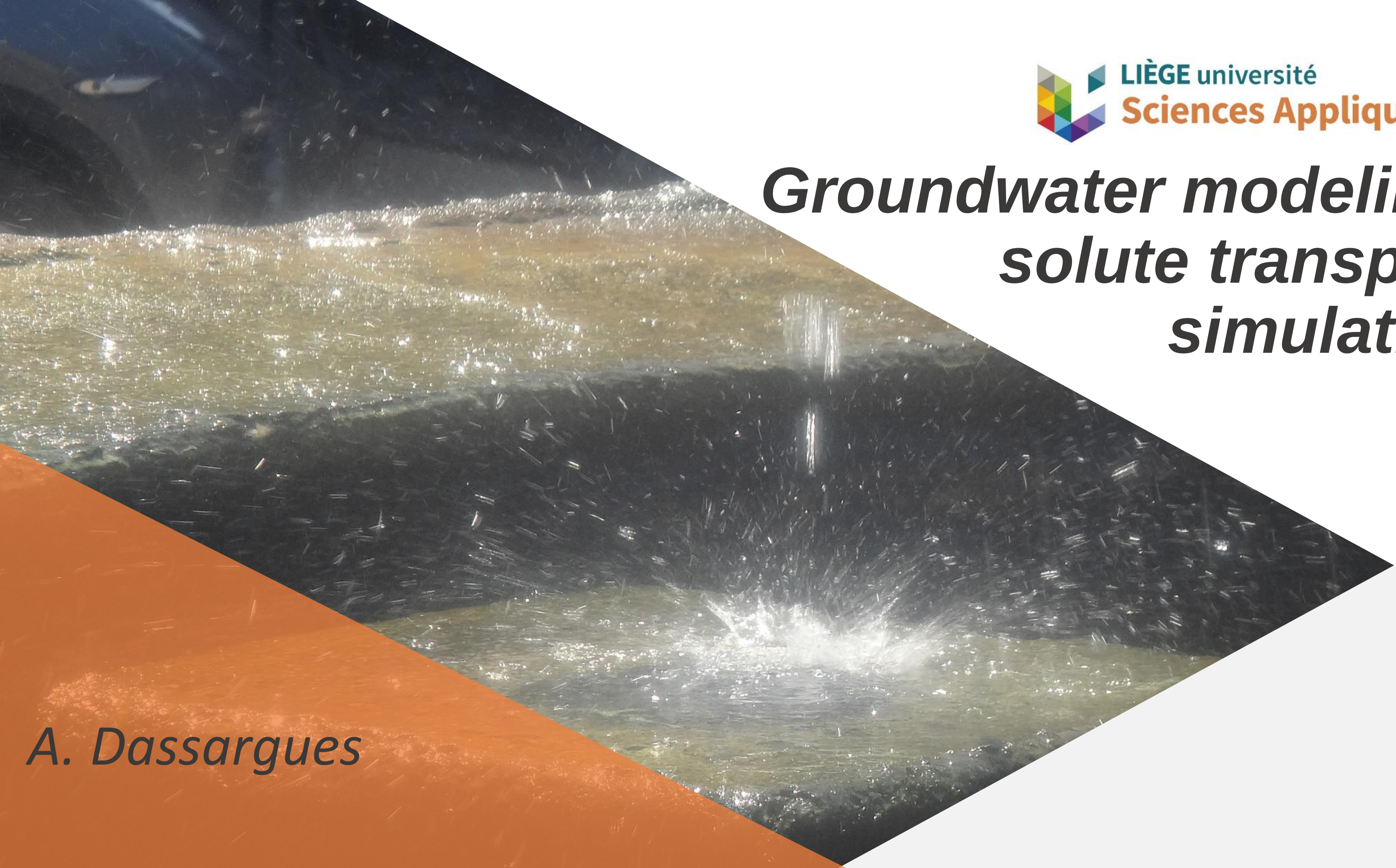

LIÈGE université
Sciences Appliquées

Groundwater modeling: solute transport simulation

A. Dassargues

References: *Dassargues A., 2018. Hydrogeology: groundwater science and engineering, 472p. Taylor & Francis CRC press (chapters 8, 12, 13)*

Dassargues A. 2020. Hydrogéologie appliquée: science et ingénierie des eaux souterraines, 512p. Dunod (chapitres 8, 12, 13)

Groundwater modeling: solute transport simulation

- *Solute transport equations*
  - *Diffusion*
  - *Advection*
  - *Mechanical dispersion*
  - *Equation of advection-dispersion*
  - *Adsorption/desorption*
  - *Degradation/decay*
  - *Solute mass conservatio eqaution*
  - *Discussion about the source/sink term*
  - *Immobile water effect/ matrix diffusion*
  - *Solute transport equations and Boussinesq approximation*
- *Transport Boundary Conditions*
  - *Dirichlet BC's*
  - *Neumann BC's*
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- *Introduction to solving methods*
  - *Introduction, Pe and Cr numbers*
  - *Time integration schemes*
  - *Eulerian techniques*
    - *upwind/upstream techniques*
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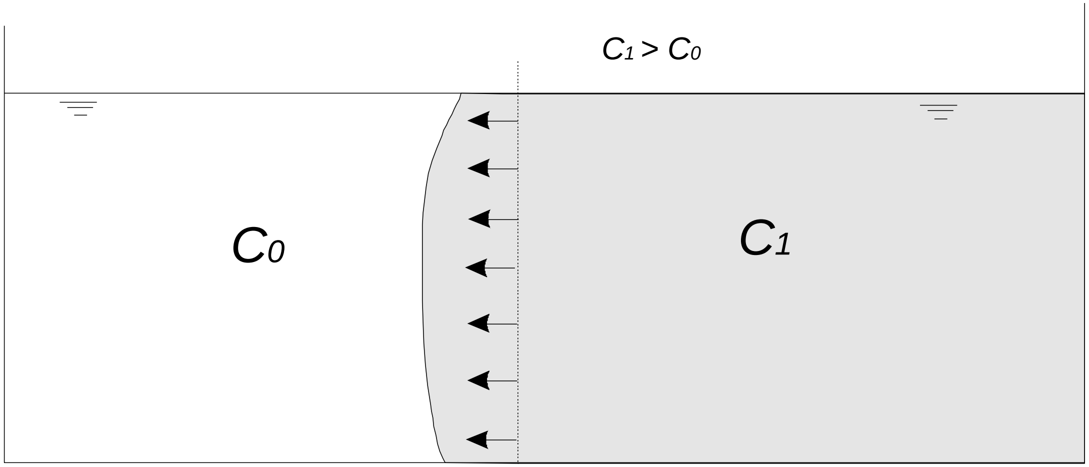
  - *Eulerian-Lagrangian techniques*
    - *MOC*
    - *MMOC*
    - *HMOC*
  - *Solving multi-reactive transport*
- *References*

Processes and equations

Molecular diffusion

… mass of solute diffusing from high to low solute concentrations



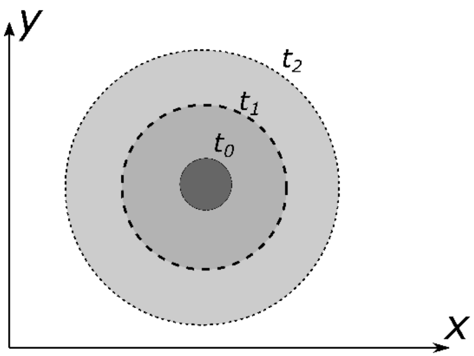
Fick law

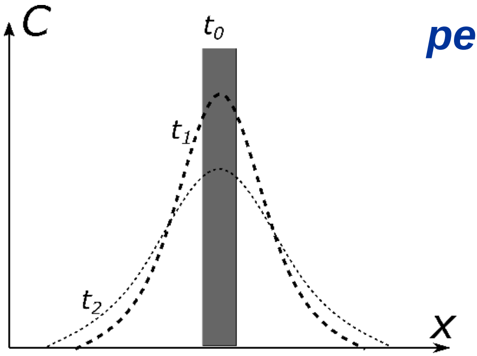
$$\boldsymbol{f_m} = -D_m \mathbf{grad}(\rho C) = -D_m \nabla(\rho C)$$

$$\boldsymbol{f_m} = -D_m \mathbf{grad}\, C^v = -D_m \nabla C^v$$

molecular diffusion mass flux per surface unit (kg/(m².s))

effective diffusion coefficient of the solute in the porous medium (m²/s)



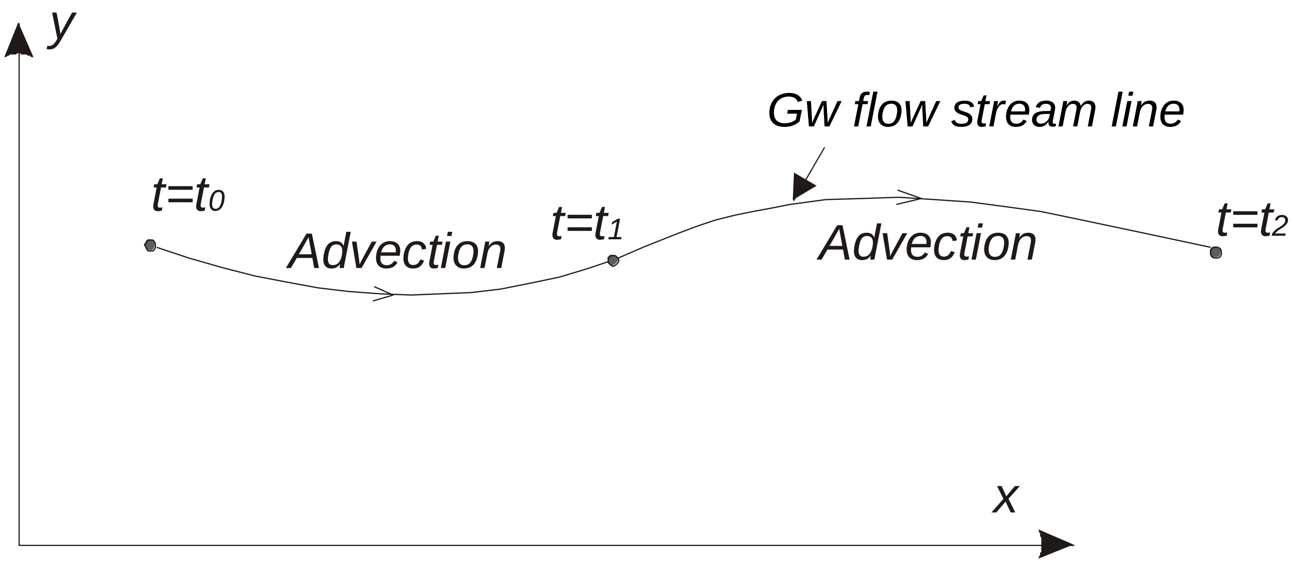


(Bear and Cheng, 2010, Fitts 2002, Rausch et al. 2005, Huysmans & Dassargues 2005, 2006, 2007, 2013)

Processes and equations

Advection

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



advection mass flux per surface unit $(kg/(m^2.s))$

$$\boldsymbol{f_a} = \boldsymbol{q}\rho C$$

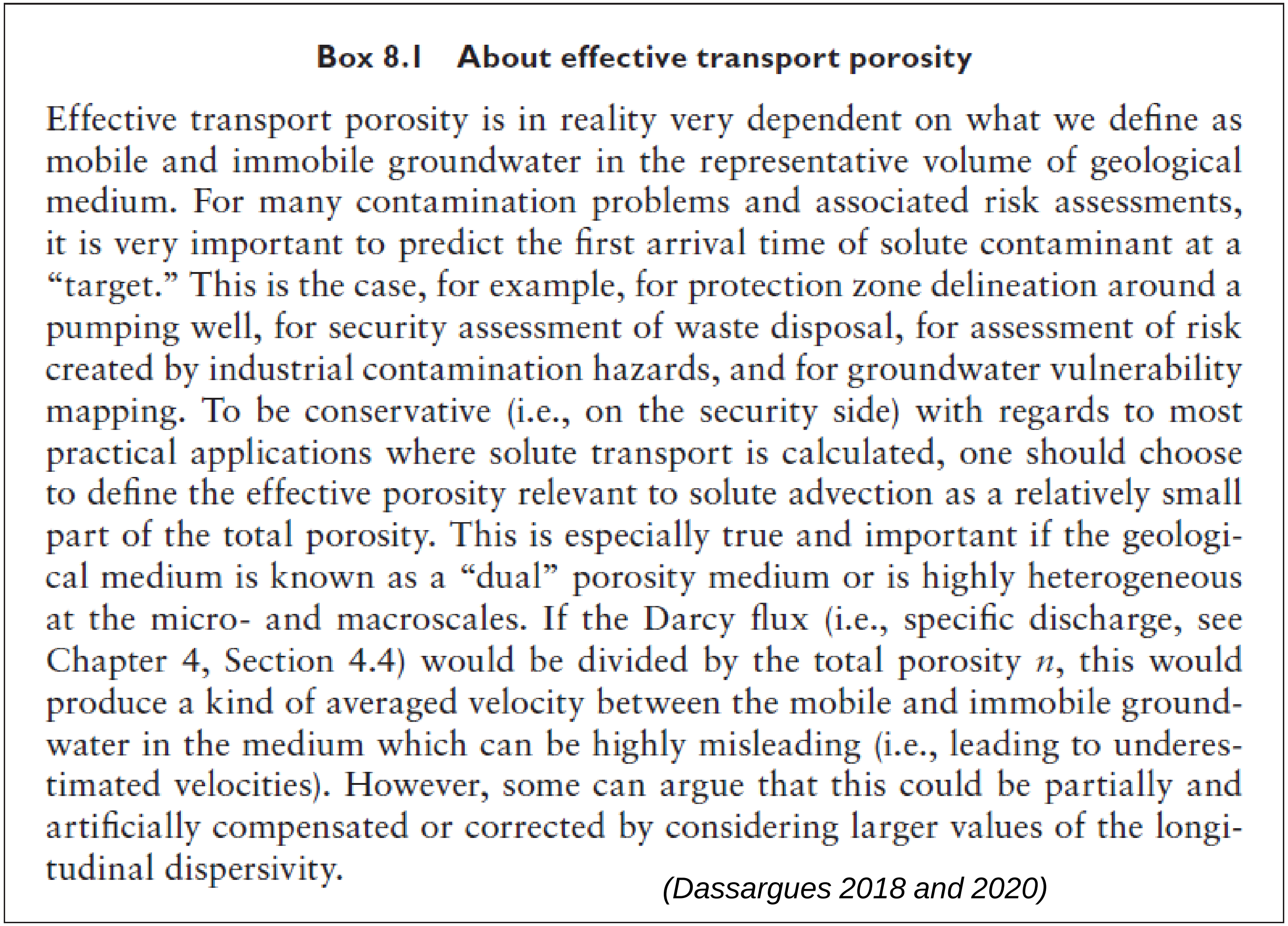
$$\boldsymbol{f_a} = \boldsymbol{q}C^v \qquad \boldsymbol{f_a} = -\boldsymbol{K} \cdot \nabla h \, C^v = -\boldsymbol{K} \cdot \nabla h \, (\rho C)$$

$$\boldsymbol{v_a} = \boldsymbol{q}/n_m$$

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)

useful porosity for solute transport is 'effective transport porosity' < drainage porosity

Processes and equations

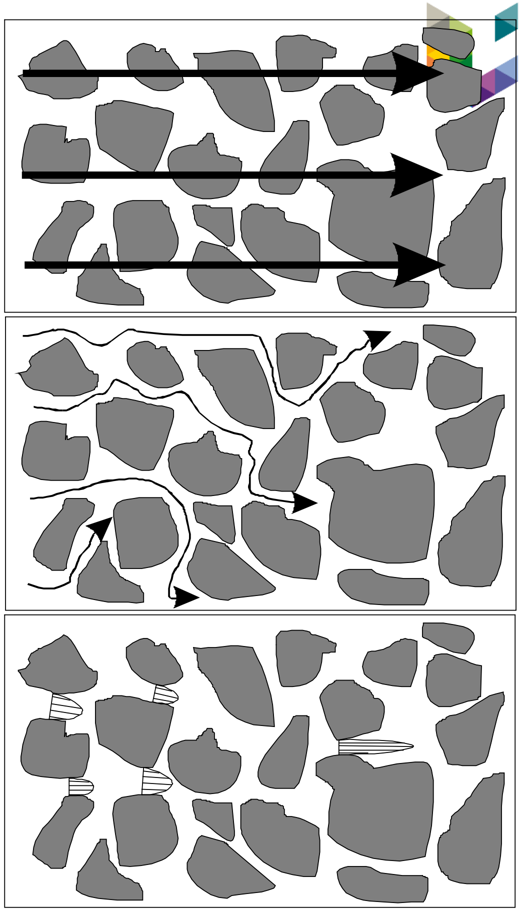
Mechanical dispersion

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

$$\boldsymbol{f_d} = -n_m \boldsymbol{D} \cdot \boldsymbol{grad}(\rho C) = -n_m \boldsymbol{D} \cdot \nabla(\rho C)$$

$$\boldsymbol{f_d} = -n_m \boldsymbol{D} \cdot \boldsymbol{grad}\, C^v = -n_m \boldsymbol{D} \cdot \nabla C^v$$

mechanical dispersion tensor (m²/s)



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

➡ a linear relation between $\boldsymbol{D}$ and $\boldsymbol{v_a}$

$$\boldsymbol{D} = \begin{bmatrix} D_{xx} & & \\ & D_{yy} & \\ & & D_{zz} \end{bmatrix}$$

longitudinal dispersivity (m)

transversal dispersivity (m)

$$D_{xx} = a_L v_{a_x},\ D_{yy} = a_T v_{a_x},\ D_{zz} = a_T v_{a_x},$$
$$\text{with } v_{a_y} = v_{a_z} = 0$$

Processes and equations

Mechanical dispersion

➡ … 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

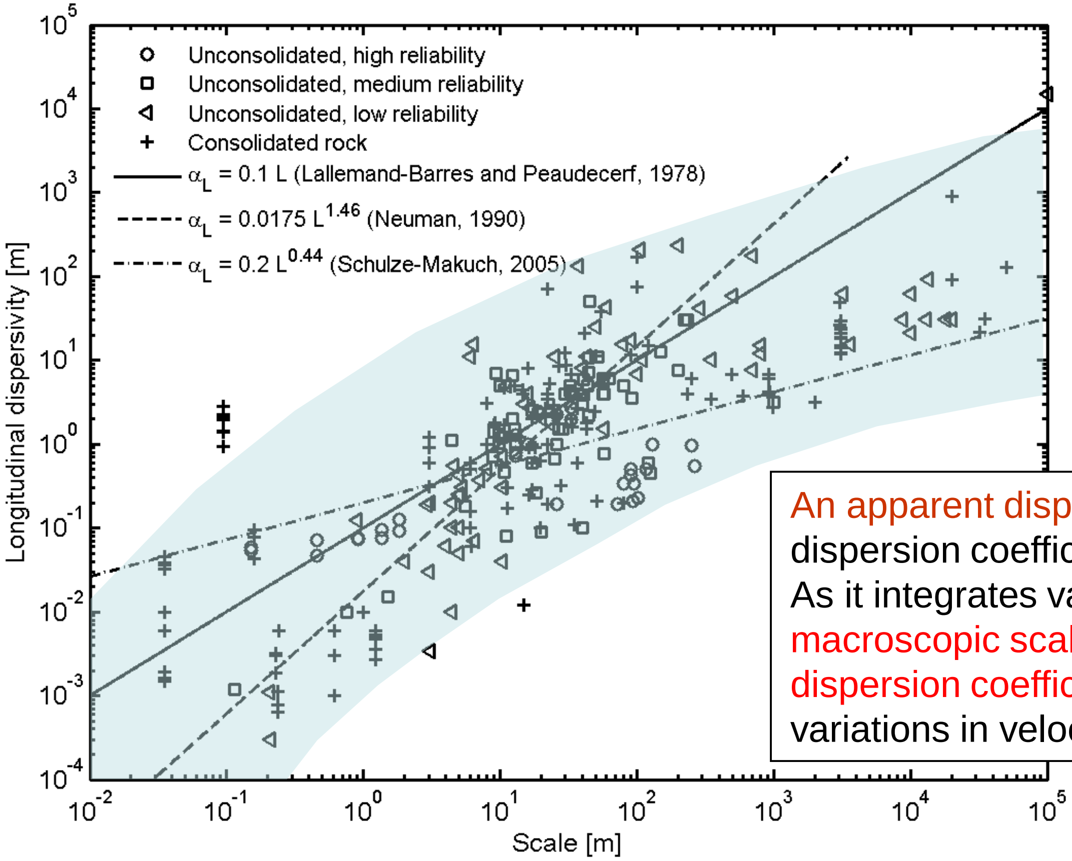
(Scheidegger 1961, Bear 1972, Bear & Verruijt 1987, Delleur 2000, Pinder & Celia 2006, Bear & Cheng, 2010)

Processes and equations

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

$$\boldsymbol{D_h} = \boldsymbol{D} + \boldsymbol{D_m} = \boldsymbol{D} + D_m\boldsymbol{I}$$

hydrodynamic dispersion tensor (m^2/s)

$$\boldsymbol{f_h} = -n_m(\boldsymbol{D_h}) \cdot \boldsymbol{grad}\,(\rho C) = -n_m(\boldsymbol{D_h}) \cdot \nabla(\rho C)$$

$$\boldsymbol{f_h} = -n_m(\boldsymbol{D_h}) \cdot \boldsymbol{grad}\,C^v = -n_m(\boldsymbol{D_h}) \cdot \nabla C^v$$

Processes and equations

Equation of advection-dispersion

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

➡ $$n_m \frac{\partial C^v}{\partial t} = -div(\boldsymbol{f_a} + \boldsymbol{f_h}) = -\nabla \cdot (\boldsymbol{f_a} + \boldsymbol{f_h})$$

➡ $$n_m \frac{\partial C^v}{\partial t} = -div(\boldsymbol{q}C^v - n_m(\boldsymbol{D_h}) \cdot \boldsymbol{grad}\, C^v) = -\nabla \cdot (\boldsymbol{q}C^v - n_m(\boldsymbol{D_h}) \cdot \nabla C^v)$$

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

$$\frac{\partial C^v}{\partial t} = -v_a \frac{\partial C^v}{\partial x} + a_L v_a \frac{\partial^2 C^v}{\partial x^2}$$

boundary cond.

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

$$C^v(0,0) = C_0^v$$

punctual injection

Instantaneous injection in x = 0

Analytical solution :

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

(Ogata and Banks 1961)

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

'Gaussian dispersion' with:

$$\begin{cases} \mu \leftrightarrow v_a t \\ \sigma^2 \leftrightarrow 2 a_L v_a t \end{cases}$$

Processes and equations

Adsorption-desorption

… in the simpliest case: isothermal conditions

$$\overline{C} = K_d . \rho . C$$

equilibrium relations in the REV

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

partitioning coefficient (m³/kg)

mass concentration of solute in groundwater

(Davis and Kent 1990)

K_d *varies from a medium to another (higher for clay)*

in the solute mass balance equation can be expressed by
$-\rho_b \mathcal{R}_{w,s}$ *(kg/m³s)*

a retardation coefficient multiplying $\frac{\partial C}{\partial t}$

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

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

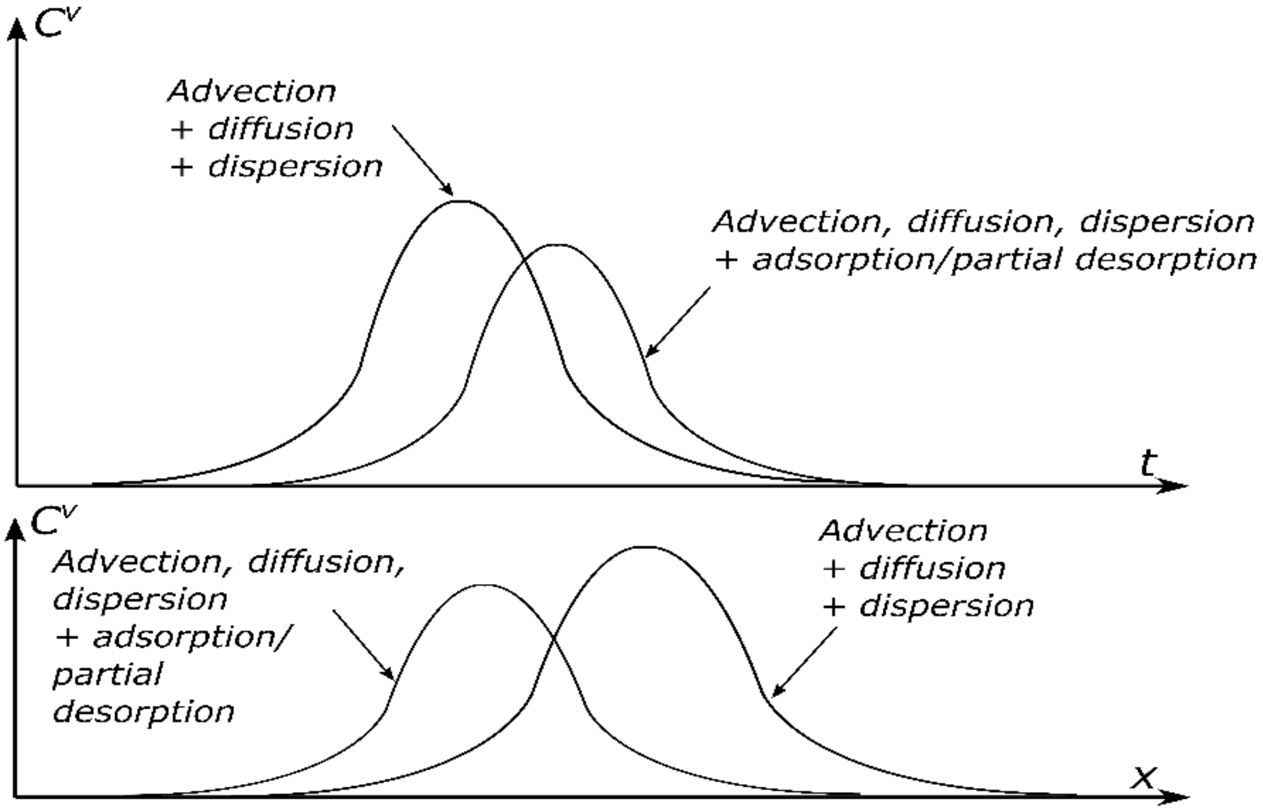
water content in volume

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})

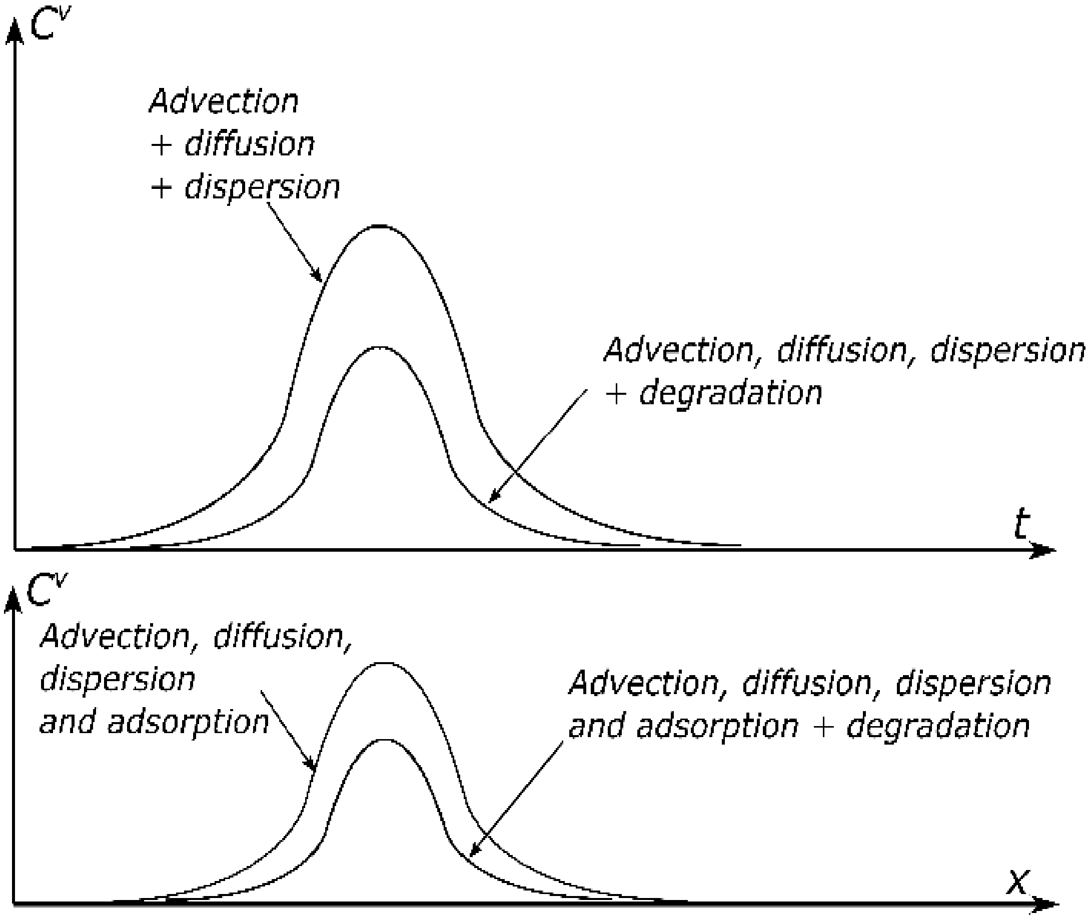
decay coefficient

$$\frac{\partial C}{\partial t} = -\Gamma .(C)^{m}$$

exponent depending on the reaction stoichiometry

Processes and equations

Degradation/decay



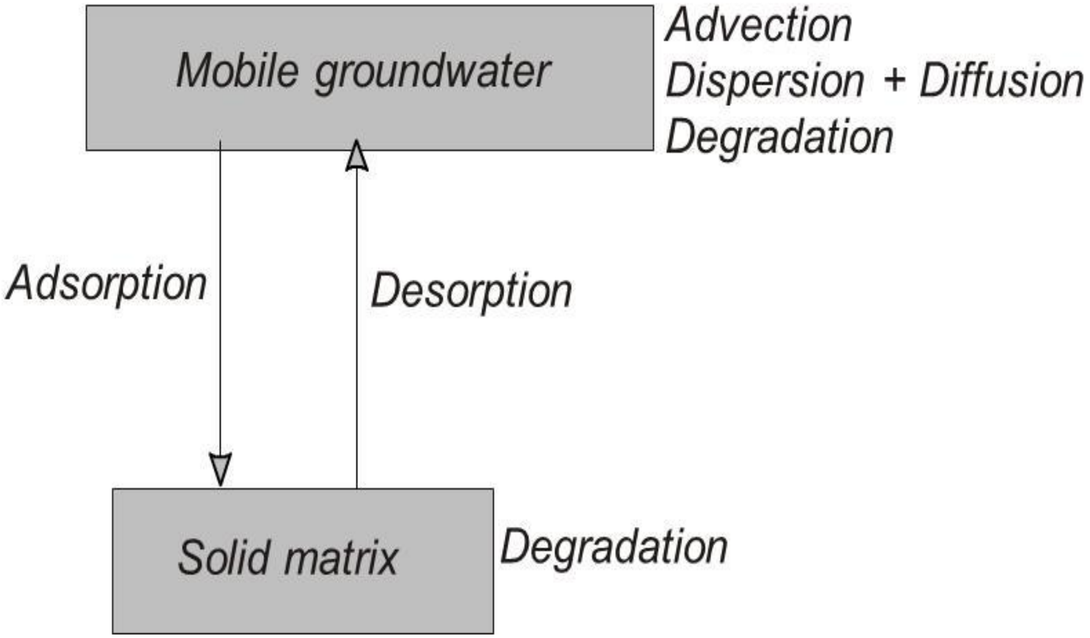
in the solute mass balance equation can be expressed by
$-n\lambda\rho C$ ***(kg/m³s)***

Processes and equations

Solute mass conservation equation

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

$$\Rightarrow \frac{\partial}{\partial t}(n_m C^v) = -\nabla \cdot (\boldsymbol{q} C^v) + \nabla \cdot n_m(\boldsymbol{D} \cdot \nabla C^v) + \nabla \cdot n(D_m \nabla C^v) - \rho_b \mathcal{R}_{w,s} - n\lambda C^v + M^v$$



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/m³s) :***

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

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

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

$$\nabla \cdot (\boldsymbol{v_a} C^v) = C^v \nabla \cdot \boldsymbol{v_a} + \boldsymbol{v_a} \cdot \nabla C^v$$

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

➡ $C^v \nabla \cdot \boldsymbol{v_a} = C^v q_s$

➡ $$R\frac{\partial C^v}{\partial t} = -\boldsymbol{v_a} \cdot \nabla C^v + \nabla \cdot (\boldsymbol{D_h} \cdot \nabla C^v) - R\lambda C^v - \frac{q_s}{n_m}(C^v - C_s^v)\Big)$$

(Rausch et al. 2005)

Processes and equations

Discussion about the source/sink term

$$R\frac{\partial C^{v}}{\partial t} = -\boldsymbol{v_{a}}\cdot\nabla C^{v} + \nabla\cdot(\boldsymbol{D_{h}}\cdot\nabla C^{v}) - R\lambda C^{v} - \frac{q_{s}}{n_{m}}(C^{v} - C_{s}^{v}\bigg)$$

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***

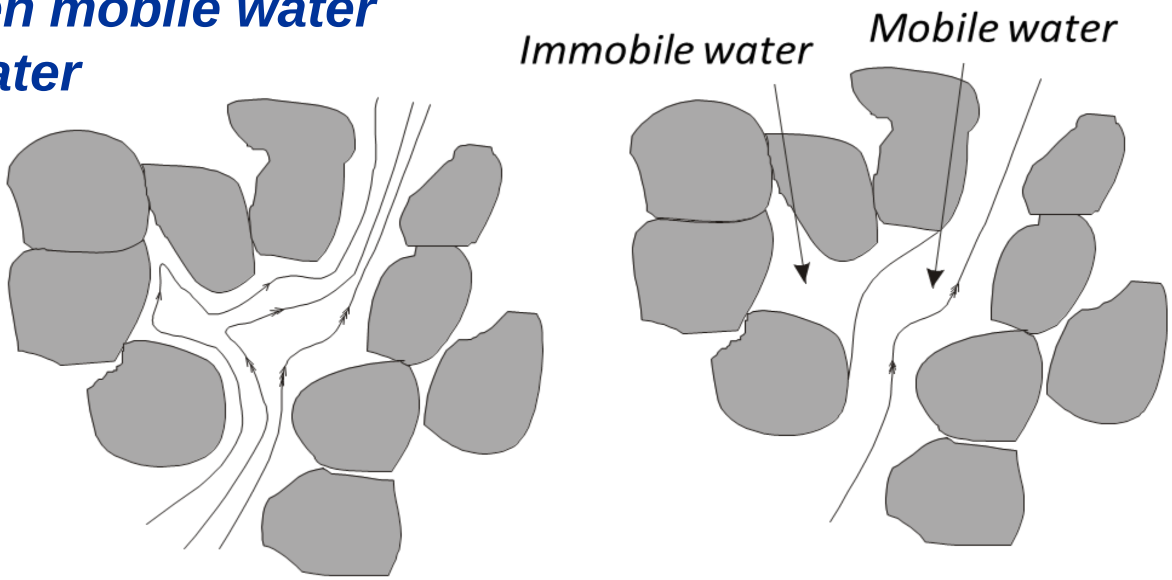
(Rausch et al. 2005)

Processes and equations

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:***

$$f_m^{im} = \alpha_d^m(\rho C - \rho_{im} C_{im})$$

$$f_m^{im} = \alpha_d^m(C^v - C_{im}^v)$$

mobile groundwater

immobile groundwater

(Gerke & van Genuchten 1993)

Processes and equations

Immobile water effect = 'matrix diffusion'

= diffusion between immobile and mobile water

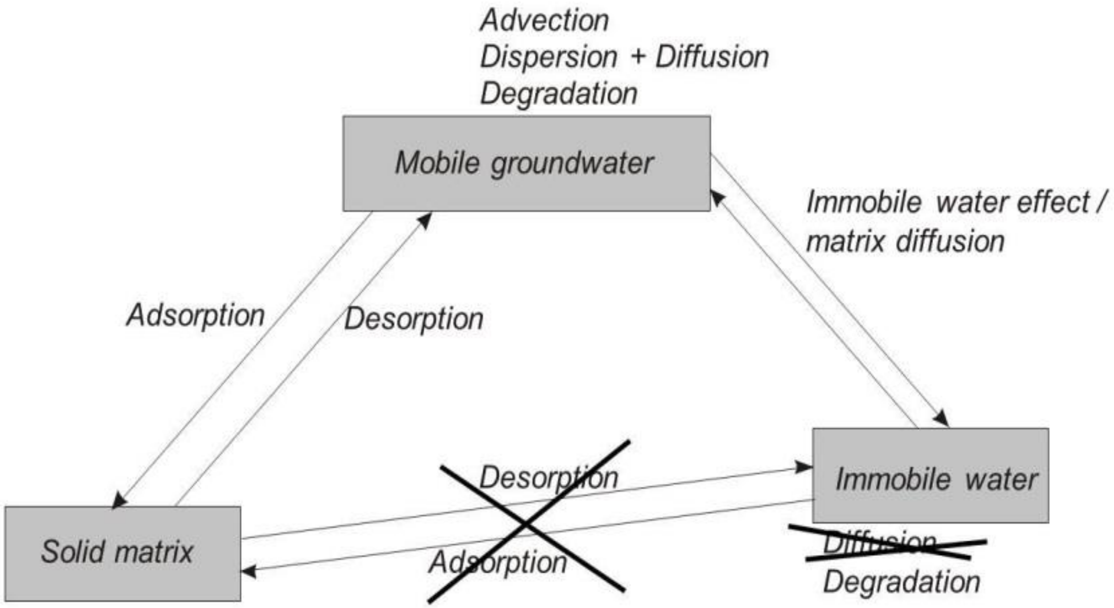
➡ ***… a solute mass balance equation in the immobile water should be used:***

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

(Coats & Smith 1964, Skopp & Warrick 1974, Rao et al. 1982, Bear and Verruijt 1987, Biver et al. 1995, Hallet & Dassargues 1998, Zheng & Wang 1999, Haerens et al. 1999, Brouyère et al. 2004, Hoffmann et al. 2021)

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

$$R_i \frac{\partial C_i^v}{\partial t} = -\boldsymbol{v}_{\boldsymbol{a}_i} \nabla C_i^v + \nabla \cdot (\boldsymbol{D}_{\boldsymbol{h}} \cdot \nabla C_i^v) - R_i \lambda_i C_i^v - \frac{q_s}{\theta_i}\left(C_i^v - C_{s_i}^v\right) \boxed{+ \frac{1}{\theta_i} \sum_{j=1}^{N_s} S_{ij}\left(C_1^v, \ldots, C_n^v\right)} \qquad i = 1, \ldots, N_s$$

can be solved separately by PHREEQC (for example)

where S_{ij} = source/sink term representing the effect of reactions (kg/m³s),

θ_i= groundwater specific volume fraction of the REV where species i is located

- ➡ ***as many equations as species in the reaction system: N_s***
- ➡ ***equations are coupled through the $S_{ij}(C_1^v, \ldots, C_n^v)$ terms***

If all reactions occur in the water phase, θ_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)

- ➡ ***homogeneous reaction system***

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

- ➡ ***heterogeneous reaction system (v_{a_i} and D_h being equal to zero for the species in those immobile phases)***

(Kinzelbach 1992, Rausch et al. 2005, Dassargues 2018, 2020)

Solute transport equations

Boussinesq approximation for density dependent flow and transport

Advection, dispersion, diffusion + adsorption/desorption + dégradation

$$R\frac{\partial(\rho(C)C)}{\partial t} = -\boldsymbol{v_a}\cdot\nabla(\rho(C)C) + \nabla\cdot\left(\boldsymbol{D_h}\cdot\nabla(\rho(C)C)\right) - R\lambda\rho(C)C - \frac{q_s}{n_m}\left(\rho(C)C - \rho(C_s)C_s\right)$$

<u>'Boussinesq approximation':</u> the only non-negligeable influence of the change in gw density is taken into account in the Darcy's law : $(\boldsymbol{v_a}\cdot\nabla C)$

$$R\frac{\partial C}{\partial t} = -\boldsymbol{v_a}\cdot\nabla C + \nabla\cdot(\boldsymbol{D_h}\cdot\nabla C) - R\lambda C - \frac{q_s}{n_m}\left(C - C_s\right)$$

(Holzbecher 1998)

$$\boldsymbol{v_a} = \frac{\boldsymbol{q}}{n_m} = -\frac{\boldsymbol{k}\rho g}{\mu n_m}\nabla h = -\frac{\boldsymbol{k}}{\mu n_m}(\nabla p + \rho g\nabla z)$$

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:

Carabin & Dassargues 2000, Peeters et al. 2004, Huysmans & Dassargues 2005, Huysmans et al. 2006, Brouyère et al. 2007, Batlle-Aguilar et al. 2009, Orban et al. 2010, Jamin et al. 2012, Huysmans & Dassargues 2013, César et al. 2014.

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

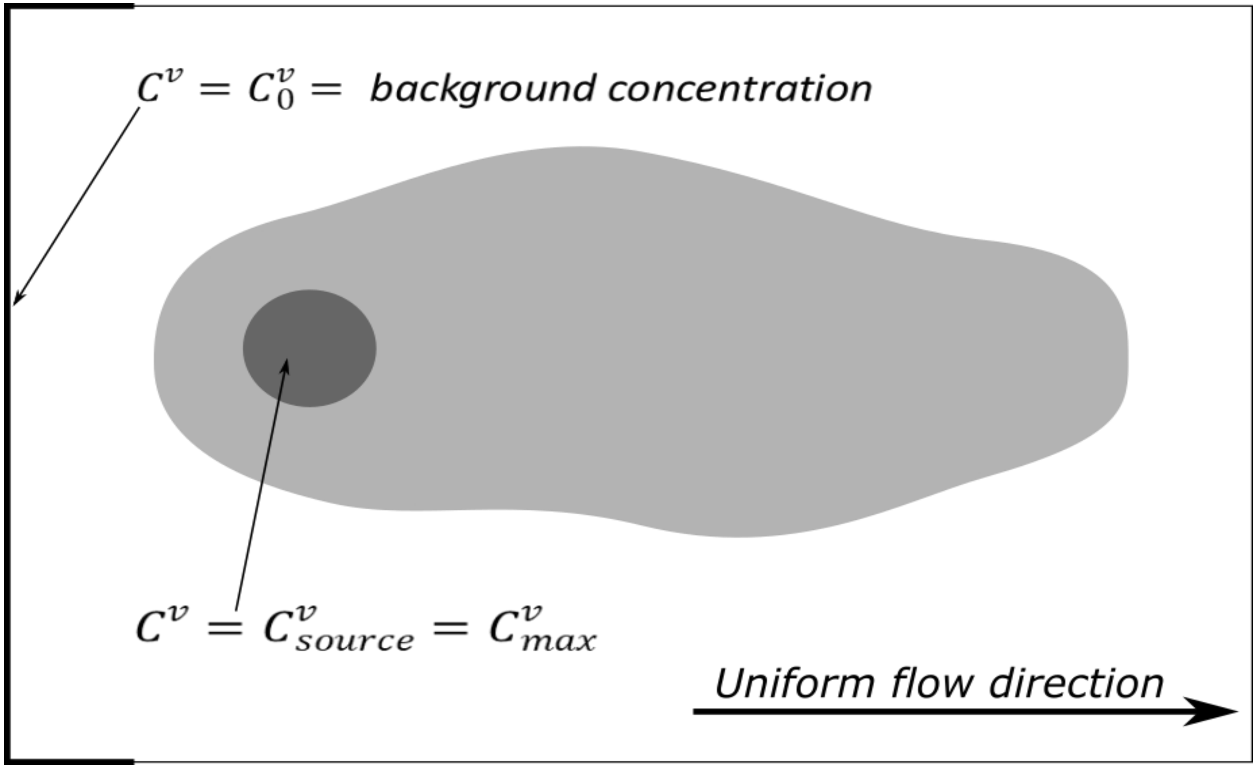
however, for numerical reasons, it induces large numerical dispersion

➡ *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)

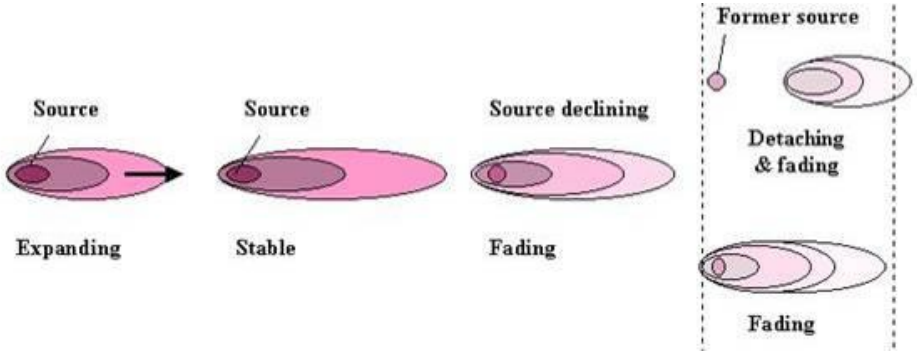
Typical case: a zero (or background) concentration prescribed upwards to the problem



also used for a source of contaminant prescribing C^v_{max} in place of $M_s = q_s C_s^v$

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)

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

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

➡ *… 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:

$$g''=0$$

➡ *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)

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

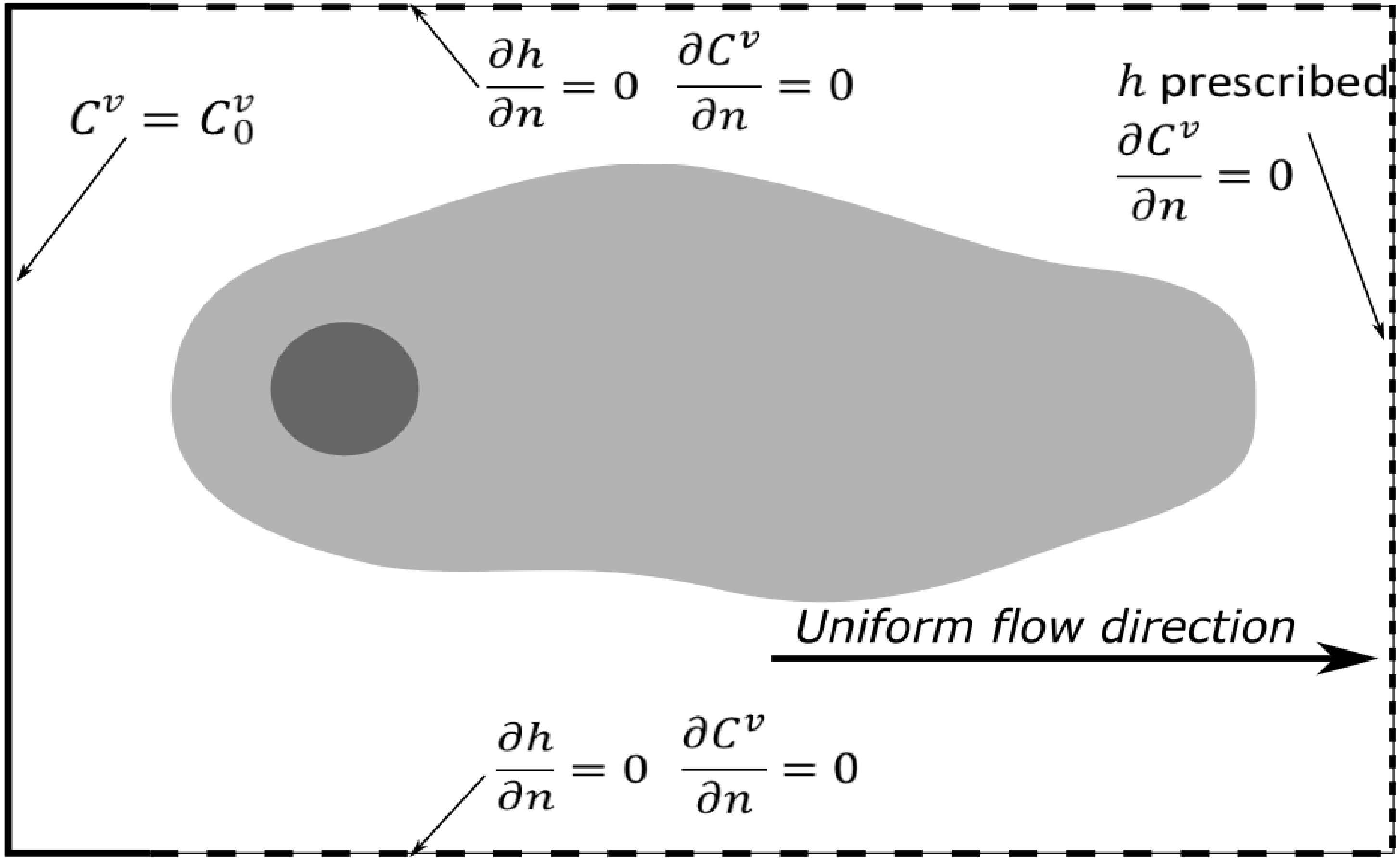
$q''(x,y,z,t)$	*diffusion-dispersion mass flux prescribed on the concerned boundary (kg/(m^2.s))*
$D_{h,n}$	*normal (to the boundary) component of the hydrodynamic dispersion tensor*

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

$\frac{\partial C^v}{\partial n} = 0$

$\frac{\partial h}{\partial n} = 0 \quad \frac{\partial C^v}{\partial n} = 0$

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 :

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

$$= q'''(x,y,z,t)$$

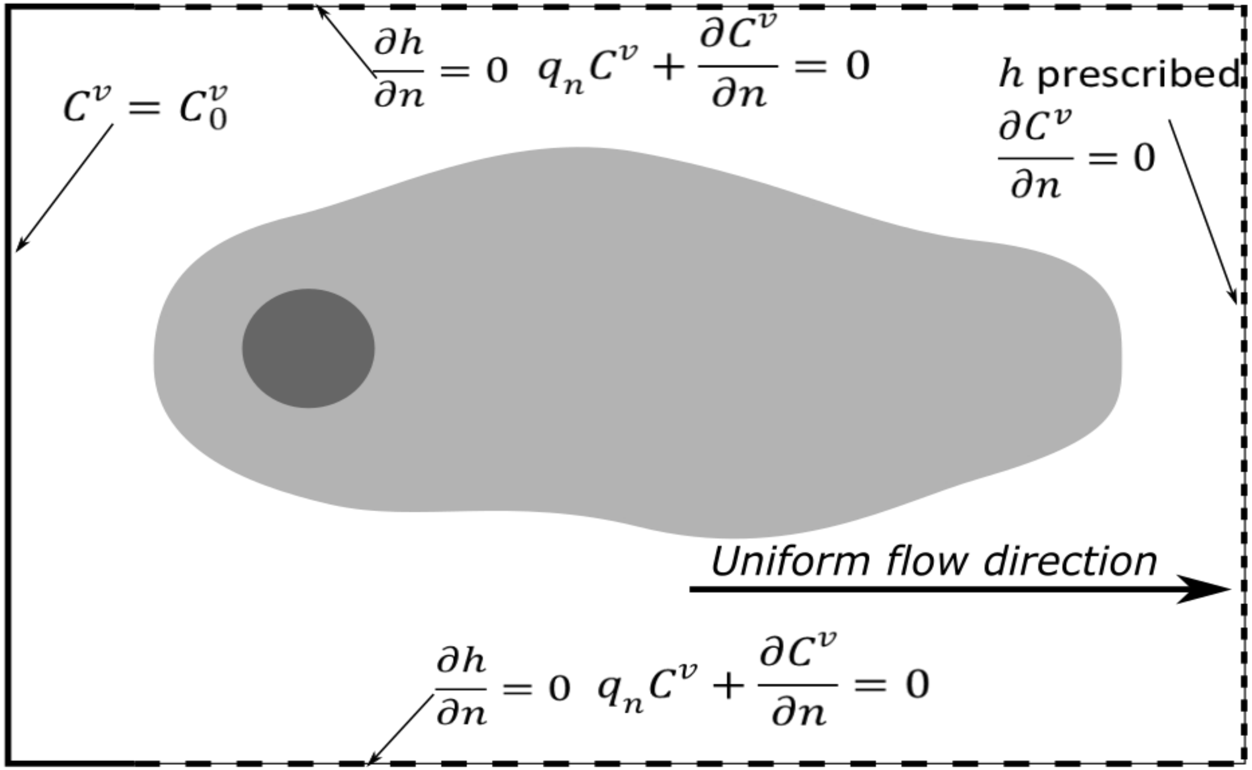
$q'''(x,y,z,t)$	*total prescribed mass flux (advection + diffusion-dispersion) normal to the concerned boundary (kg/(m^2.s))*

… 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)*



… 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*

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, elliptic and hyperbolic equation)*

→
- *numerical dispersion*
- *artificial oscillations*
- *more memory*
- *more CPU*

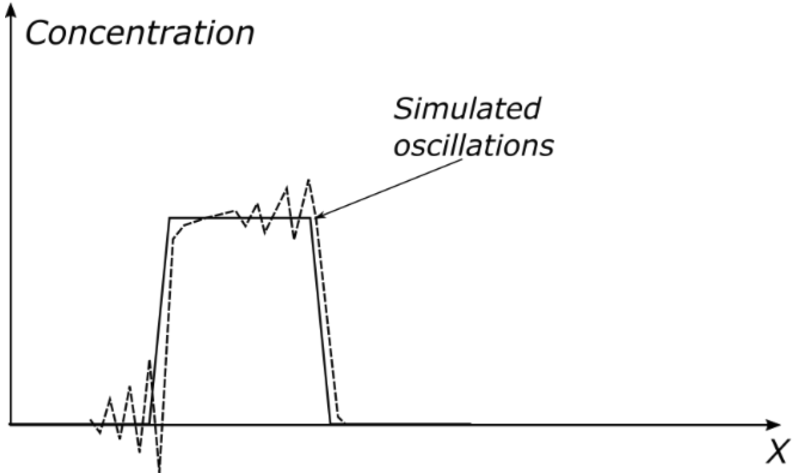
- *Introduction*
- *Pe and Cr numbers*
- *Eulerian methods*
- *Eulerian-Lagrangian methods*
- *Multi-reactive transport*

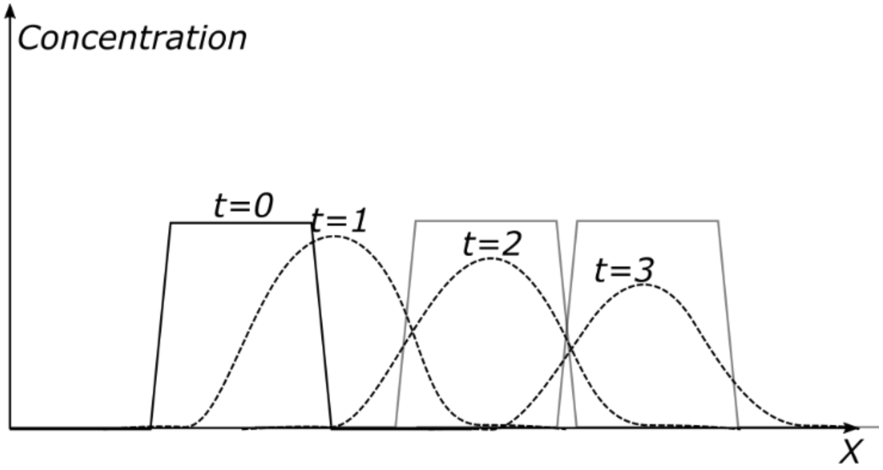
Introduction to solute transport solving methods

… 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)

- *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 and even hyperbolic)*

with regards to a fixed axis system

with regards to a moving axis system (referential) at v_a /R velocity along a streamline

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

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* *(Price et al. 1966)*

- *dimensionless Cr number = ratio between advection travel during a time step and the grid dimension* $Cr = \frac{v_a \Delta t}{\Delta x}$

(Daus & Frind 1985, Rausch et al. 2005)

➡ $Cr < 1$ *to allow the transfer of information from a grid cell (element) to the next without losing information*

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:*

central-in-space

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

where α *is the upwind coefficient,* $\alpha \in [0,1]$

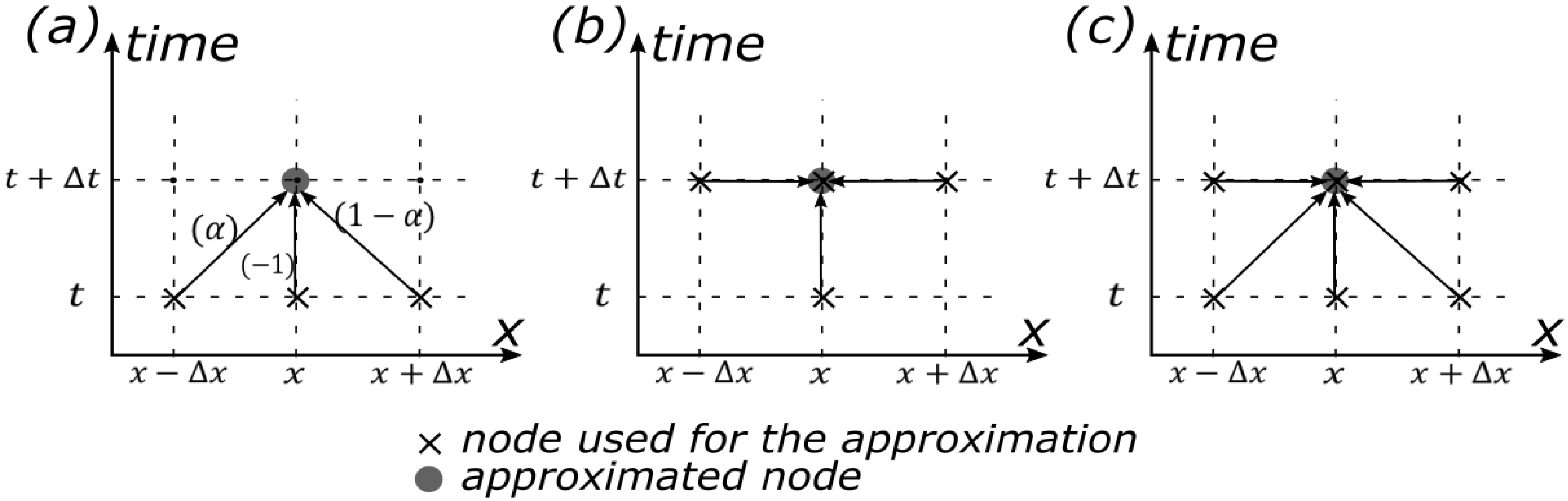
$$\frac{\partial C}{\partial x} \approx \frac{(1-\alpha)C(x+\Delta x)-C(x)+\alpha C(x-\Delta x)}{\Delta x}$$

α *must be chosen larger than 0.5 to create an upwind weighting*

Solving methods

Eulerian methods: *combined with different time integration schemes*

central-in-space



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

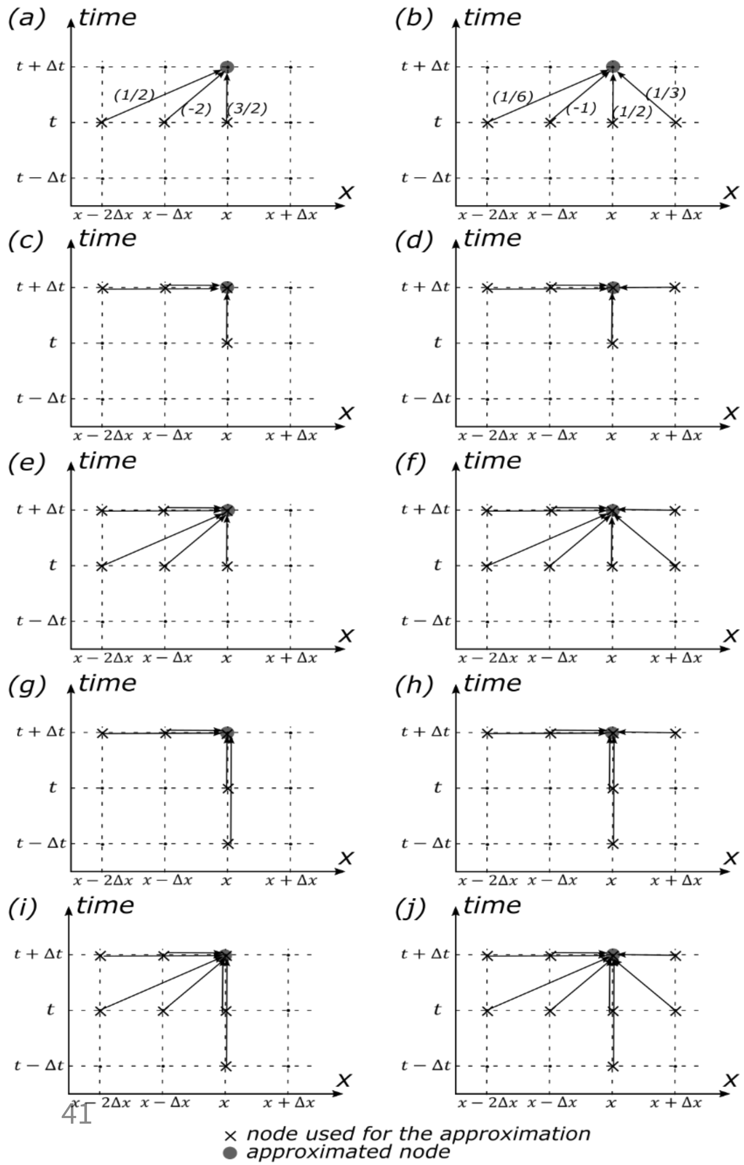
- *(a) an explicit*
- *(b) an implicit*
- *(c) a Crank-Nicolson time integration scheme*

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

2^{nd} order *3^{rd} order*



Time scheme

Explicit θ =0

Implicit θ = 1

Crank-Nicolson θ =0.5

1st order BDF implicit θ = 1

BDF = Backward Differentiation Formula (family of implicit methods)

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

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

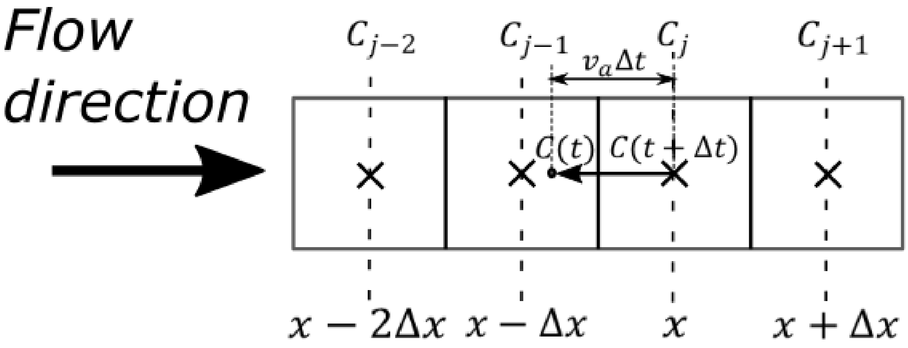
Eulerian methods: TVD method (Total Variation Diminishing)

(Cox and Nishikawa 1991, Zheng 1990, Zheng and Bennet 1995, Zheng and Wang 1999)

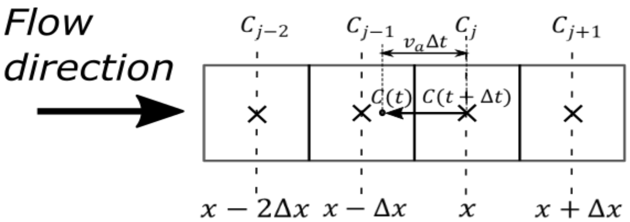
- *can be implemented in FDM-, FVM- and FEM-based models to solve advection dominated transport*
- *known as more accurate than standard central-in-space weighting and upstream methods for simulating sharp concentration variations*
- *wise to apply them only if Pe < 2 and Cr < 1*
- *in a FD regular grid,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

$$\Rightarrow \quad C(x, t+\Delta t) = C(x - v_a t, t)$$

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



Eulerian methods: TVD method (Total Variation Diminishing)



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

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

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

$$\boxed{Cr = \frac{v_a \Delta t}{\Delta x}}$$

- *may lead to oscillations in advection dominated problems*
- *a 'flux limiter' is activated when the spatial concentration profile does not show a monotonic evolution* *(Leonard and Niknafs 1990 and 1991, Zheng and Wang 1999)*

- *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

PDE

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

➡ ***in a Lagrangian approach:***

ODE

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

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

(Zheng 1990, Bear and Cheng 2010)

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

Solving methods

Eulerian Lagrangian methods

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

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

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

(Zheng 1990)

1) Solving advection by a ‘characteristic’ method

2) Solving the 2nd term by classical method with explicit, implicit, Crank-Nicolson or Galerkin time integration

Solving methods

Eulerian Lagrangian methods

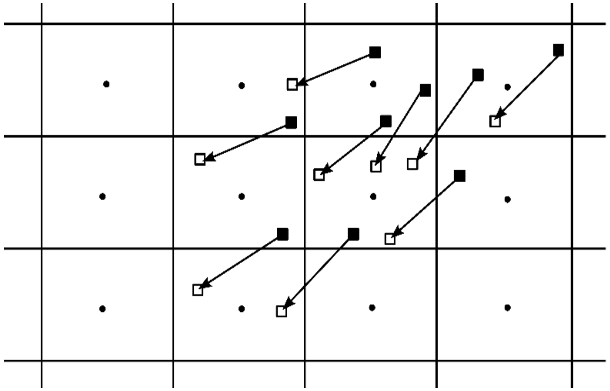
C^{v*} = *'intermediate' concentration at time* $(t + \Delta t)$

… 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 *(Garder et al. 1964, Konikow and Bredehoeft 1978, Zheng 1990)*



- *• cell centered node*
- *■ particle at time t*
- *□ particle at time t+Δt*

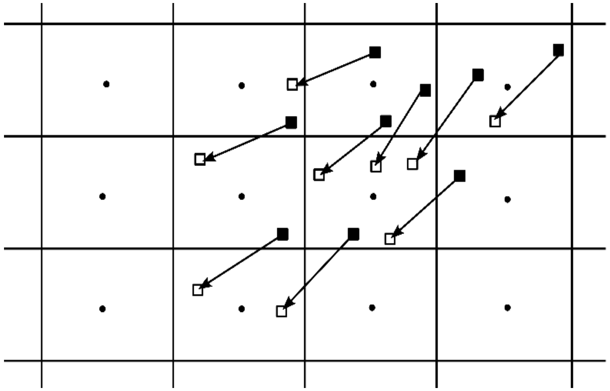
$$\tilde{C}_i^{v*}(t+\Delta t) = \frac{1}{np_i}\sum_{k=1}^{np_i} C_k^v(t)$$

$$C_i^{v*}(t+\Delta t) = \omega\tilde{C}_i^{v*}(t+\Delta t) + (1-\omega)\,C_i^v(t)$$

- *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)*



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

$$C_i^{v*}(t+\Delta t) = \omega\tilde{C}_i^{v*}(t+\Delta t) + (1-\omega)\, C_i^v(t)$$

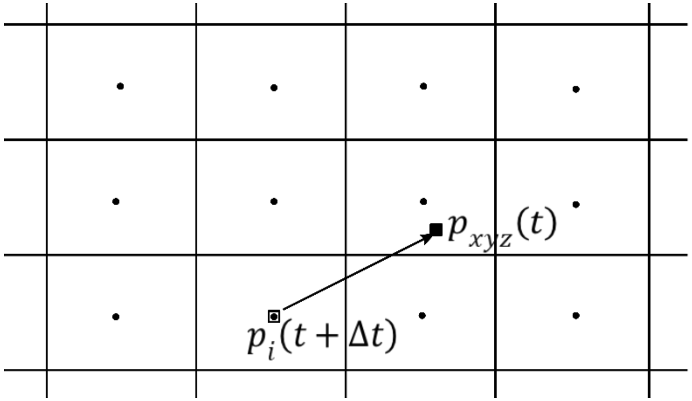
(Zheng and Wang 1999, Rausch et al. 2005)

- *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*

Eulerian Lagrangian methods

MMOC

(Ewing et al. 1983, Cheng et al. 1984, Molz et al. 1986, Zheng and Wang 1999)



- • 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

(Neuman 1981 and 1984, Zheng and Wang 1999)

- *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

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

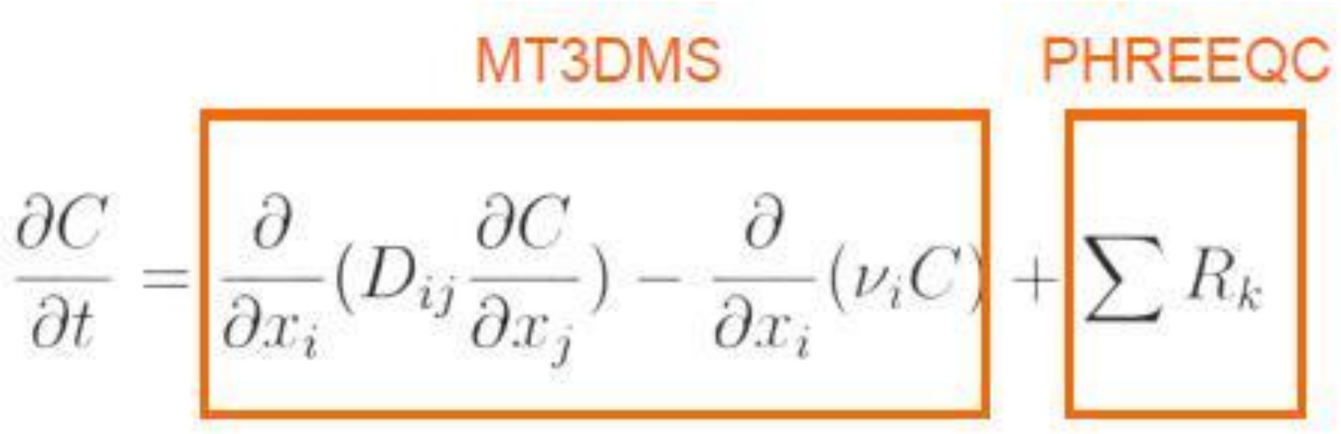
C^{v*} = *'intermediate' concentration at time* $(t+\Delta t)$

1) Solving advection by MOC, MMOC or HMOC

2) Solving the 2nd term by classical method with explicit, implicit, Crank-Nicolson or Galerkin time integration

Solving a solute transport problem

with multi-reactive transport



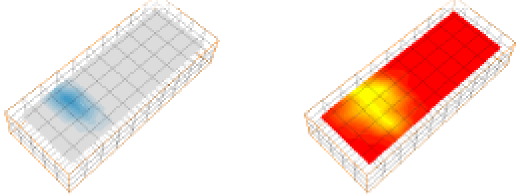
$$\frac{\partial C}{\partial t} = \overset{\text{MT3DMS}}{\boxed{\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(\nu_i C)}} + \overset{\text{PHREEQC}}{\boxed{\sum R_k}}$$

- (temporal) operator-splitting method: separate solutions for the "transport step" and "reaction step(s)"
- Rk'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

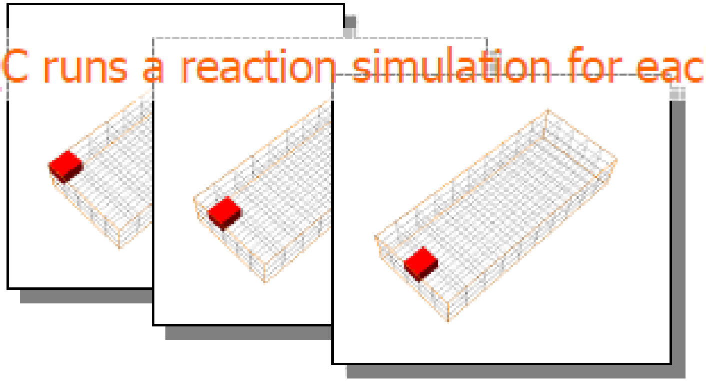
Multi-reactive transport

MT3MS simulates the transport of n components for a timestep Δt



Comp 1 Comp 2 … Comp n

PHREEQC runs a reaction simulation for each grid cell



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