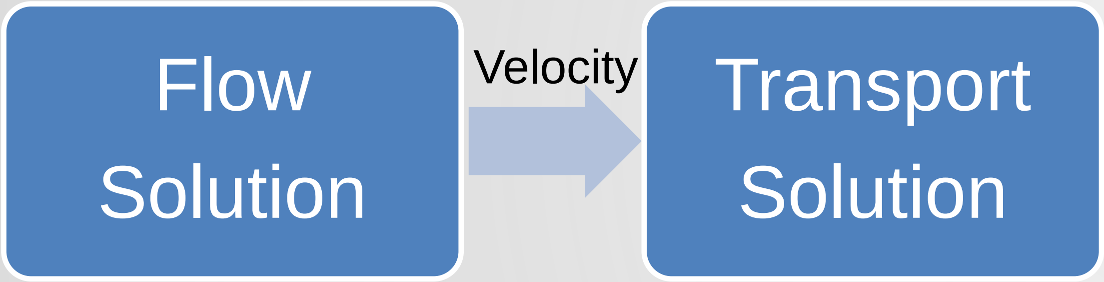
Dispersion

Source/Sink

- θ= porosity of the aquifer (-),
- C^k= dissolved concentration of solute k $[M/L^3]$,
- t= time $[T]$,
- D_{ij}= dispersion coefficient tensor $[L^2/T]$-both hydrodynamics and molecular diffusions ,
- v_i= linear pore water velocity $[L/T]$ from a groundwater flow model,
- q_s= volumetric flow rate per unit volume representing sources or sinks $[1/T]$,
- C_s^k=source or sink concentration of solute k $[M/L^3]$

Approach

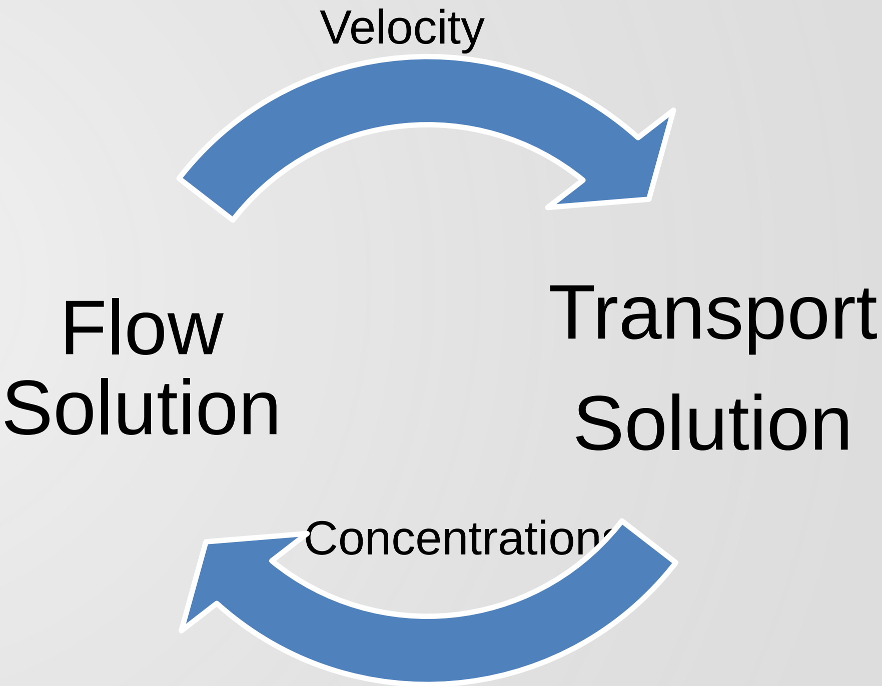
Water Quality Simulations



One way coupled (loosely coupled)

Concentrations are small (<5 000 mg/l) -> Does not impact the flow density

Seawater Intrusion Simulations



Two way coupled (tightly coupled)

Higher concentrations (>5 000 mg/l) -> Flow field is impacted by concentrations

Density dependent flow simulations

Challenges of solving Advection-Dispersion Equation

- Governing Advection-dispersin equation
  - *hyperbolic* when advection is dominant
  - *parabolic* when dispersion is dominant
- No single numerical solution works for all conditions
- Many field conditions are advection dominated (*Grid Peclet number, Pe>1*)
  - Numerical dispersion issue
  - Spurious oscillation near sharp fronts (under and over shoot)
- Stabilization methods are needed for advection dominated conditions in Eulerian methods such as Finite Elements
  - Lagrangian methods-no numerical dispersion or spurious oscillations-more computational time

$$P_e = \frac{|v| L}{D}$$

$\lvert v \rvert$	is the magnitude of the seepage velocity vector, LT^{-1};
L	is a characteristic length, commonly taken as the grid cell width, L;
D	is the dispersion coefficient, L^2T^{-1}.

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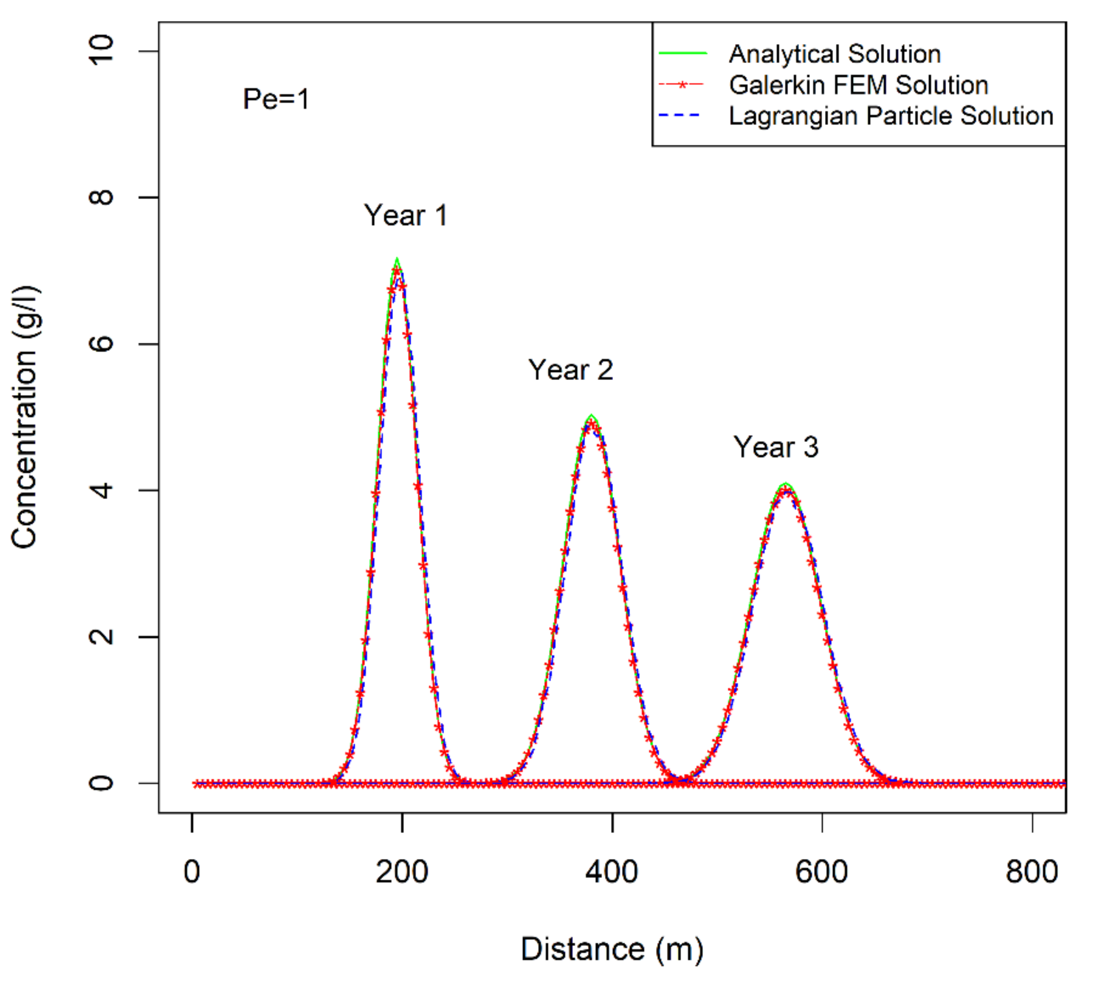
Stabilization methods of Finite Elements for advection dominated cases

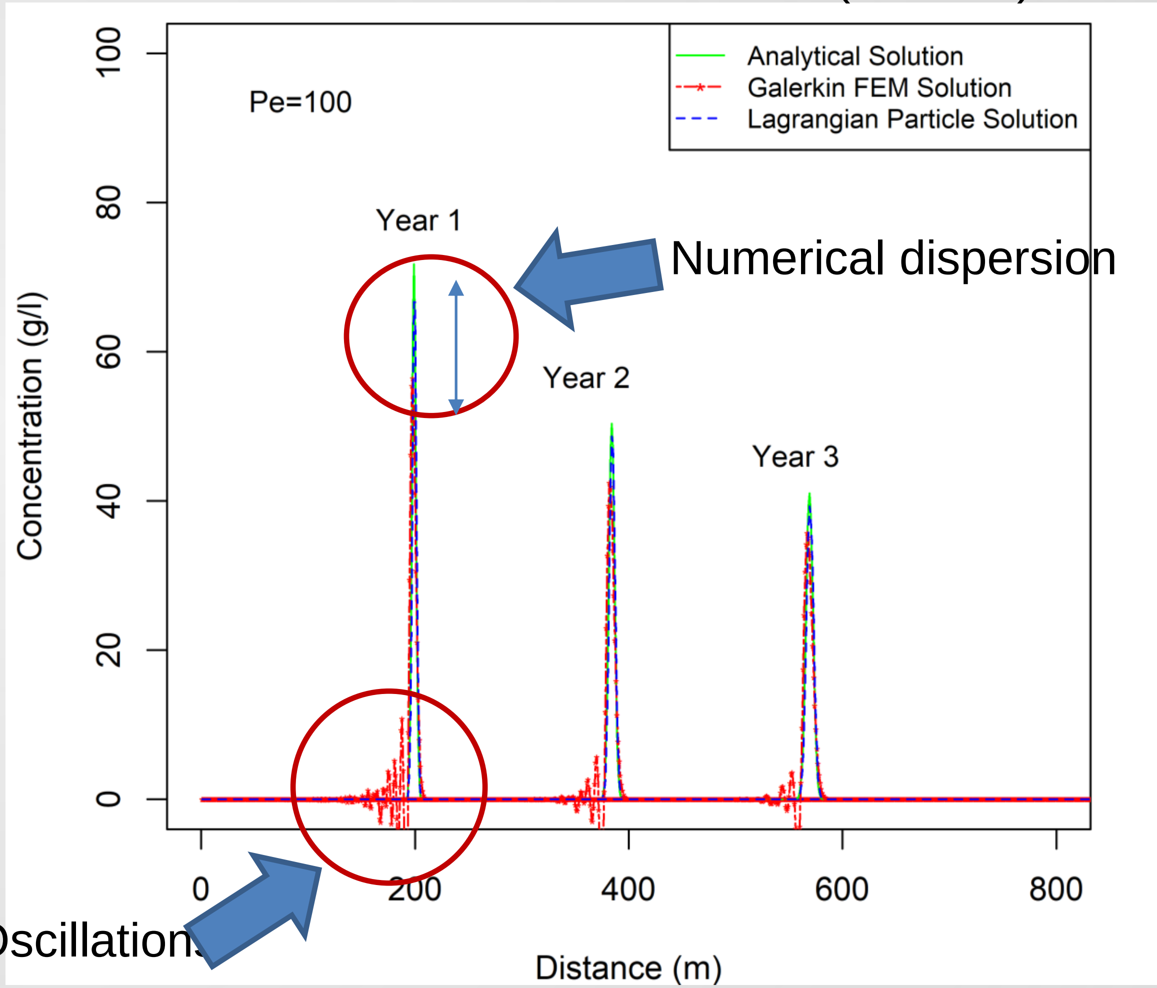
- 1-D: Petrov Galerkin (PG)
  - Artificial diffusion is added to overcome the instability near sharp fronts through unwinding
- 2-D: Streamline Upwind Petrov Galerkin-SUPG (Brooks and Huges, 1982)
  - For 2D case excessive cross diffusion (perpendicular to the flow) in Petrov Galerkin method corrupts the results
  - Upwind effect is added only in the direction of flow-SUPG

Instantaneous Release of a Contaminant-1D

Not advection dominated (Pe=1)



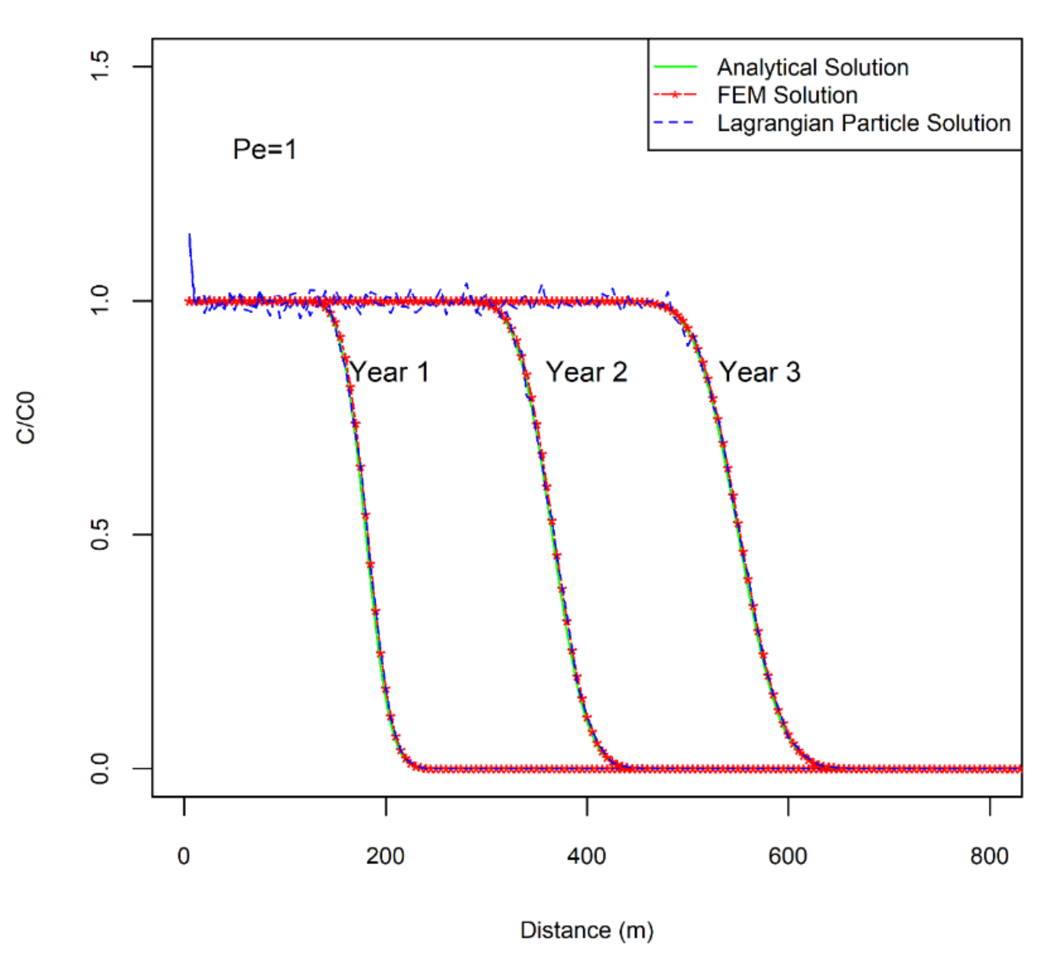
Advection dominated (Pe=100)



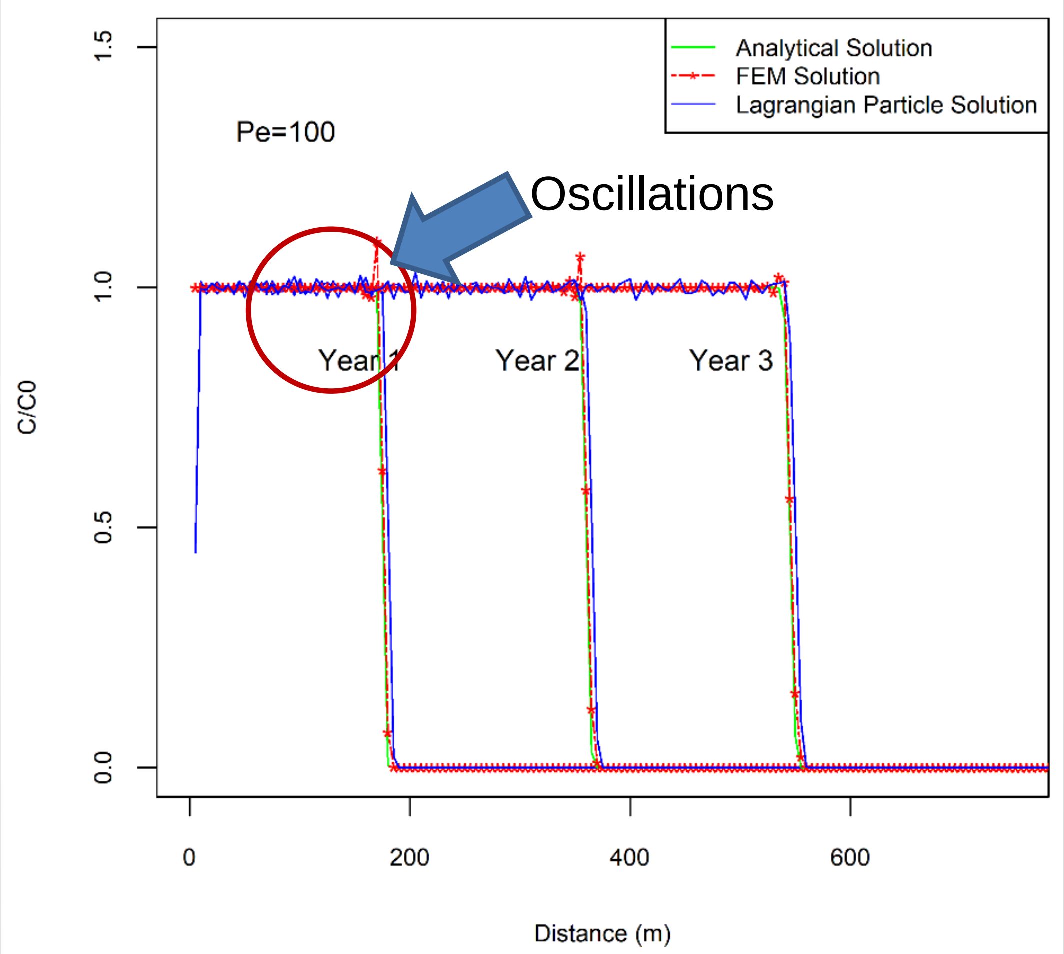
Analytical Solution Bear, 1979

Continuous Release of a Contaminant-1D

Not advection dominated (Pe=1)



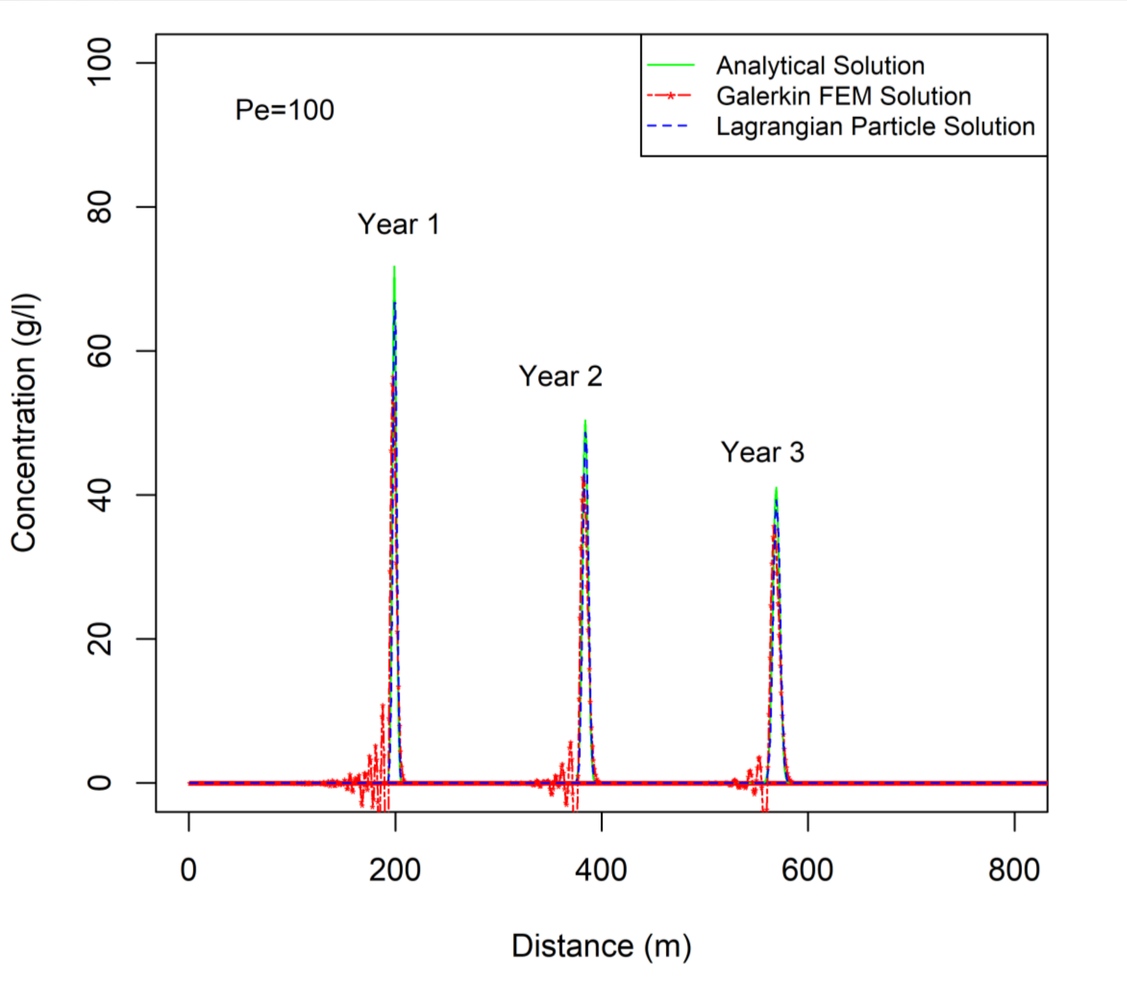
Advection dominated (Pe=100)



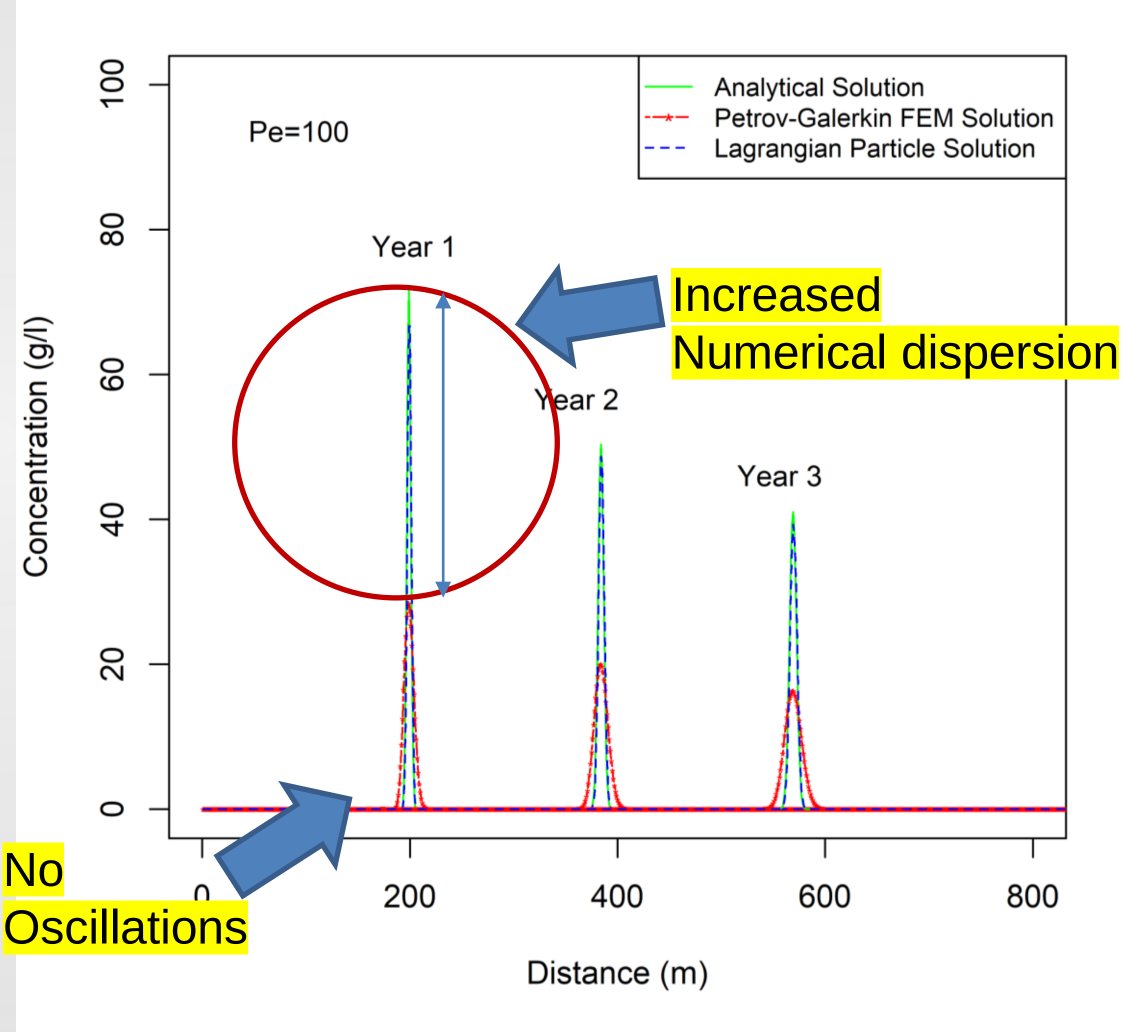
Analytical Solution Van Genuchten and Alves (1982)

Petrov Galerkin Stabilization Results

Galerkin (Pe=100)

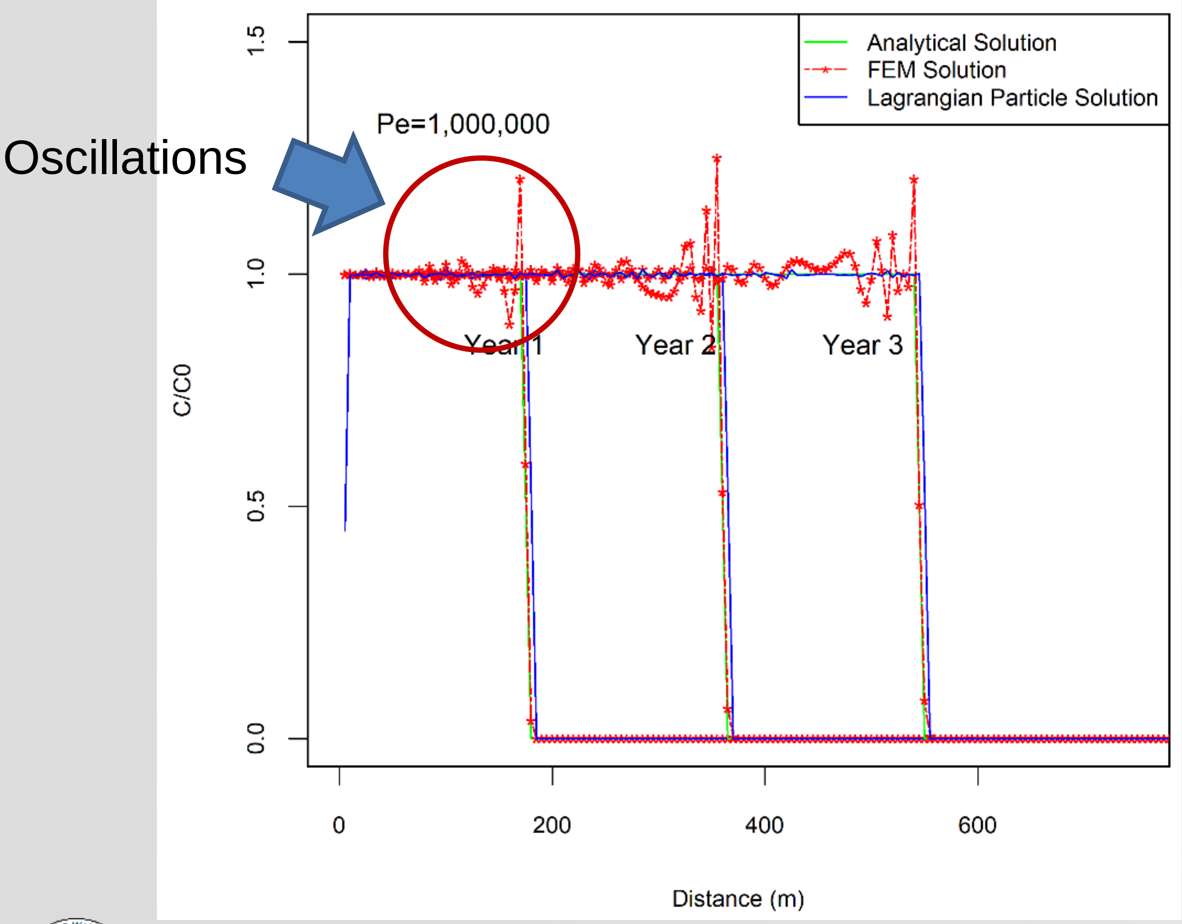


Petrov-Galerkin (Pe=100)

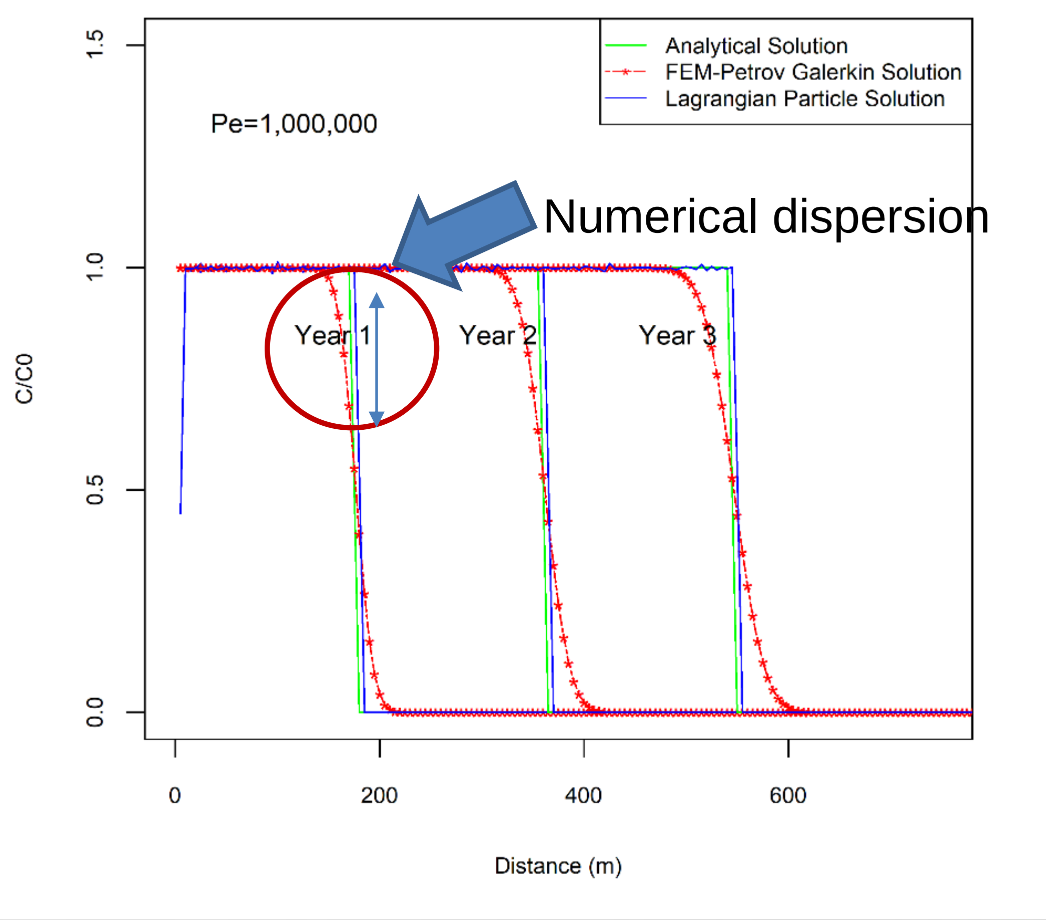


Petrov Galerkin Stabilization-Results-Pure advection case

Galerkin (Pe=1,000,000)



Petrov-Galerkin (Pe=1,000,000)



Oscillations issue can be resolved at the expense of some numerical dispersion

Instantaneous Release of a Contaminant

MT3D example-2D (Wilson and Miller, 1978): Pe=1

Uni-directional flow

Cell width along rows (Δx) = 10 m	
Cell width along columns (Δy) = 10 m	
Layer thickness (Δz) = 10 m	
Groundwater seepage velocity (v) = 1/3 m/day	X-dir. only
Porosity (θ) = 0.3	
Longitudinal dispersivity = 10 m	
Ratio of transverse to longitudinal dispersivity = 0.3	
Volumetric injection rate = 1 m^3/day	
Concentration of the injected water = 1000 ppm	
Simulation time (t) = 365 days	

$$Pe_{xx} = \frac{u_x dx}{D_x} \qquad Pe_{yy} = \frac{u_y dy}{D_y}$$

$$D_{xx} = \alpha_L \frac{{u_x}^2}{|V|} + \alpha_T \frac{{u_y}^2}{|V|}$$

$$D_{yy} = \alpha_L \frac{{u_y}^2}{|V|} + \alpha_T \frac{{u_x}^2}{|V|}$$

$$where \quad |V| = \sqrt{{u_x}^2 + {u_y}^2}$$

D_{xx} =10*(1/3)^2/(1/3)+0=10/3

D_{yy} =0+10*0.3*(1/3)/(1/3)=0.3

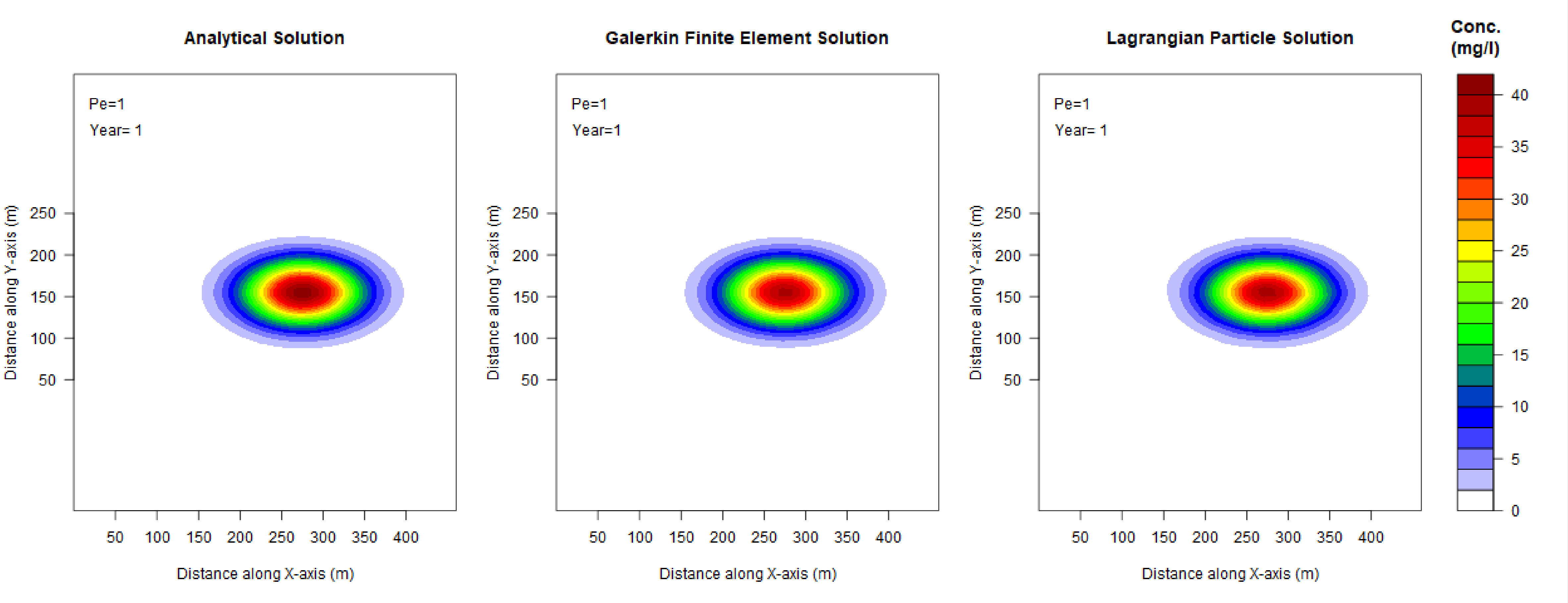
Pe_x=(1/3)*10/(10/3)=1

Pe_y=0*10/(0.3)=0

Pe_x=max(Pe_x, Pe_y) = 1

Concentrations - after 1 yr (Pe=1)

Release location (150 m, 150 m) dt=1 day, dx= dy=10 m



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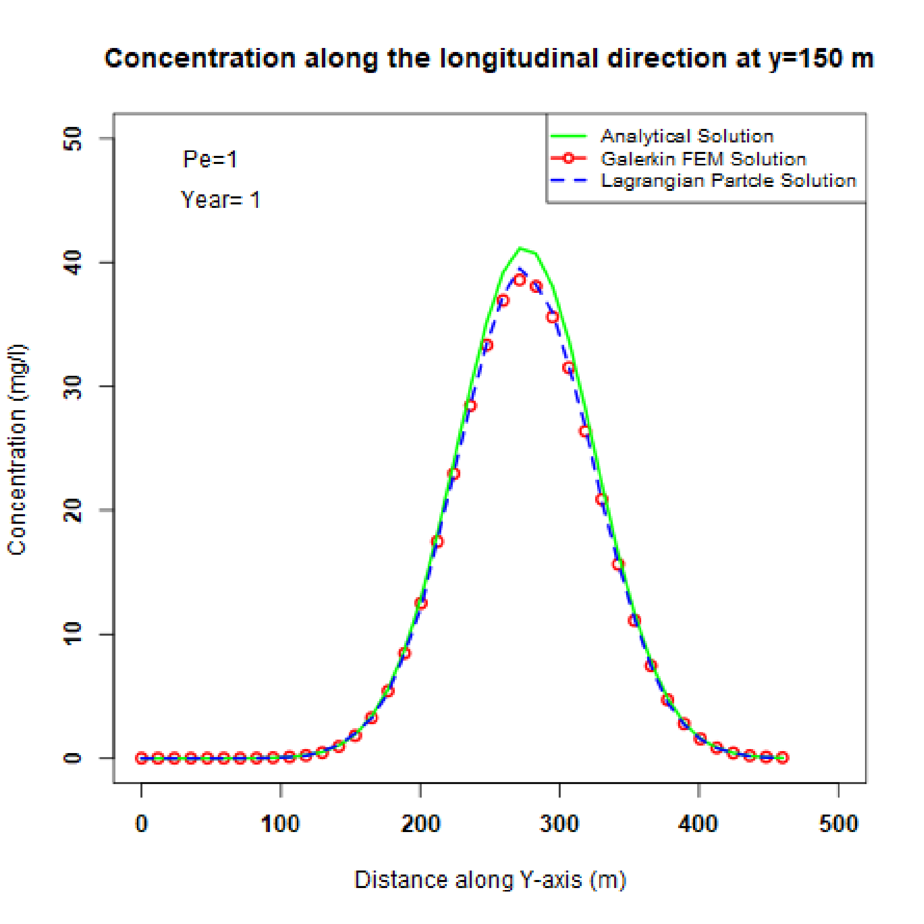
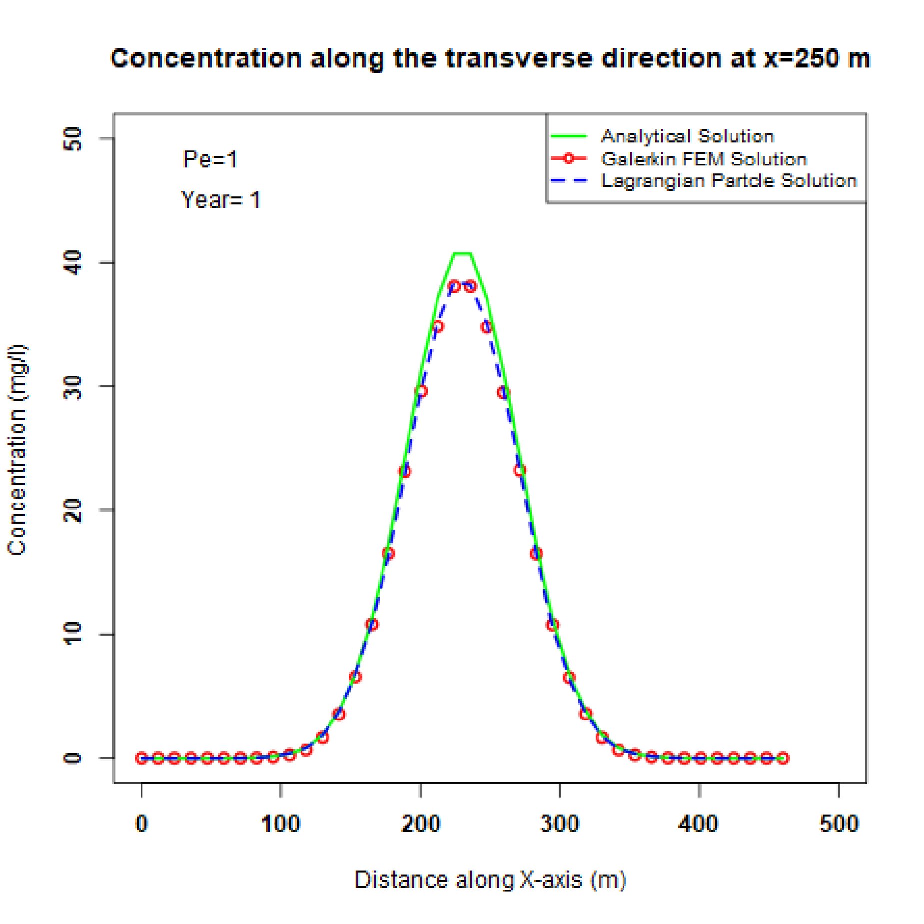
Analytical Solution by Wilson and Miller, 1978

Concentrations - after 1 yr (Pe=1)

Release location (150 m, 150 m)   dt=1 day, dx= dy=10 m





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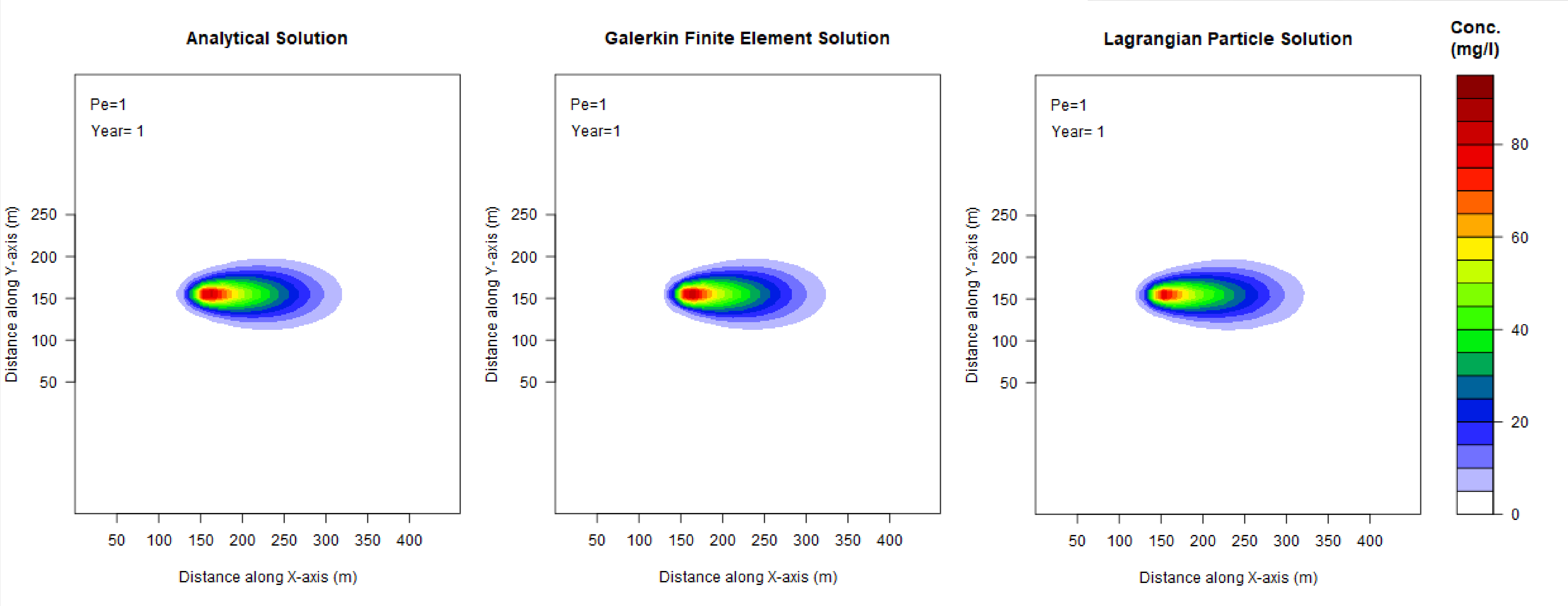
Continuous Release-Concentrations - after 1 year (Pe=1)

Uni-directional flow

Release location (150 m, 150 m)

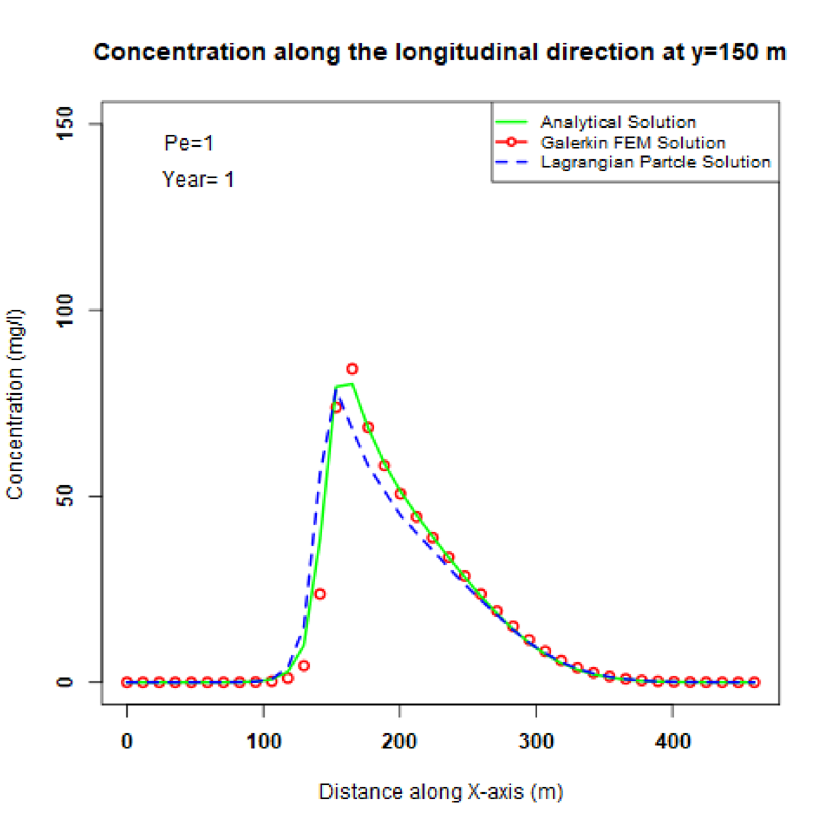
dt=1 day, dx= dy=10 m

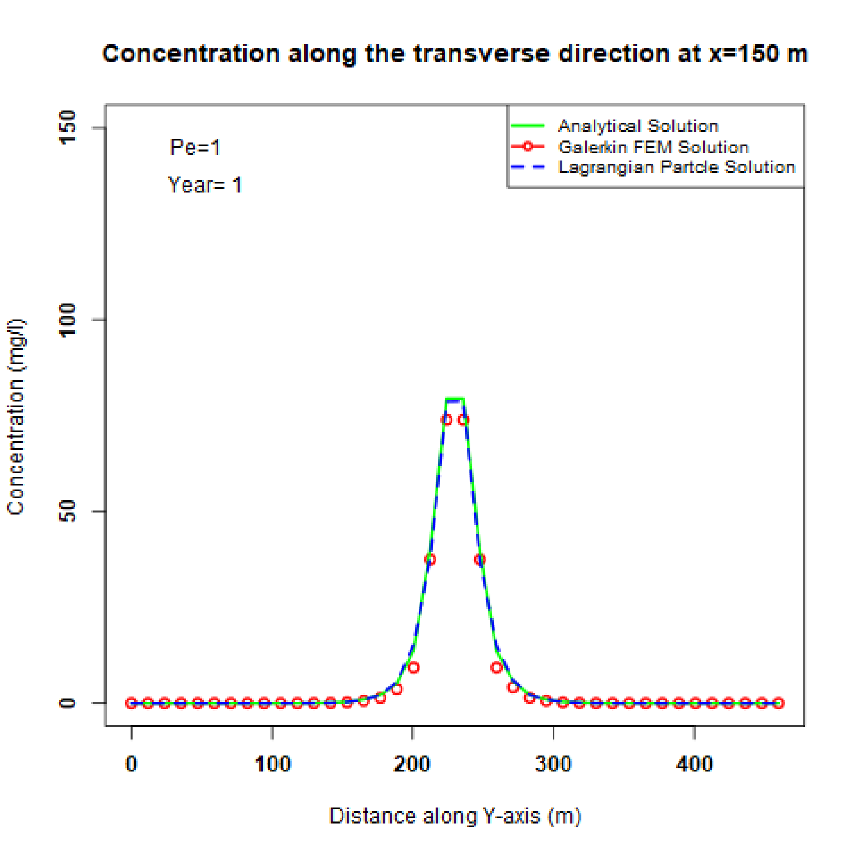


Analytical Solution by Wilson and Miller, 1978

Continuous Release-Concentration Profiles - after 1 year (Pe=1)

Release location (150 m, 150 m)





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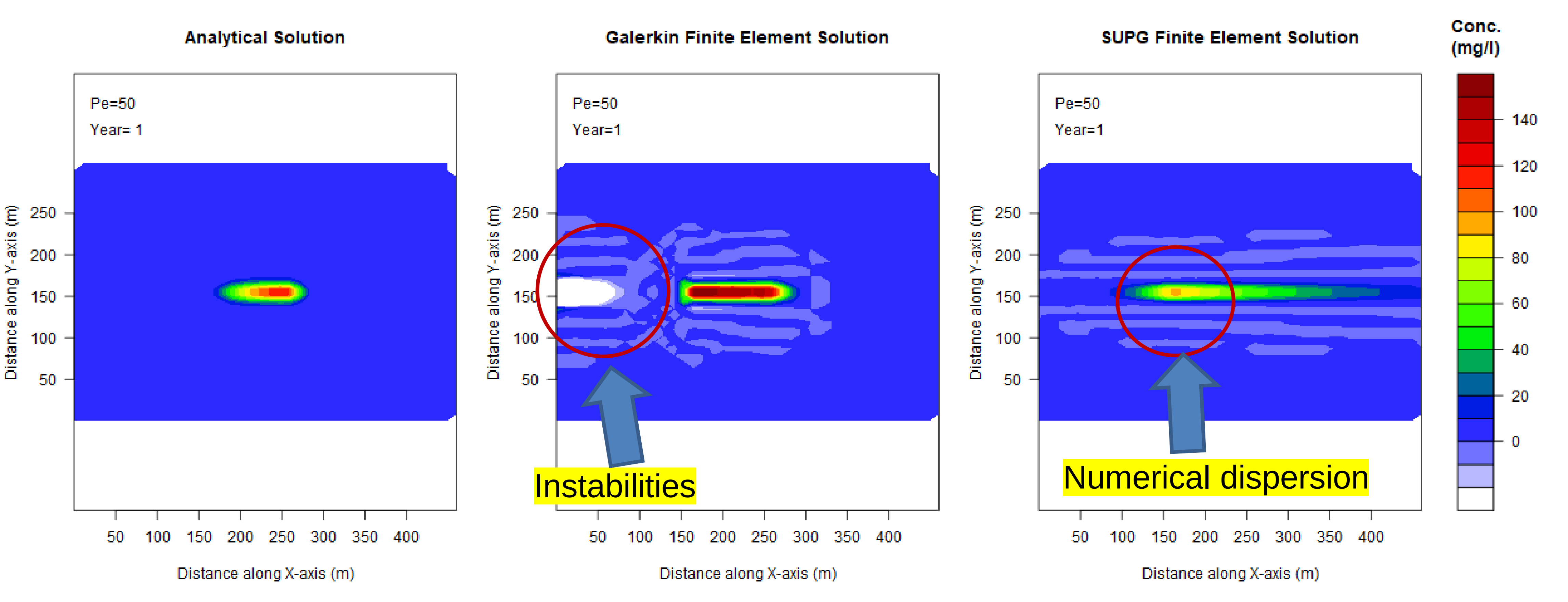
Continuous Release-Concentrations - after 1 year SUPG Stabilization (Pe=50)

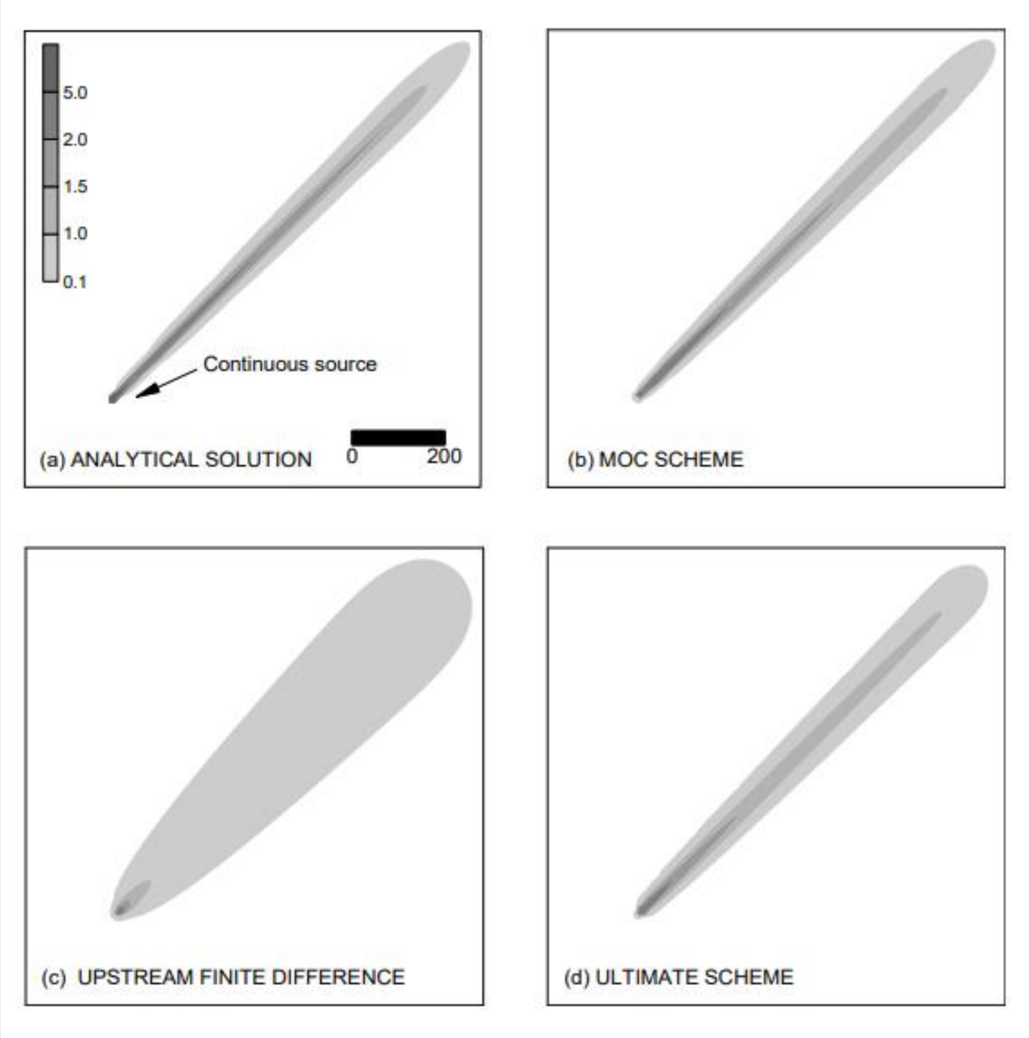
Release location (150 m, 150 m)

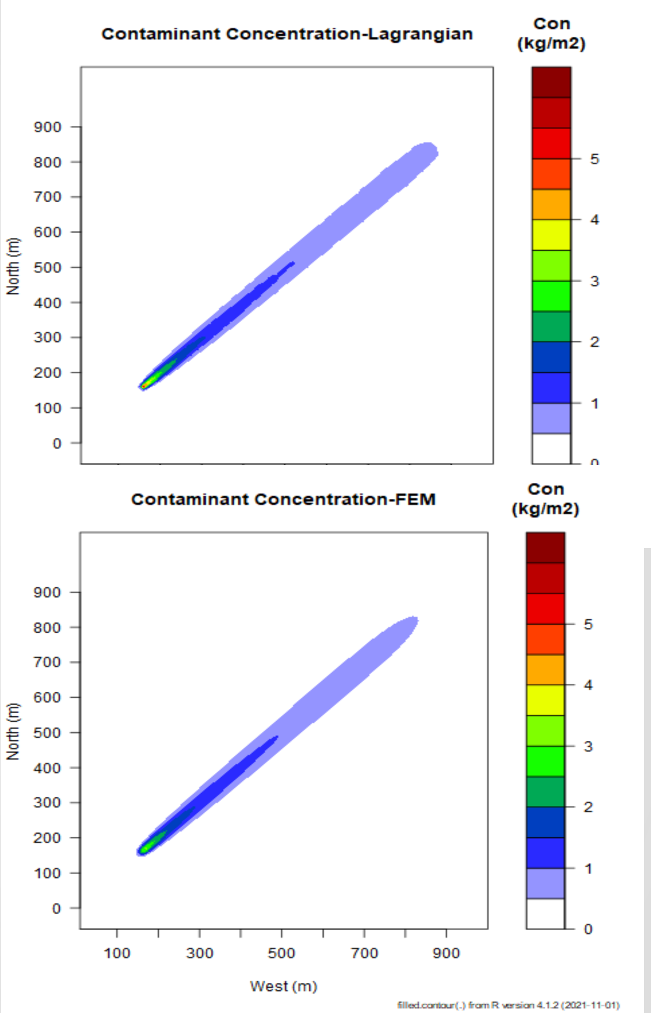


Instabilities can be resolved at the expense of some numerical dispersion

MT3D Example : Diagonal Flow Field

Multi-directional flow





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Colorado Rocky Mountain Arsenal (RMA) site-

Konikow-1979

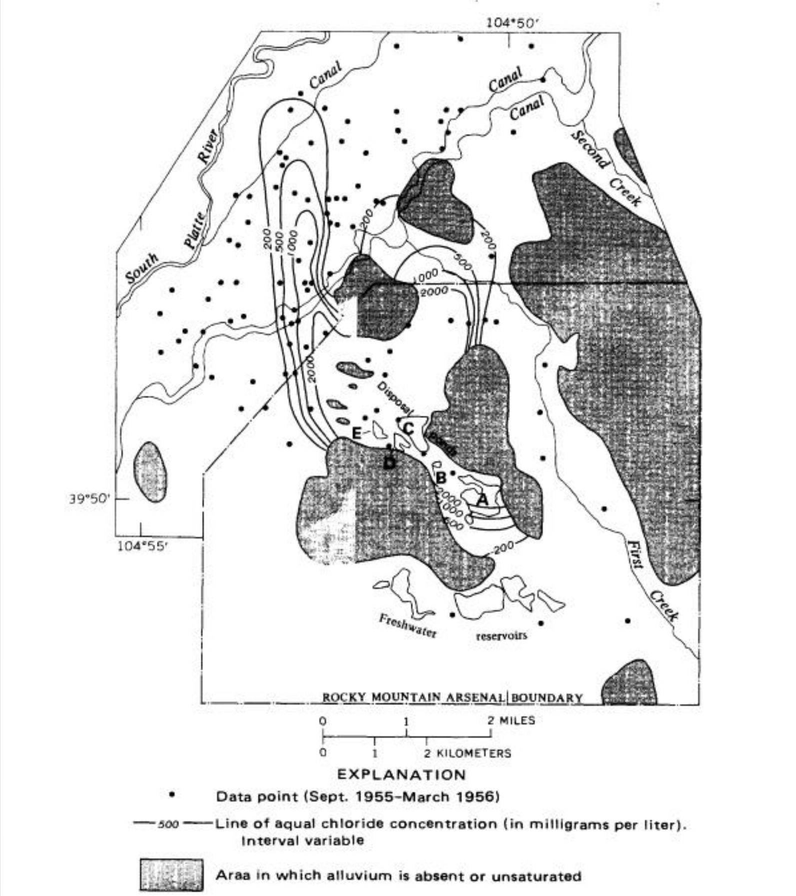


FIGURE 3.— Observed chloride concentration, 1956.

SUTRA-simplified conceptualization

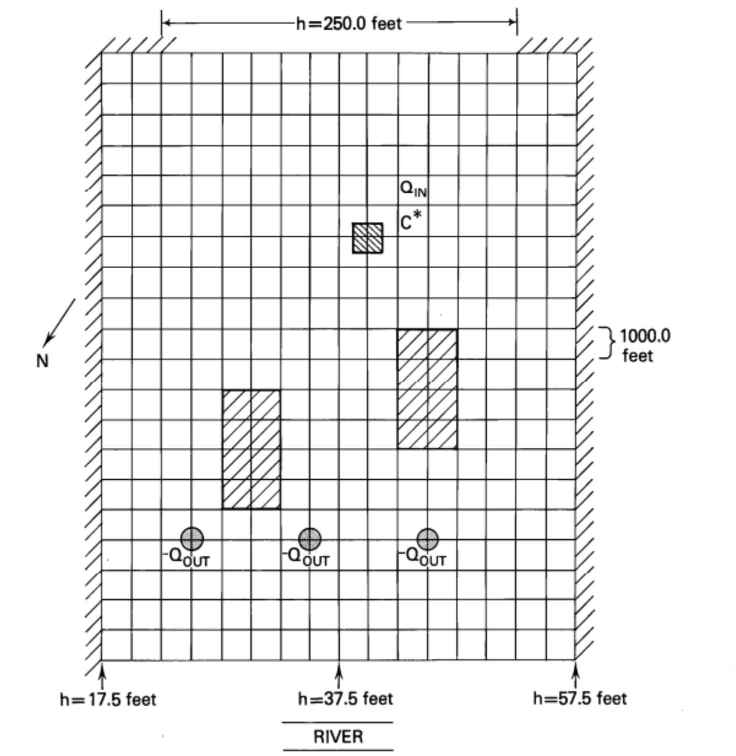
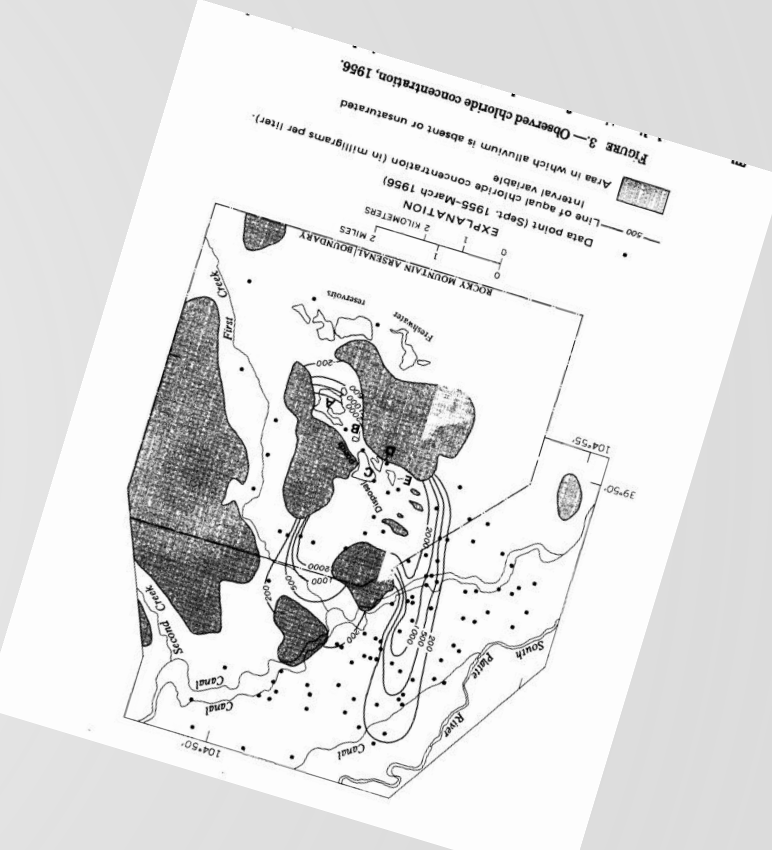


Figure 6.6. Idealized representation for example at Rocky Mountain Arsenal, and finite-element mesh. Upper shaded square is the pond, shaded rectangles are impermeable zones, and three circles are wells.



Discharge concentration=1000-mg/l
Aquifer thickness= 18 m
Horizontal Dispersivity= 100 m
Transverse Dispersivity=100 m
Effective Porosity=0.3

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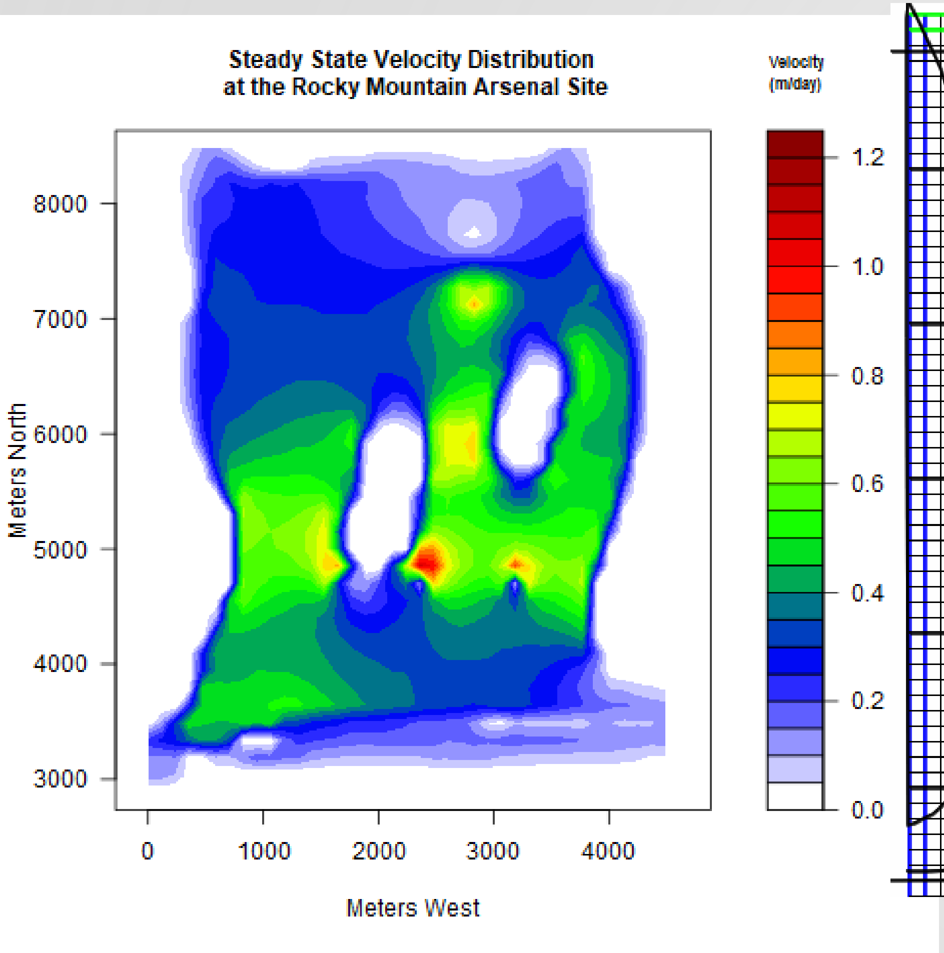
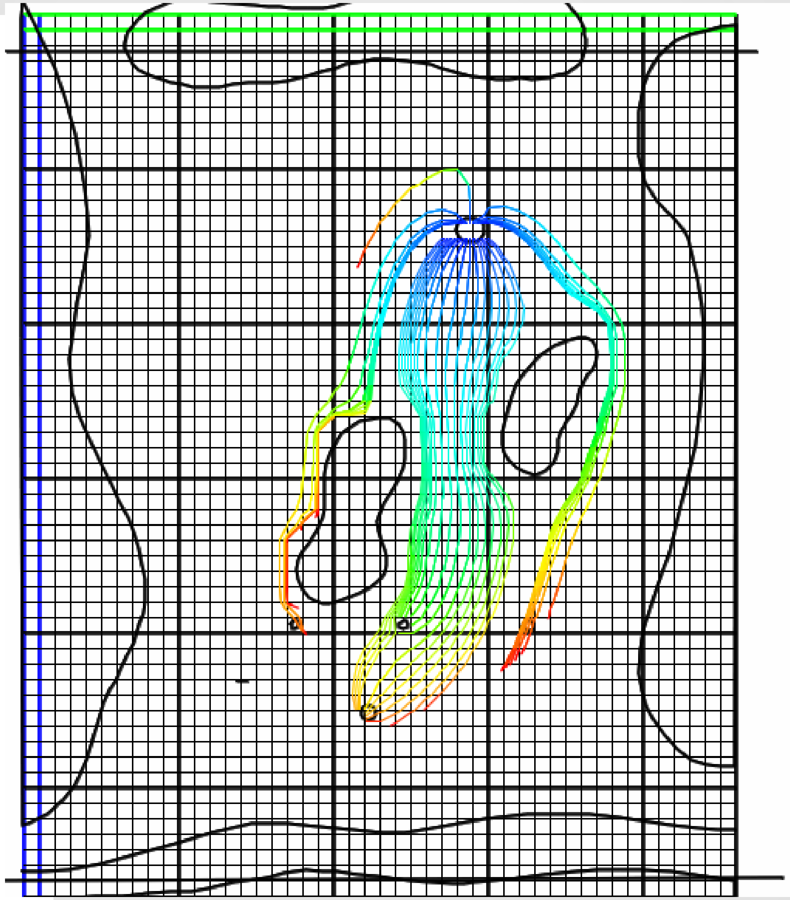
Rocky Mountain Arsenal (RMA) site- MODFLOW simulation

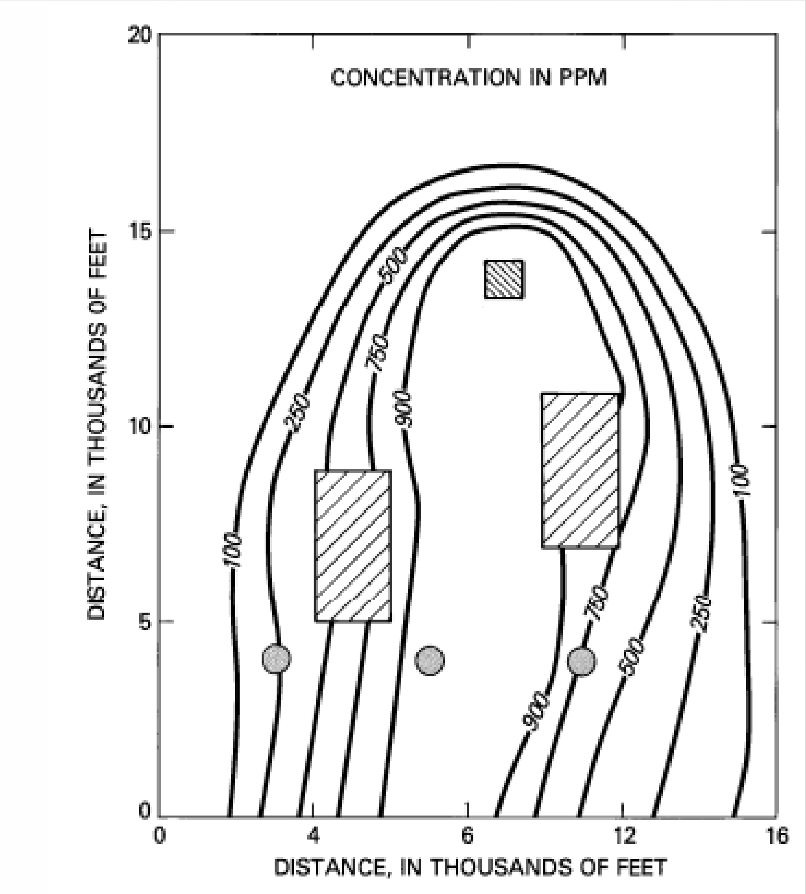
MODFLOW Velocity Distribution



MODPATH Distribution



SUTRA-steady state concentrations



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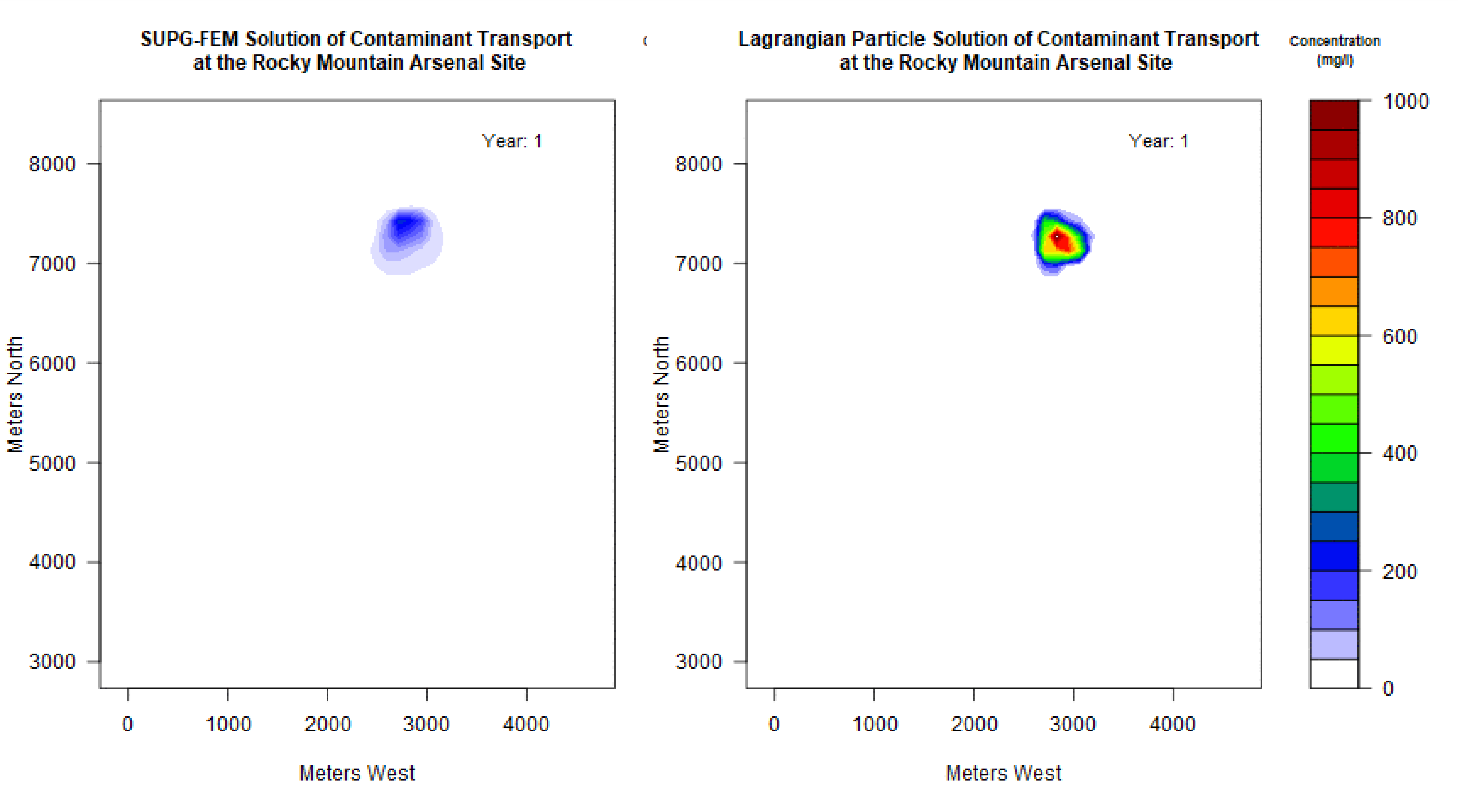

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Summary & Next Steps

- Finite Element and Lagrangian based solutions for solute transport problems are developed and verified
- Next: Integration with IWFM
  - Time step level integration
  - Implement solute transport within streamflow module
  - Multi-species transport
  - Testing and verification with field data
  - Expected completion by Spring of 2024
- Long term goal: Density dependent flow model
  - Required for the saltwater intrusion modeling
  - Solute concentration impacts the flow field and vice versa-fully coupled run
  - Requires changing flow equation in IWFM code to account for variable density