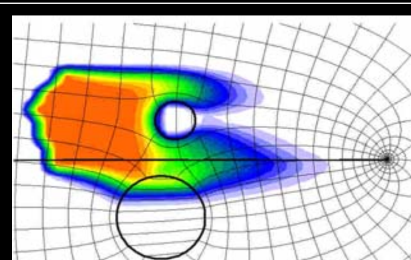
An Overview of Using Analytic Element Flow Solutions for Contaminant Transport Simulation



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Background: AEM & Transport

- AEM is conventionally used for water resources rather than water quality investigations
  - Capture zone delineation
  - SW/GW interaction
  - Water budgets
- Groundwater flow models are increasingly used for the sole purpose of developing a contaminant transport model
  - AEM can, and should, be part of this

Background: AEM & Transport

- Strack (1992); Strack & Fairbrother (1997)
  - Moving front dispersion models
- Rumbaugh (1993)
  - Finite element (2D) (WinFlow-WinTran)
- Grasshoff et al. (1994)
  - Finite difference methods (3D) (MLAEM-STYX)
- Soule (1997)
  - Streamline-based air venting
- Everybody
  - Particle tracking, a bit of random walk

- Recent research has addressed how best to simulate reactive contaminant transport using general 2D AEM flow solutions – standard ADRE (Craig PhD 2005)

Overview

- Current scope of research
- AEM-based discrete modeling*
  - Finite element
  - Finite difference
- AEM-based semi-discrete modeling
  - Random walk
  - Streamline methods
- AEM-based continuous modeling
  - Coordinate-mapped transport solutions
  - AEM for transport??
- Future Research

Current Focus

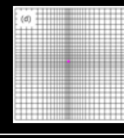
- 2D (vertically-averaged) reactive transport in single layer systems
  - Conceptually consistent with 2D D-F assumption
  - Concentration averaged over saturated thickness, *h*, of aquifer

$$h\theta\frac{\partial C}{\partial t} = -Q_x\frac{\partial C}{\partial x} - Q_y\frac{\partial C}{\partial y} + \frac{\partial}{\partial x}\left(h\theta D_{xx}\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial x}\left(h\theta D_{xy}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial y}\left(h\theta D_{yx}\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(h\theta D_{yy}\frac{\partial C}{\partial y}\right) + N_t^+\left(c_t^+ - C\right) + N_b^+\left(c_b^+ - C\right)$$

Discrete modeling

- Translate analytic element flow solutions to a discrete analog for use as input to FD/FE transport simulators
  - Finite element (FE)
  - Finite difference (FD)
  - Eulerian-Lagrangian methods
    - Characteristic Methods (e.g., MMOC, ELLAM)
    - Flux-limiting methods (TVD)
- Requires significant bookkeeping/geometric processing
  - Primary difficulty is the maintenance of the exact water balance during translation

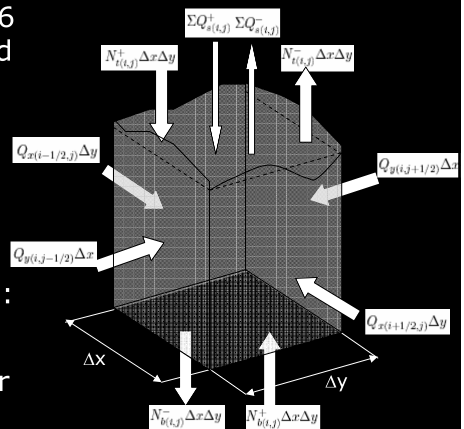
Finite difference Methods



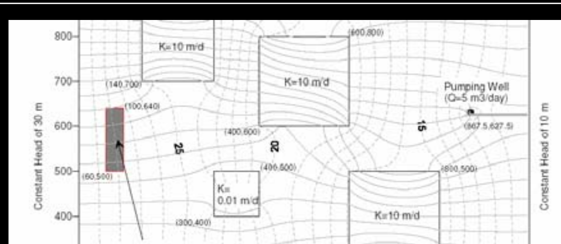
- Craig and Rabideau, 2006
- Fluxes may be discretized along cell faces (stream function or analytic integration)

$$\int_{z_1}^{z_2} Q_\eta(z)\,\mathrm{d}z = \sum_{e=1}^{N_E} \int_{z_1}^{z_2} \underset{e}{Q_\eta(z)}\,\mathrm{d}z$$

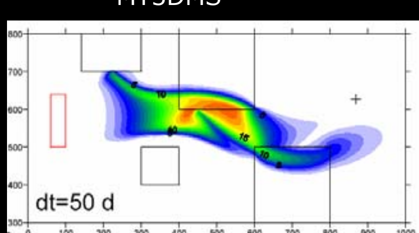
- Cell-averaged saturated thicknesses may be used: method just needs to be consistent, not exact
- Can maintain exact water balance! → Exact solute mass balance
- Grid orientation effects still an issue



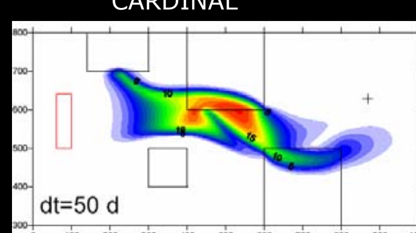
Finite Difference Methods



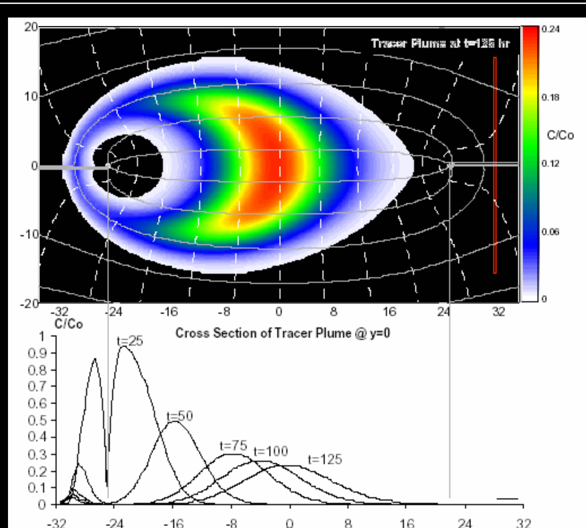
MT3DMS



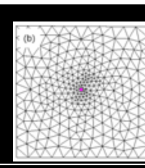
CARDINAL



Finite Difference Methods

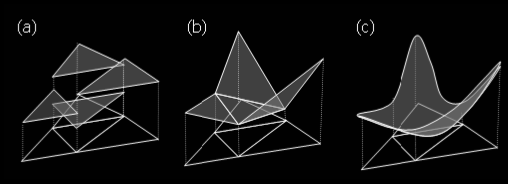


Finite Element methods



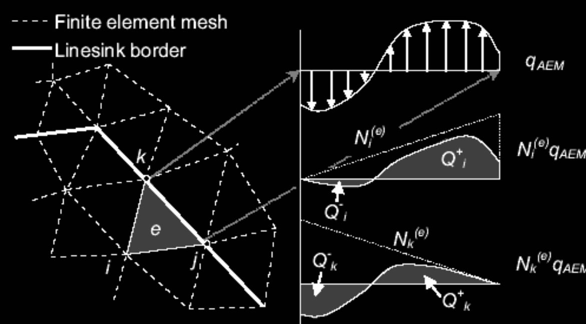
- Craig & Rabideau (in review)
- Minimizes space-integrated error between approximate solution (composed of superimposed basis functions) and exact PDE
- Translation requires clever evaluation of finite element residual expressions:
  - Methods for distributing linesink, area sink fluxes
  - Methods for integrating singular residuals (v~1/r)
  - Discretization rules:
    - Finite element sides coincide with analytic element sides
    - Special unstructured mesh generator developed
  - Means of handling AEM-based discontinuities in saturated thickness (e.g., Leaky wall)
- Important result:
  - ***Cannot*** export nodal heads from AEM flow solution to standard FE simulator and still have accurate transport
  - ***Can*** export element-averaged velocities, *if* singular flow is minimal
  - Best option: FE simulator has full knowledge of AEM solution

Finite Element Methods



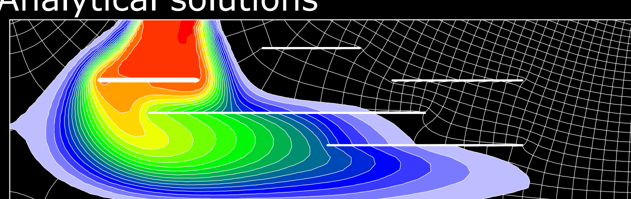
Velocity distributions
(a) piecewise
(b) nodal
(c) continuous

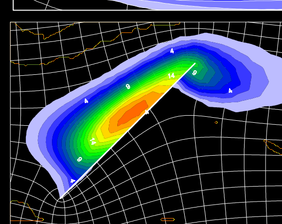
Flux distributions to finite element nodes using standard basis functions & numerical integration

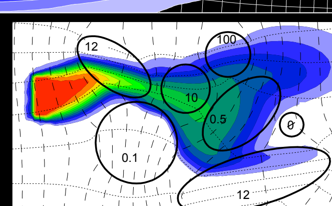


Finite Element Methods

- Benchmarked against FEFlow, MT3DMS, Analytical solutions







Semi-Continuous Methods

- Random walk
  - Easy to implement, no translation required
  - Number of required particles is prohibitive; tracking is expensive for difficult models
- Deterministic streamline methods
  - 1D transport equation solved along streamlines (neglects transverse dispersion)
  - Streamline geometry benefits from exact flow field
  - Translation is simple, mass balance inexact
- Both methods would benefit from faster tracking routines (Taylor Series/Superblocks for tracking?)

Fully Continuous Methods

- Is it possible to have fully analytical flow and transport?
- Unlikely, but we can come pretty close

Coordinate Mapping

- Particular Solutions (2D):
  - If we can get z=f(Ω), we can obtain approximate steady-state (SS) transport solutions for some special cases
- In the Ω domain, the SS-ADE can be approximated with constant coefficients :

$$-\frac{\partial C}{\partial \Phi}+\overline{D}_l\frac{\partial^2 C}{\partial \Phi^2}+\overline{D}_t\frac{\partial^2 C}{\partial \Psi^2}=0$$

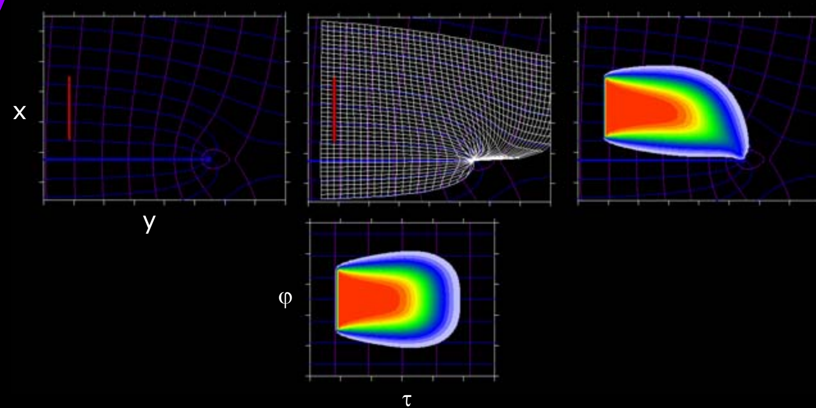
- z=f(Ω)
  - SS Injection Well & Decay?
  - SS Pumping Doublet w/ decay?

Coordinate Mapping

- z=f(Ω) is unattainable for complex systems
  - recharge, branch cuts, multiple roots…
- Mappings are still possible in terms of numerically-calculated time-of-flight (τ)
  - TOF, τ , obtained from AEM-generated pathlines
  - Revised constant-coefficient ADE in τ-φ coordinate system
    - Amenable to analytical or semi-analytical solutions in transformed domains
    - Exact when transverse dispersion is negligible

Coordinate mapping

- $$\frac{\partial C}{\partial T} = -\left(1 - \alpha_l \frac{N}{\overline{Q}_s}\right)\frac{\partial C}{\partial \tau} + \frac{\alpha_l}{\overline{v}_s}\frac{\partial^2 C}{\partial \tau^2} + \alpha_t \overline{v}_s \frac{\partial^2 C}{\partial \psi^2} - NC$$



Conclusions

- Multiple methods for AEM-based transport simulation have been developed
  - Translation is not trivial
  - Grid-free nature of AEM is beneficial
- Future Research
  - Multilayer systems
  - 3D transport in 2D D-F systems**
  - 3D transport in 3D AEM models
  - Further development of streamline models
  - Further development of coordinate-mapped analytic solutions
  - Specific methods:
    - Transport through drain elements
    - Better handling of distributed singular flow (FE)