1D Diagenetic modelling - Porous Media

Arthur Capet, Eric Delhez, Marilaure Grégoire

July 11, 2017

Reaction-Transport Models

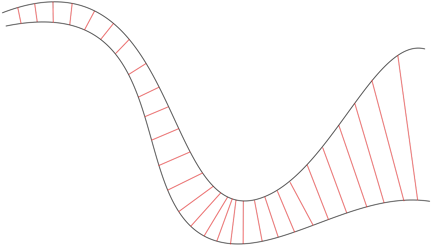
Transport Reaction Equation

$$\frac{\partial C}{\partial t} = T + R$$

C	Concentration	mass/m^3
t	Time	time
T	Transport	mass/m^3/time
R	Reaction	mass/m^3/time

1D spatial contexts

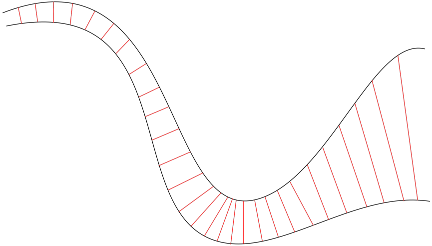
Ex.: Rivers



- $C(t) \rightarrow C(t, x)$

1D spatial contexts

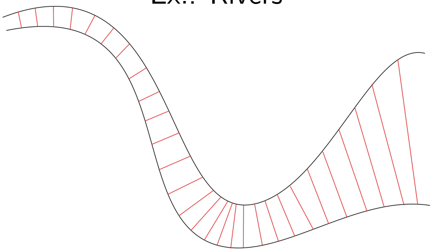
Ex.: Rivers



- $C(t) \to C(t,x)$
- x is the axis of largest spatial variability

1D spatial contexts

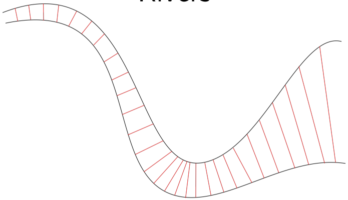
Ex.: Rivers



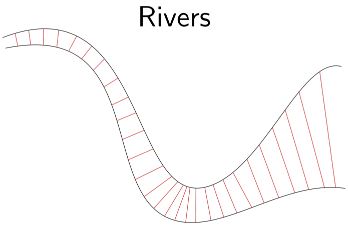
- $C(t) \rightarrow C(t, x)$
- x is the axis of largest spatial variability
- C can be considered homogeneous along the other dimension

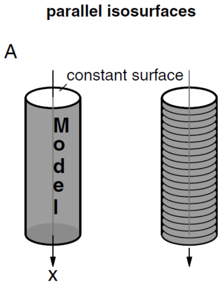
1D spatial contexts

Rivers

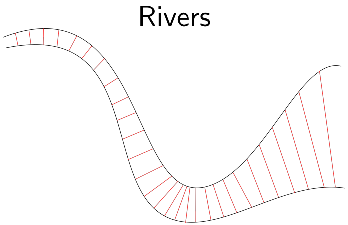


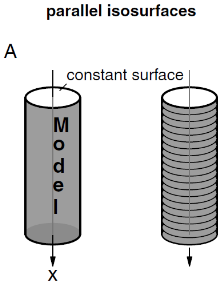
1D spatial contexts

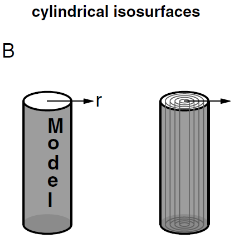




1D spatial contexts

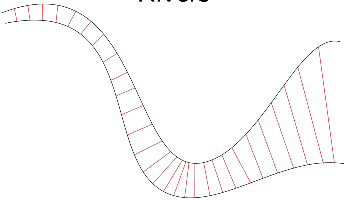






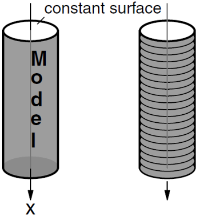
1D spatial contexts

Rivers



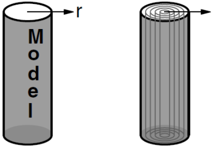
parallel isosurfaces

A



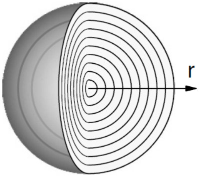
cylindrical isosurfaces

B



spherical isosurfaces

D



Reaction-Transport Models in 1D

Transport Reaction Equation in 1D

$$\frac{\partial C}{\partial t} = \underbrace{-\frac{1}{A_x}\frac{\partial (A_x . J)}{\partial x}}_{\text{Transport}} + R$$

C	Concentration	mass/m^3
t	Time	time
R	Reaction	mass/m^3/time
A_x	Surface	m^2
J	Flux	mass/m^2/time

Reaction-Transport Models in 1D

Transport Reaction Equation in 1D

$$\frac{\partial C}{\partial t} = \underbrace{-\frac{1}{A_x}\frac{\partial (A_x . J)}{\partial x}}_{\text{Transport}} + R$$

C	Concentration	mass/m^3
t	Time	time
R	Reaction	mass/m^3/time
A_x	Surface	m^2
J	Flux	mass/m^2/time

General flux expression

$$J = \underbrace{-D\frac{\partial C}{\partial x}}_{\text{Diffusion}} + \underbrace{vC}_{\text{Advection}}$$

D	Diffusion Coefficient	m^2/time
v	Advection rate	m/time

Reaction-Transport Models in 1D

$$\frac{\partial C}{\partial t} = -\frac{1}{A_x}\frac{\partial (A_x . J)}{\partial x} + R \qquad (1)$$

$$J = -D\frac{\partial C}{\partial x} + vC \qquad (2)$$

Reaction-Transport Models in 1D

$$\frac{\partial C}{\partial t} = -\frac{1}{A_x}\frac{\partial (A_x . J)}{\partial x} + R \qquad (1)$$

$$J = -D\frac{\partial C}{\partial x} + vC \qquad (2)$$

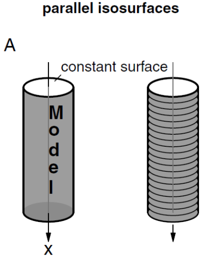
(1) + (2) → General 1D Diffusion-Advection-Reaction equation

$$\frac{\partial C}{\partial t} = \frac{1}{A_x}\frac{\partial}{\partial x}\left[A_x . D\frac{\partial (C)}{\partial x} - A_x . vC\right] + R$$

Reaction-Transport Models in 1D

$$\frac{\partial C}{\partial t} = -\frac{1}{A_x}\frac{\partial (A_x . J)}{\partial x} + R \qquad (1)$$

$$J = -D\frac{\partial C}{\partial x} + vC \qquad (2)$$



Assumptions

- Horizontal homogeneity $\rightarrow$ Constant surface $A_x = A$

(1) + (2) $\rightarrow$ General 1D Diffusion-Advection-Reaction equation

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left[D\frac{\partial (C)}{\partial x} - vC\right] + R$$

Multiple phases !

Until now :

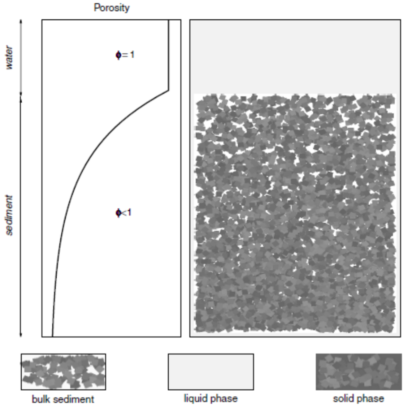
Concentration : mass / Volume

Multiple phases !

Until now :

Concentration : mass / Volume

Bulk Sediments = Solid + Liquid



Multiple phases !

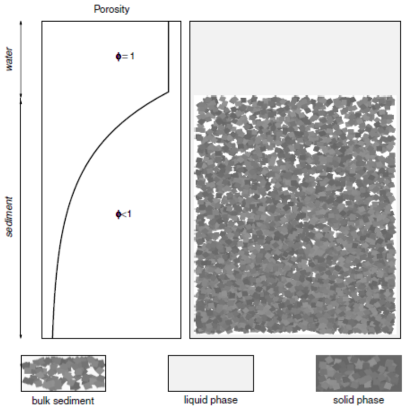
Until now :

Concentration : mass / Volume

Bulk Sediments = Solid + Liquid

More convenient to use

- for Solutes
  mass / Vol. of liquid
- for Solids
  mass / Vol. of solid



Multiple phases !

Until now :

Concentration : mass / Volume

Bulk Sediments = Solid + Liquid

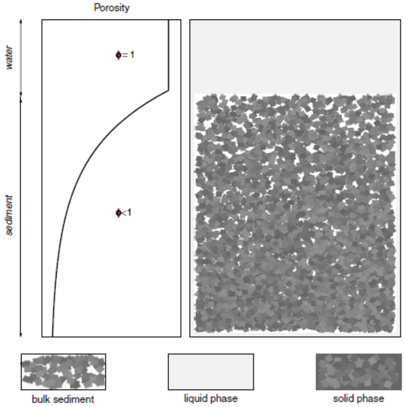
More convenient to use

- for Solutes
  mass / Vol. of liquid
- for Solids
  mass / Vol. of solid

Porosity :

ϕ = Vol. Liquid / Vol. Bulk

$1 - \phi$ = Vol. Solid / Vol. Bulk



Multiple phases !

Porosity :

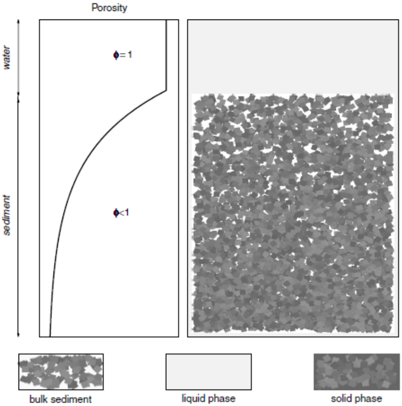
$\phi =$ Vol. Liquid / Vol. Bulk

$1 - \phi =$ Vol. Solid / Vol. Bulk

if R_s is a solid-phase reaction rate [mmol/m^3_{solid}/time]

The effect on liquid phase will be :

$R_s.(1-\phi)/(\phi)$



Multiple phases : Transport terms

for liquids :

- Diffusion is due to molecular diffusion
- Advection is due to liquid flow

$$J_{Liq.} = -D_{sed}\frac{\partial C}{\partial x} + v_L C$$

Multiple phases : Transport terms

for liquids :

- Diffusion is due to molecular diffusion
- Advection is due to liquid flow

for solid :

- Diffusion is due to bioturbation
- Advection is due to solid advection (sedimentation or compression)

$$J_{Liq.} = -D_{sed}\frac{\partial C}{\partial x} + v_L C \qquad\qquad J_{Sol.} = -D_b\frac{\partial C}{\partial x} + v_S C$$

Reactive Transport in Porous Media

for liquids :

$$\frac{\partial \phi_x C}{\partial t} = \frac{\partial}{\partial x} \left[\phi_x J_L\right] + \phi_x R_L$$

for solids :

$$\frac{\partial (1-\phi_x) S}{\partial t} = \frac{\partial}{\partial x} \left[(1-\phi_x) J_S\right] + (1-\phi_x) R_S$$

Reactive Transport in Porous Media

for liquids :

$$\frac{\partial \phi_x C}{\partial t} = \frac{\partial}{\partial x}\left[\phi_x J_L\right] + \phi_x R_L$$

$$\frac{\partial \phi_x C}{\partial t} = \frac{\partial}{\partial x}\left[\phi_x(-D_{sed}\frac{\partial C}{\partial x} + v_L C)\right] + \phi_x R_L$$

for solids :

$$\frac{\partial (1-\phi_x) S}{\partial t} = \frac{\partial}{\partial x}\left[(1-\phi_x) J_S\right] + (1-\phi_x) R_S$$

$$\frac{\partial (1-\phi_x) S}{\partial t} = \frac{\partial}{\partial x}\left[(1-\phi_x)(-D_b\frac{\partial C}{\partial x} + v_S C)\right] + (1-\phi_x) R_S$$

Reactive Transport in Porous Media

for liquids :

$$\frac{\partial \phi_x C}{\partial t} = \frac{\partial}{\partial x}\left[\phi_x J_L\right] + \phi_x R_L$$

$$\frac{\partial \phi_x C}{\partial t} = \frac{\partial}{\partial x}\left[\phi_x(-D_{sed}\frac{\partial C}{\partial x} + v_L C)\right] + \phi_x R_L$$

$$\frac{\partial C}{\partial t} = \frac{1}{\phi_x}\frac{\partial}{\partial x}\left[\phi_x(-D_{sed}\frac{\partial C}{\partial x} + v_L C)\right] + R_L$$

for solids :

$$\frac{\partial (1-\phi_x) S}{\partial t} = \frac{\partial}{\partial x}\left[(1-\phi_x) J_S\right] + (1-\phi_x) R_S$$

$$\frac{\partial (1-\phi_x) S}{\partial t} = \frac{\partial}{\partial x}\left[(1-\phi_x)(-D_b\frac{\partial C}{\partial x} + v_S C)\right] + (1-\phi_x) R_S$$

$$\frac{\partial S}{\partial t} = \frac{1}{1-\phi_x}\frac{\partial}{\partial x}\left[(1-\phi_x)(-D_b\frac{\partial C}{\partial x} + v_S C)\right] + R_S$$

- We only consider dissolved oxygen, only the liquid phase.
- Permeable sediments $\rightarrow$ No liquid flow, no advection.
- Constant oxygen consumption rate as a function of depth.

$$\frac{\partial O_2(z)}{\partial t} = \frac{1}{\phi}\frac{\partial}{\partial z}[\phi D \frac{\partial C}{\partial z}] - \gamma(z) \tag{3}$$

$$\gamma(z) = \begin{cases} \gamma_0, \text{if } z \leq L \\ 0, \text{if } z > L \end{cases} \tag{4}$$