Groundwater modeling: solute transport simulation

A. Dassargues

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Groundwater modeling: solute transport simulation

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**Processes and equations**

**Molecular diffusion**

... mass of solute diffusing from high to low solute concentrations

\[ f_m = -D_m \nabla (\rho C) = -D_m \nabla (\rho C) \]

\[ f_m = -D_m \nabla C^v = -D_m \nabla C^v \]

- molecular diffusion mass flux per surface unit (kg/(m².s))
- effective diffusion coefficient of the solute in the porous medium (m²/s)

Processes and equations

Advection

… solute motion at the same velocity than water = effective groundwater velocity

\[ f_a = q \rho C \]
\[ f_a = q C^v \]
\[ f_a = -K \cdot \nabla h \, C^v = -K \cdot \nabla h \, (\rho C) \]

\[ \nu_a = q / n_m \]

effective (transport) porosity (-)
...about mobile water porosities

the ‘mobile water porosity’ to be considered for groundwater flow is typically higher than the ‘mobile water porosity’ acting in solute transport processes (Payne et al. 2008, Hadley and Newell, 2014)

Box 8.1 About effective transport porosity

Effective transport porosity is in reality very dependent on what we define as mobile and immobile groundwater in the representative volume of geological medium. For many contamination problems and associated risk assessments, it is very important to predict the first arrival time of solute contaminant at a “target.” This is the case, for example, for protection zone delineation around a pumping well, for security assessment of waste disposal, for assessment of risk created by industrial contamination hazards, and for groundwater vulnerability mapping. To be conservative (i.e., on the security side) with regards to most practical applications where solute transport is calculated, one should choose to define the effective porosity relevant to solute advection as a relatively small part of the total porosity. This is especially true and important if the geological medium is known as a “dual” porosity medium or is highly heterogeneous at the micro- and macroscales. If the Darcy flux (i.e., specific discharge, see Chapter 4, Section 4.4) would be divided by the total porosity \( n \), this would produce a kind of averaged velocity between the mobile and immobile groundwater in the medium which can be highly misleading (i.e., leading to underestimated velocities). However, some can argue that this could be partially and artificially compensated or corrected by considering larger values of the longitudinal dispersivity.

(Dassargues 2018 and 2020)
Processes and equations

Mechanical dispersion

... dispersion mass flux most often described by a Fick law:

\[ f_d = -n_m D \cdot \nabla (\rho C) = -n_m D \cdot \nabla \rho C \]
\[ f_d = -n_m D \cdot \nabla C^v = -n_m D \cdot \nabla C^v \]

mechanical dispersion tensor \((m^2/s)\)

... in a uniform velocity gw flow and with an axis // to the velocity vector

a linear relation between \(D\) and \(v_a\)

\[
D = \begin{bmatrix}
D_{xx} & D_{yy} \\
D_{yy} & D_{zz}
\end{bmatrix}
\]

longitudinal dispersivity \((m)\)

transversal dispersivity \((m)\)

\[ D_{xx} = a_L v_{a_x}, \quad D_{yy} = a_T v_{a_x}, \quad D_{zz} = a_T v_{a_x}, \]
with \(v_{a_y} = v_{a_z} = 0\)
... in practice, it is not easy to determine the longitudinal and transversal dispersivities in most cases:

\[ 3 \leq \frac{a_L}{a_T} \leq 10 \]

... in the case where this ratio is < 3 or >10 (on the basis of laboratory or tracer tests)

anisotropy of the fissured or porous medium

Mechanical dispersion

The scale effect in longitudinal dispersivity

As a result, measured (or apparent) values of the longitudinal dispersion coefficient $D_L^*$ increase accordingly.

An apparent dispersion coefficient is a dispersion coefficient measured in the field. As it integrates variations in velocity at a macroscopic scale, it is larger than the local dispersion coefficient, corresponding to variations in velocity at a microscopic scale.

As spatial scale increases, a contaminant plume experiences more and more heterogeneities.

(Pinder & Celia 2006, Zech et al. 2015, 2016, )
Processes and equations

**Mechanical dispersion + diffusion = hydrodynamic dispersion**

\[
D_h = D + D_m = D + D_m I
\]

**Hydrodynamic dispersion tensor \((m^2/s)\)**

\[
f_h = -n_m(D_h) \cdot \text{grad} \ (\rho C) = -n_m(D_h) \cdot \nabla (\rho C)
\]

\[
f_h = -n_m(D_h) \cdot \text{grad} \ C^v = -n_m(D_h) \cdot \nabla C^v
\]
Processes and equations

Equation of advection-dispersion

... mass balance equation for the solute with advection-dispersion:

\[ n_m \frac{\partial C^v}{\partial t} = -\text{div}(f_a + f_h) = -\nabla \cdot (f_a + f_h) \]

\[ n_m \frac{\partial C^v}{\partial t} = -\text{div}(qC^v - n_m(D_h) \cdot \text{grad } C^v) = -\nabla \cdot (qC^v - n_m(D_h) \cdot \nabla C^v) \]

in 1D (direction supposed // to the gw flow velocity):

\[ \frac{\partial C^v}{\partial t} = -v_a \frac{\partial C^v}{\partial x} + a_L v_a \frac{\partial^2 C^v}{\partial x^2} \quad \text{boundary cond.} \]

\[ \lim_{x \to \pm \infty} C^v(x, t) = 0 \]

\[ C^v(0,0) = C_0^v \]

punctual injection

Analytical solution:

\[ C^v(x, t) = \frac{C_0^v}{2} \text{erfc} \left[ \frac{x - v_a t}{\sqrt{4a_L v_a}} \right] \]

(Ogata and Banks 1961)

'Gaussian dispersion' with:

\[ \mu \leftrightarrow v_a t \]
\[ \sigma^2 \leftrightarrow 2a_L v_a t \]
Processes and equations

Adsorption-desorption

... in the simplest case: isothermal conditions

\[ \bar{C} = K_d \cdot \rho \cdot C \]

equilibrium relations in the REV

mass concentration adsorbed on the solid per mass unit of solid (-)

mass concentration of solute in groundwater

(Davis and Kent 1990)

partitioning coefficient (m³/kg)

\[ K_d \] varies from a medium to another (higher for clay)

in the solute mass balance equation can be expressed by

\[ -\rho_b R_{w,s} \text{ (kg/m}^3\text{s)} \]

a retardation coefficient multiplying

\[ R = \left[ 1 + \left( \frac{\rho_b}{\theta} \right) K_d \right] \]

bulk-density \( \rho_b = (1 - n) \rho_s \)

water content in volume
Processes and equations
Adsorption-desorption

... many more intricated equilibrium or non-equilibrium relations

many physical processes and chemical reactions can be introduced similarly creating a delay of the contamination
Processes and equations

Degradation/decay

... tens of reactions or part of reactions
... equilibrium or non-equilibrium conditions
... locally very different equilibrium conditions, depending on the nature of the medium and of the gw flow velocity

Rough approximation:

- linear decay of the solute
- non-linear decay of the solute

\[ \frac{\partial C}{\partial t} = -\lambda C \]

linear decay constant \((s^{-1})\)

decay coefficient

\[ \frac{\partial C}{\partial t} = -\Gamma (C)^m \]

exponent depending on the reaction stoichiometry
Processes and equations
Degradation/decay

in the solute mass balance equation can be expressed by

\[-n\lambda \rho C \ (kg/m^3s)\]
Processes and equations

Solute mass conservation equation

\[ \frac{\partial}{\partial t} (n_m C^v) = -\nabla \cdot f_a - \nabla \cdot f_d - \nabla \cdot f_m - \rho_b \mathcal{R}_{w,s} - n\lambda C^v + M^v \]

\[ \frac{\partial}{\partial t} (n_m C^v) = -\nabla \cdot (q C^v) + \nabla \cdot n_m (D \cdot \nabla C^v) + \nabla \cdot n (D_m \nabla C^v) - \rho_b \mathcal{R}_{w,s} - n\lambda C^v + M^v \]
Processes and equations

- most often \( n \) is reduced to \( n_m \) in the solute mass balance equation (diffusion and degradation considered only in the mobile water)

- solute mass balance expressed on the solid

solute mass balance equation in the mobile water (kg/m\(^3\)s):

\[
R \frac{\partial C^v}{\partial t} = -\nabla \cdot (\nu_a C^v) + \nabla \cdot (D_h \cdot \nabla C^v) - R\lambda C^v + \frac{M^v}{n_m}
\]

with:

\[
R = \left(1 + \frac{\rho_b}{n_m} K_d \right)
\]
Processes and equations

Discussion about the source/sink term

\[ M^v = q_s C_s^v \]

- \( q_s \) = volumetric flow rate per unit volume of porous medium (s\(^{-1}\)) flowing into \((q_s > 0)\) or flowing out from \((q_s < 0)\)
- \( C_s^v \) = the associated concentration (kg/m\(^3\))

- if \( q_s < 0 \), automatically \( C_s^v = C^v \) because any groundwater flowing out is assigned the local concentration

\[ R \frac{\partial C^v}{\partial t} = - \nabla \cdot (v_a C^v) + \nabla \cdot (D_h \cdot \nabla C^v) - R \lambda C^v + \frac{M^v}{n_m} \]

\[ \nabla \cdot (v_a C^v) = C^v \nabla \cdot v_a + v_a \cdot \nabla C^v \]

- if groundwater is assumed incompressible (as previously), the only internal change in \( v_a \) is due to sources or sinks

\[ C^v \nabla \cdot v_a = C^v q_s \]

\[ R \frac{\partial C^v}{\partial t} = - v_a \cdot \nabla C^v + \nabla \cdot (D_h \cdot \nabla C^v) - R \lambda C^v - \frac{q_s}{n_m} \left( C^v - C_s^v \right) \]

(Rausch et al. 2005)
Processes and equations

Discussion about the source/sink term

\[ R \frac{\partial C^v}{\partial t} = -v_a \cdot \nabla C^v + \nabla \cdot (D_h \cdot \nabla C^v) - R \lambda C^v - \frac{q_s}{n_m} (C^v - C^s) \]

Remarks:

1) if \( C_s^v = C^v \) (outflowing groundwater)
   - last term = 0 (concentrations are not influenced)
2) if \( C_s^v < C^v \) injection at lower concentration than existing
   - dilution of the solute = decreasing concentration in the system
3) if \( C_s^v > C^v \) injection at a higher concentration than existing
   - increase of local concentration in the domain

(Rausch et al. 2005)
Immobile water effect = ‘matrix diffusion’

... a part of groundwater is not so mobile with regards to mobile water in preferential pathways or fissures

Diffusion between mobile water and immobile water

Linear relation:

\[ f_{m}^{im} = \alpha_d^m (\rho C - \rho_{im} C_{im}) \]
\[ f_{m}^{im} = \alpha_d^m (C^v - C_{im}^v) \]

(Gerke & van Genuchten 1993)
**Processes and equations**

**Immobile water effect** = ‘matrix diffusion’  
= diffusion between immobile and mobile water

... a solute mass balance equation in the immobile water should be used:

$$\frac{\partial}{\partial t} (n_{im} C_{im}^v) = f_{m}^{im} - \lambda n_{im} C_{im}^v$$


**neglecting diffusion within immobile water and adsorption-desorption between immobile water and solid matrix**

**term to be added to the solute mass balance equation in the mobile water**
Solute transport equations

multi-species reactive transport in mobile groundwater

\[
R_i \frac{\partial C_i^v}{\partial t} = -v_{a_i} \nabla C_i^v + \nabla \cdot (D_h \cdot \nabla C_i^v) - R_i \lambda_i C_i^v - \frac{q_s}{\theta_i} (C_i^v - C_{s_i}^v) + \frac{1}{\theta_i} \sum_{j=1}^{N_s} S_{ij}(C_1^v, ..., C_n^v)
\]

where \( S_{ij} = \) source/sink term representing the effect of reactions (kg/m\(^3\)s), \( \theta_i = \) groundwater specific volume fraction of the REV where species \( i \) is located

\[ \rightarrow \text{as many equations as species in the reaction system: } N_s \]
\[ \rightarrow \text{equations are coupled through the } S_{ij}(C_1^v, ..., C_n^v) \text{ terms} \]

If all reactions occur in the water phase, \( \theta_i \) are all equal to \( n_m \) and the components of \( v_{a_i} \) are all equal to \( v_a \) (i.e. the advection velocity)

\[ \rightarrow \text{homogeneous reaction system} \]

On the contrary, if a part of the involved species is on the solid matrix or in the immobile water

\[ \rightarrow \text{heterogeneous reaction system } (v_{a_i} \text{ and } D_h \text{ being equal to zero for the species in those immobile phases}) \]

Solute transport equations

Boussinesq approximation for density dependent flow and transport

Advection, dispersion, diffusion + adsorption/desorption + dégradation

\[ R \frac{\partial (\rho(C)C)}{\partial t} = - \mathbf{v}_a \cdot \nabla (\rho(C)C) + \nabla \cdot (\mathbf{D}_h \cdot \nabla (\rho(C)C)) - R\lambda \rho(C)C \\
- \frac{q_s}{n_m} (\rho(C)C - \rho(C_s)C_s) \]

‘Boussinesq approximation’: the only non-negligeable influence of the change in gw density is taken into account in the Darcy’s law : \((\mathbf{v}_a \cdot \nabla C)\)

\[ R \frac{\partial C}{\partial t} = - \mathbf{v}_a \cdot \nabla C + \nabla \cdot (\mathbf{D}_h \cdot \nabla C) - R\lambda C - \frac{q_s}{n_m} (C - C_s) \]

(Holzbecher 1998)

\[ \mathbf{v}_a = \frac{q}{n_m} = - \frac{k \rho g}{\mu n_m} \nabla h = - \frac{k}{\mu n_m} (\nabla p + \rho g \nabla z) \]
Transport Boundary Conditions

Full analogy with gw flow problem, 3 kinds of BC’s:

- Prescribed concentration (Dirichlet condition)
- First derivative of the concentration is prescribed (Neumann condition)
- A relation between the concentration and its first derivative is prescribed (Cauchy or mixed condition)

Practical examples where groundwater flow and solute transport BCs are discussed on various practical cases are available from the experience of the author and researchers from his team in the following references:

**BC’s for a solute transport problem**

**Prescribed concentration (Dirichlet BC)**

\[ C(x, y, z, t) = g'(x, y, z, t) \]

\( g' \) can vary in space and time

(one value per concerned node and per time step)

in some cases, a non zero prescribed concentration is used for simulating a continuous (long term) source of contamination

however, for numerical reasons, it induces large numerical dispersion

a huge concentration gradient is prescribed abruptly to the system inducing artificial (numerical) dispersion
**BC’s for a solute transport problem**

**Prescribed concentration (Dirichlet BC)**

*Typical case: a zero (or background) concentration prescribed upwards to the problem*

\[ C^v = C_0 = \text{background concentration} \]

\[ C^v = C^v_{\text{source}} = C^v_{\text{max}} \]

*also used for a source of contaminant prescribing \( C^v_{\text{max}} \) in place of \( M_s = q_s C^v_s \)
BC’s for a solute transport problem

- main discussion point: how to translate in the model the actual source of contaminant corresponding to the pollution?
- through the source/sink term? or through prescribed concentrations?
- conceptually, 3 periods in a pollution event
  - First release … recent contamination
  - Possible stable period
  - Decline period … old contamination
BC’s for a solute transport problem

Prescribed first derivative of the concentration
(Neumann BC)

\[ \nabla C^v \cdot \mathbf{n} = \frac{\partial C^v}{\partial n} (x, y, z, t) = g''(x, y, z, t) \]

\( g'' \) the concentration gradient normal to the boundary can vary in space and in time (one value per node and per time step)

\( g'' = 0 \)

… a way of prescribing the dispersion mass flux (hydrodynamic dispersion) on the boundary

In practice, this kind of condition is often used with a zero value for the diffusion-dispersion mass flux through the boundary:

the advective component of the mass flux is computed on the boundary by the code
**BC’s for a solute transport problem**

**Prescribed first derivative of the concentration**

(Neumann BC)

\[ n \cdot (-n_m D_h \cdot \nabla C^v) = -n_m D_{h,n} \frac{\partial C^v}{\partial n} (x, y, z, t) = q''(x, y, z, t) \]

\[ q''(x, y, z, t) \text{ diffusion-dispersion mass flux prescribed on the concerned boundary (kg/(m}^2\cdot\text{s})) \]

\[ D_{h,n} \text{ normal (to the boundary) component of the hydrodynamic dispersion tensor} \]
BC’s for a solute transport problem
Prescribed first derivative of the concentration
(Neumann BC)

example:

\[ C^v = C_0^v \]
\[ \frac{\partial h}{\partial n} = 0 \quad \frac{\partial C^v}{\partial n} = 0 \]

h prescribed
\[ \frac{\partial C^v}{\partial n} = 0 \]

Uniform flow direction

\[ \frac{\partial h}{\partial n} = 0 \quad \frac{\partial C^v}{\partial n} = 0 \]
BC’s for a solute transport problem

**Prescribed relation linking concentration and its first derivative** (Cauchy or mixed Neumann BC)

A linear combination of the concentration and its first derivative is prescribed on the concerned boundary:

$$a \frac{\partial C^v}{\partial n} (x, y, z, t) + b C^v (x, y, z, t) = g''' (x, y, z, t)$$

$g'''$ can vary in space and time
(one value per concerned node and per time step)

A combination (most often the sum) of advection and hydrodynamic dispersion mass fluxes is prescribed
**BC’s for a solute transport problem**

**Prescribed relation linking concentration and its first derivative (Cauchy or mixed Neumann BC)**

**Advection + diffusion-dispersion:**

\[ n \cdot (qC^v - n_m D_h \cdot \nabla C^v) = q_n C^v(x, y, z, t) - n_m D_{h,n} \frac{\partial C^v}{\partial n} (x, y, z, t) \]

\[ = q'''(x, y, z, t) \]

\[ q'''(x, y, z, t) \] total prescribed mass flux (advection + diffusion-dispersion) normal to the concerned boundary (kg/(m².s))

… mostly used for prescribing a zero total flux on a boundary:

\[ g''' = 0 \]
BC’s for a solute transport problem

Prescribed relation linking concentration and its first derivative (Cauchy or mixed Neumann BC)

\[ C^v = C_0^v \]

\[ \frac{\partial h}{\partial n} = 0 \quad q_n C^v + \frac{\partial C^v}{\partial n} = 0 \quad h \text{ prescribed} \]

\[ \frac{\partial C^v}{\partial n} = 0 \]

… equivalent to a zero flux (Neumann) gw flow BC associated with a transport zero Neumann BC:

no advection and no diffusion-dispersion through the boundary

a totally impervious boundary
Introduction

Pe and Cr numbers

Eulerian methods

Eulerian-Lagrangian methods

Multi-reactive transport

Solute transport solving methods

... solving the transport equation is never a simple operation ...

Partial derivatives of the 1\textsuperscript{st} and 2\textsuperscript{nd} order in the same equation (parabolic, elliptic and hyperbolic equation)

- numerical dispersion
- artificial oscillations
- more memory
- more CPU
Introduction to solute transport solving methods

... solving the transport equation is never a simple operation ...

- partial derivatives of the $1^{st}$ and $2^{nd}$ order in the same equation (parabolic and elliptic equation)
- numerical dispersion
- artificial oscillations
- more memory
- more CPU
Introduction to solute transport solving methods

... solving the transport equation is never a simple operation ...

- partial derivatives of the 1st and 2nd order in the same equation (parabolic and elliptic equation and even hyperbolic)

- Pe and Cr numbers
- Eulerian methods
- Eulerian-Lagrangian methods
- Multi-reactive transport

- with regards to a fixed axis system
- with regards to a moving axis system (referential) at $v_a/R$ velocity along a streamline
Numerical Peclet and Courant numbers

- dimensionless Peclet number = ratio between advection and dispersion
  \[ Pe = \frac{v_a \Delta x}{D} \]
  simplified in
  \[ Pe = \frac{v_{a_x} \Delta x}{a_L v_{a_x}} = \frac{\Delta x}{a_L} \]
  \[ \Delta x < 2a_L \] to avoid oscillations when using classical grid-based numerical methods

- dimensionless Cr number = ratio between advection travel during a time step and the grid dimension
  \[ Cr = \frac{v_a \Delta t}{\Delta x} \]
  \[ Cr < 1 \] to allow the transfer of information from a grid cell (element) to the next without losing information

(Price et al. 1966)
(Daus & Frind 1985, Rausch et al. 2005)
Time integration schemes

- explicit integration schemes ($\theta < 0.5$) : conditionally stable
- time integration on the implicit side ($\theta \geq 0.5$): unconditionally stable
- Crank-Nicolson scheme ($\theta = 0.5$) provides 2nd order accuracy (i.e. proportional to $(\Delta t)^2$) and is just unconditionally stable
  
  the reduction of the time step by a factor of 2 reduces the approximation error by a factor of 4.

- time weighting can be combined to different spatial weighting (i.e. upstream weighting) for a variety of different methods
- in general, weighting more toward the implicit side will produce less oscillations but more numerical dispersion
- Crank-Nicolson scheme is often adopted as a compromise
- with spatial and temporal discretizations adequately chosen in relation to Peclet and Courant constraints
Solving methods

Eulerian methods

concentration calculated at a given node should be more influenced by the concentration at the upstream node (i.e. with respect to the advective transport) than by concentrations at the other neighboring nodes

- more weight should be given to upstream values in the finite difference or finite element approximations of the advective term
- other terms of the solute transport PDE are treated by the standard approximations (i.e. similarly to what is done for solving the flow equation

- a series of upwind or upstream numerical techniques to decrease oscillations but at the cost of creating numerical dispersion (using upstream information artificially smooths the simulated gradients, which corresponds to numerical dispersion)
- Note: in many numerical books, oscillations = ‘dispersive error’ and numerical dispersion = ‘diffusive error’
**Solving methods**

### Eulerian methods

- similar when applied to FDM, FVM and FEM
- upwind or upstream techniques require to compute beforehand the advection direction (i.e. groundwater flow direction) for the time step
- two types of upwind techniques: central-in-space upwind weighting and upstream weighting
- combined with different time integration schemes gives rise to a series of different methods
- for FD with uniform grid:

\[
\frac{\partial C}{\partial x} \approx (1 - \alpha) \frac{C(x + \Delta x) - C(x)}{\Delta x} + \alpha \frac{C(x - \Delta x) - C(x)}{\Delta x}
\]

where \(\alpha\) is the upwind coefficient, \(\alpha \in [0,1]\)

\[
\frac{\partial C}{\partial x} \approx \frac{(1 - \alpha)C(x + \Delta x) - C(x) + \alpha C(x - \Delta x)}{\Delta x}
\]

\(\alpha\) must be chosen larger than 0.5 to create an upwind weighting
Solving methods
Eulerian methods: combined with different time integration schemes

(a) time
(b) time
(c) time

t + ∆t
t
x - ∆x x x + ∆x

central-in-space

node used for the approximation
approximated node

nodal contributions to the approximated C(x,t+∆t) with a central-in-space upwind weighting combined with

- (a) an explicit
- (b) an implicit
- (c) a Crank-Nicolson time integration scheme

The weight of each nodal contribution is not mentioned for implicit schemes as it depends on the combination of the spatial with the temporal weighting.
**Eulerian methods:** higher order upstream weighting

**Spatial weighting**

**2nd order**

- Explicit $\theta = 0$

- Implicit $\theta = 1$

- Crank-Nicolson $\theta = 0.5$

**3rd order**

- 1st order BDF implicit $\theta = 1$

- 3rd order BDF partially explicit $\theta = \frac{1}{3}$

**Time scheme**

- Explicit $\theta = 0$

- Implicit $\theta = 1$

- Crank-Nicolson $\theta = 0.5$

- 1st order BDF implicit $\theta = 1$

- 3rd order BDF partially explicit $\theta = \frac{1}{3}$

---

$x$ node used for the approximation
° approximated node
Eulerian methods: first order and higher order upstream weighting

\[
\frac{\partial C}{\partial x} \approx \frac{(1 - \alpha)C(x + \Delta x) - C(x) + \alpha C(x - \Delta x)}{\Delta x}
\]

- these upstream techniques reduce oscillations but create numerical dispersion
- wise to apply them only if \( Pe < 2 \) and \( Cr < 1 \)
- an additional check about sensitivity to changes in longitudinal and transverse dispersivities

good way to assess the relative parts of numerical and physical dispersion in the simulated results
Solving methods

Eulerian methods: TVD method (Total Variation Diminishing)

- can be implemented in FDM-, FVM- and FEM-based models to solve advection dominated transport
- known as more accurate than standard central-in-space weighting and upstream methods for simulating sharp concentration variations
- wise to apply them only if Pe < 2 and Cr < 1
- in a FD regular grid, considering only 1D advection:

\[ C(x, t + \Delta t) = C(x - v_a t, t) \]

- point found by interpolation from the concentrations at the 4 neighboring nodes: a 3rd order polynomial is used

Flow direction

\( x - 2\Delta x \) \( x - \Delta x \) \( x \) \( x + \Delta x \)


**Eulerian methods: TVD method** *(Total Variation Diminishing)*

\[ C_j(t + \Delta t) = C_j(t) - Cr\left[ \left( \frac{C_{j+1}(t)}{3} + \frac{C_j(t)}{2} - C_{j-1}(t) + \frac{C_{j-2}(t)}{6} \right) \right. \]

\[ \left. - Cr \left( \frac{C_{j+1}(t) - 2C_j(t) + C_{j-1}(t)}{2} \right) \right. \]

\[ + Cr^2 \left( \frac{C_{j+1}(t) - 3C_j(t) + 3C_{j-1}(t) - C_{j-2}(t)}{6} \right) \]

- may lead to oscillations in advection dominated problems
- a ‘flux limiter’ is activated when the spatial concentration profile does not show a monotonic evolution  

- TVD scheme is explicit, subject to stability constraints
- other terms of the solute transport equation solved by an explicit or an implicit procedure
- mostly mass conservative!
Solving methods

Eulerian Lagrangian methods

\[
\frac{\partial C^v}{\partial t} = -\frac{v_a}{R} \cdot \nabla C^v + \frac{1}{R} \nabla \cdot (D_h \cdot \nabla C^v) - \lambda C^v - \frac{q_s}{R n_m} (C^v - C_s^v)
\]

in a Lagrangian approach:

\[
\frac{dC^v}{dt} = \frac{1}{R} \nabla \cdot (D_h \cdot \nabla C^v) - \lambda C^v - \frac{q_s}{R n_m} (C^v - C_s^v)
\]

\[
\frac{dC^v}{dt} = \frac{\partial C^v}{\partial t} + \frac{v_a}{R} \cdot \nabla C^v
\]

(Zheng 1990, Bear and Cheng 2010)

the left hand side is Lagrangian while the right hand side remains Eulerian
Solving methods

Eulerian Lagrangian methods

\[ \frac{dC^v}{dt} \approx \frac{C^v(t + \Delta t) - C^v(t + \Delta t)}{\Delta t} \]

\[ C^v(t + \Delta t) \approx C^v(t + \Delta t) + \Delta t \left[ \frac{1}{R} \nabla \cdot (D_h \cdot \nabla C^v) - \lambda C^v - \frac{q_s}{R \ n_m} (C^v - C^s) \right] \]

\( C^v = \text{'intermediate' concentration at time} \ (t + \Delta t) \)

(Zheng 1990)

1) Solving advection by a ‘characteristic’ method
2) Solving the 2\textsuperscript{nd} term by classical method with explicit, implicit, Crank-Nicolson or Galerkin time integration
Solving methods

Eulerian Lagrangian methods

\[ C^v* = \text{‘intermediate’ concentration at time } (t + \Delta t) \]

... can be calculated by a particle tracking or a method of characteristics

- ‘Method Of Characteristics’ MOC
- ‘Modified Method Of Characteristics’ MMOC
- ‘Hybrid Method Of Characteristics’ HMOC
**Eulerian Lagrangian methods**

**‘Method Of Characteristics’ MOC**

\[ \tilde{C}_i^v (t + \Delta t) = \frac{1}{n_p_i} \sum_{k=1}^{n_p_i} C_k^v (t) \]

\[ C_i^v (t + \Delta t) = \omega \tilde{C}_i^v (t + \Delta t) + (1 - \omega) C_i^v (t) \]

- initial ‘set’ of particles: an initial position and a concentration given to each of them
- small time step, particles moving along streamlines
- at the end of the time step, concentration computed by counting the arrived particles in the concerned cell
- nearly no numerical dispersion but time consuming and memory consuming with many particles
- if too few particles: mass conservation problems
Eulerian Lagrangian methods

‘Method Of Characteristics’ MOC (Garder et al. 1964, Konikow and Bredehoeft 1978, Zheng 1990)

- no numerical dispersion even for large Pe number
- errors coming from the interpolation of the velocity field from the groundwater flow model
- discrete nature of the particles (and counting of them in each cell/element after each time step) induces local mass conservation problems
- more particles ➔ increasing rapidly the computing load and memory storage
- too heavy for highly heterogeneous and complex non linear problems

\[
\tilde{C}_i^v (t + \Delta t) = \frac{1}{np_i} \sum_{k=1}^{np_i} C_k^v (t)
\]

\[
C_i^v (t + \Delta t) = \omega \tilde{C}_i^v (t + \Delta t) + (1 - \omega) C_i^v (t)
\]

Eulerian Lagrangian methods

**MMOC**


- cell centered node
- particle at time $t$
- particle at time $t + \Delta t$

Backward unique particle tracking

$p_{xyz}(t) = p_i(t + \Delta t) - v_a(p_i(t + \Delta t))\Delta t$

$C_i^v(t + \Delta t) = C^v(p_{xyz}(t), t)$

- $C^v(p_{xyz}(t), t)$ is calculated using a linear (bilinear in 2D or trilinear in 3D) interpolation of neighboring nodal values at time $t$

- reduced memory requirements if lower order interpolation scheme

- faster than MOC but same mass conservation problem than MOC

- main issue = numerical dispersion with lower order interpolations

- higher order interpolation schemes lead to better results but induce oscillations when simulating sharp concentration gradients
Eulerian Lagrangian methods

**HMOC**

- optimizing the choice between MOC and MMOC
- an automatic change of the technique as function of the local concentration gradients
- MOC applied in regions of the domain with steep concentration gradients
- MMOC applied elsewhere
Solving methods

Eulerian Lagrangian methods

\[ C^v(t + \Delta t) \approx C^v^*(t + \Delta t) + \Delta t \left[ \frac{1}{R} \nabla \cdot (D_h \cdot \nabla C^v) - \lambda C^v - \frac{q_s}{R n_m} (C^v - C_s^v) \right] \]

\( C^v^* \) = ‘intermediate’ concentration at time \((t + \Delta t)\)

1) Solving advection by MOC, MMOC or HMOC
2) Solving the 2\(^{nd}\) term by classical method with explicit, implicit, Crank-Nicolson or Galerkin time integration
Solving a solute transport problem with multi-reactive transport

- (temporal) operator-splitting method: separate solutions for the “transport step” and “reaction step(s)”
- $R_k$’s are independent from neighbouring grid cells and might be computed in parallel mode.
- Splitting introduces “error”
- Iteration between the steps would reduce this “error”
Solving a solute transport problem

Multi-reactive transport

MT3MS simulates the transport of \( n \) components for a timestep \( \Delta t \)

Comp 1  Comp 2  ...  Comp \( n \)

PHREEQC runs a reaction simulation for each grid cell
References


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References


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