1D Diagenetic modelling - Porous Media

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Reaction-Transport Models

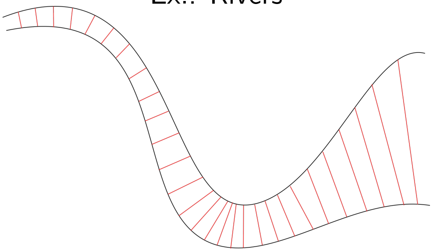
Transport Reaction Equation

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

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



- $C : C(x, t)$

1D spatial contexts

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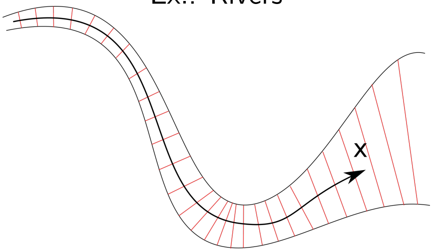
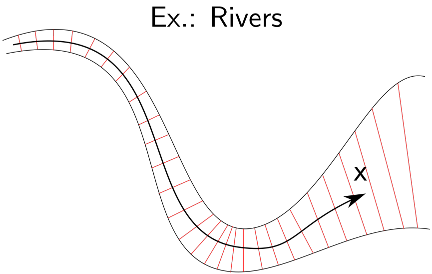


- $C : C(x, t)$
- x: main axis of spatial variability

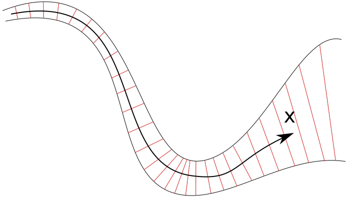
1D spatial contexts



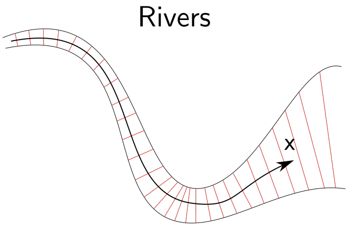
- $C : C(x, t)$
- x: main axis of spatial variability
- C is considered homogeneous along the other dimensions

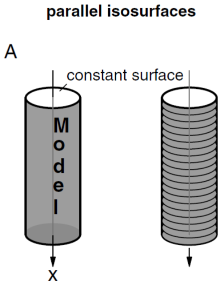
1D spatial contexts

Rivers



1D spatial contexts





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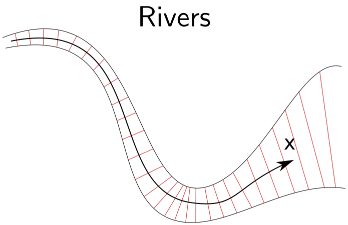

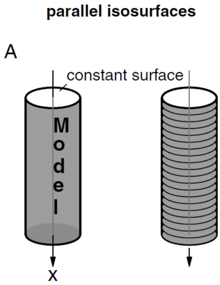

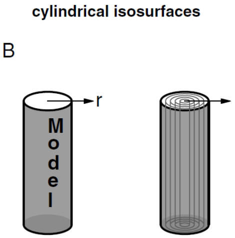

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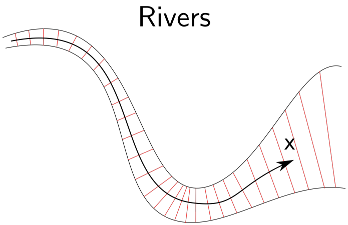

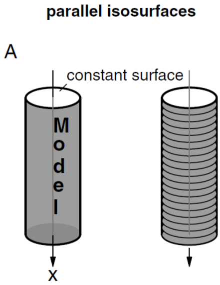

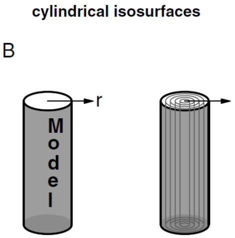

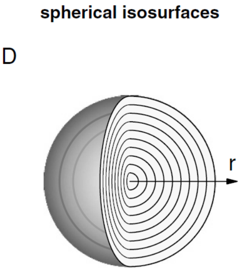

Reaction-Transport Models in 1D

Transport Reaction Equation in 1D

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

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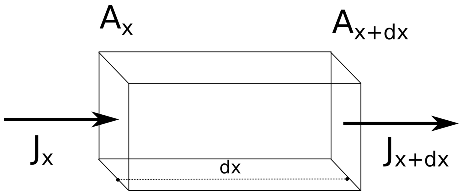
t	Time	time
R	Reaction	mass/m^3/time
A_x	Surface	m^2
J	Flux	mass/m^2/time



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General flux expression

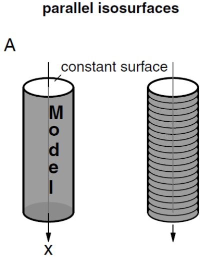
$$J = \underbrace{-D\frac{\partial C}{\partial x}}_{\text{Diffusion}} + \underbrace{vC}_{\text{Advection}}$$

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

Reaction-Transport Models in 1D

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

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



Spatial context

Horizontal homogeneity

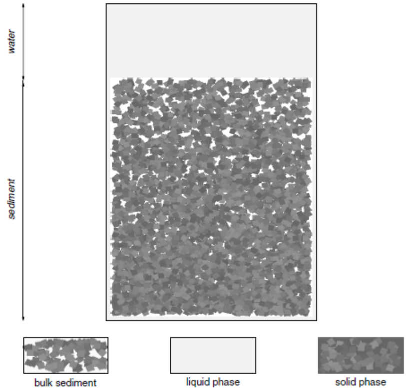
- Depth as the main axis → Constant surface $A_x = A$

(1) + (2) → 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

Bulk Sediments = Solid + Liquid



Multiple phases
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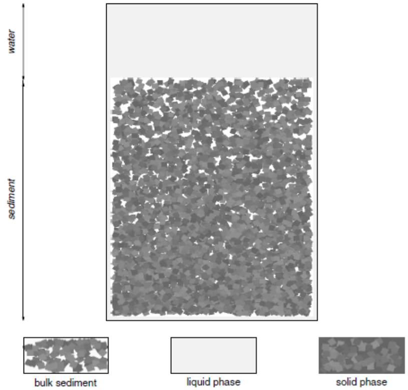
Until now :

- Concentrations
  Mass / Vol. of Bulk Sediments



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Until now :

- Concentrations
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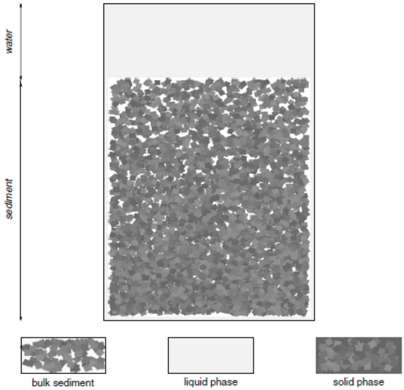
Different transport processes
→ need to express different phases.

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



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  Mass / Vol. of liquid
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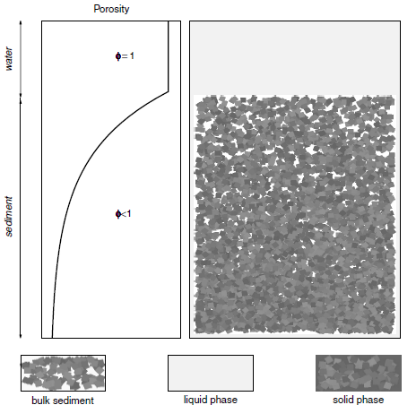
Useful for conversion: Porosity (ϕ)

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



Multiple phases : porosity

Porosity : $\phi = \frac{\text{volume of pore waters}}{\text{volume sediments}}$

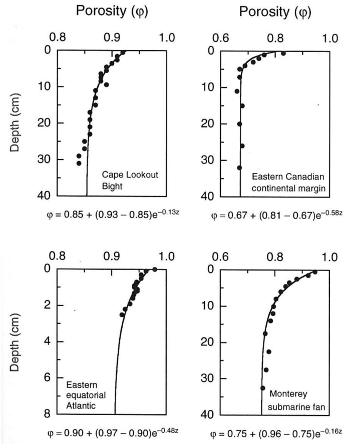


Figure 1: Examples of porosity profiles

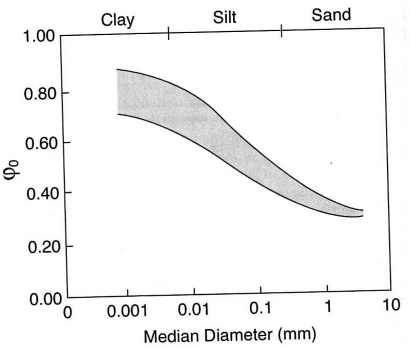


Figure 2: Upper porosity and grain size

Multiple phases : porosity

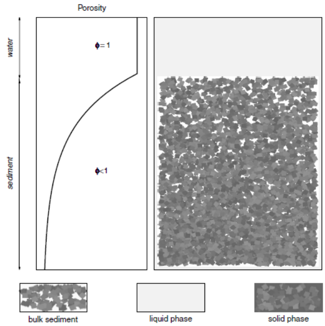
Porosity :

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

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

Example : Solid Dissolution

$S(\text{solid}) \xrightarrow{\gamma} C(\text{dissolved})$



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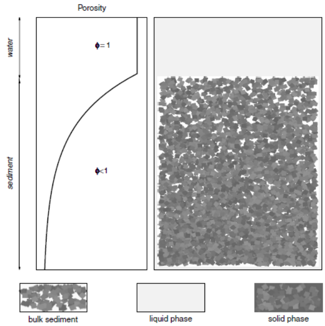
$\frac{\partial S}{\partial t} = -\gamma S$ (No Transport)

S	Conc. in solid	[mmol m_{solid}^{-3}]
γ	diss. rate	[d^{-1}]
C	Conc. in liquid	[mmol m_{liquid}^{-3}]



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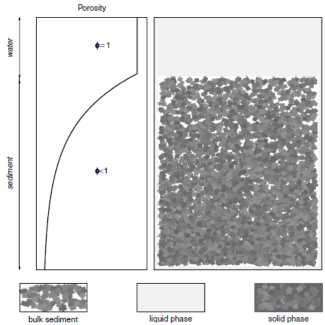
S	Conc. in solid	$[\text{mmol } m^{-3}_{solid}]$
γ	diss. rate	$[d^{-1}]$
C	Conc. in liquid	$[\text{mmol } m^{-3}_{liquid}]$

The effect on liquid phase will be :

$\frac{\partial C}{\partial t} = \gamma S . \frac{1-\phi}{\phi}$



Multiple phases : Different transport processes

Liquids

- Diffusion is due to molecular diffusion
- Advection is due to liquid flow with respect to the SWI.

Liquids

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

Tortuosity

$$D_{sed} = \frac{D_{sea\ water}}{1 - ln(\phi^2)}$$

Boudreau, 1996

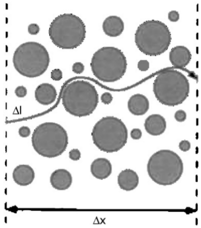


Fig. 1. Convolute diffusion path in a sediment from Boudreau (1996).

Multiple phases : Different transport processes

Liquids

- Diffusion is due to molecular diffusion
- Advection is due to liquid flow with respect to the SWI.
  - Sedimentation
  - Compaction
  - Biological activity
  - Pressure gradients in permeable sediments.

Liquids

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

Multiple phases : Different transport processes

Liquids

- Diffusion is due to molecular diffusion
- Advection is due to liquid flow with respect to the SWI.

Solid

- Diffusion is due to bioturbation
- Advection is due to solid advection with respect to the SWI (sedimentation or compression)

Liquids

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

Solids

$$J_{Sol.} = -D_b\frac{\partial S}{\partial x} + v_S S$$

Bioirrigation

Flushing of burrows with overlying waters

Allows diffusive exchanges between bottom waters and porewaters at depth, through burrow walls

$\rightarrow$ 3D(2D) context.
However, Boudreau (1984) showed the equivalence of

- 3D set-up with cylindrical burrows
- 1D vertical set-up with non-local exchange of pore waters

Reactive Transport in Porous Media

Solutes

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

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

Solutes

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

Solids

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

Reactive Transport in Porous Media

Solutes

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

Solids

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

Reactive Transport in Porous Media

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Boundary Conditions (usual)

Solutes

Solids

Reactive Transport in Porous Media

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Boundary Conditions (usual)

Solutes

- Upper boundary $(x = 0)$
  Imposed conc. ($C_{bot.\,waters}$).

Solids

- Upper boundary $(x = 0)$
  Imposed flux (sedimentation).

Reactive Transport in Porous Media

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Boundary Conditions (usual)

Solutes

- Upper boundary ($x = 0$)
  Imposed conc. ($C_{bot.\,waters}$).
- Lower boundary ($x = \infty$)
  Zero Gradient

Solids

- Upper boundary ($x = 0$)
  Imposed flux (sedimentation).
- Lower boundary ($x = \infty$)
  Zero Gradient

Organic Matter Lability I

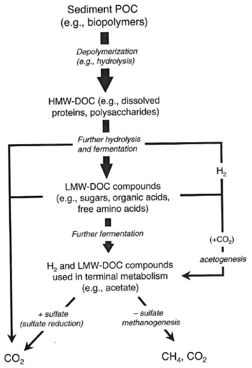


Figure 3: Example of Org. C degradation

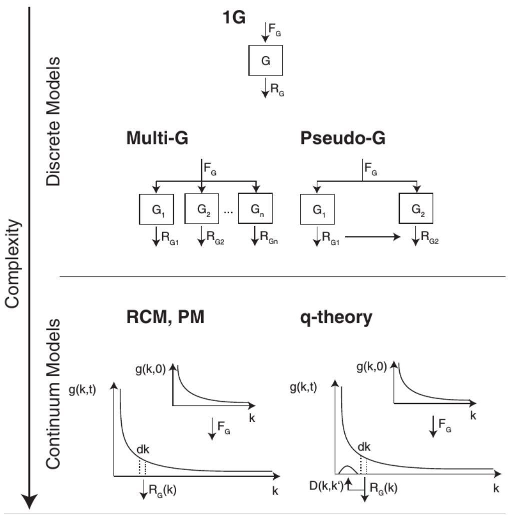
Large chain generally replaced by one step reaction $Part.\, OrgC \xrightarrow{R_G} DIC$

$$R_G = k.G.\sum_i F_{TEM,i} F_{BIO,i} F_{TEA,i} F_{IN,i} F_{T,i}$$

G	Organic Matter
R_G	Degradation rate,
k	max degradation rate,
i	metabolic pathways,
$F_{TEM,i}$	Temperature effect
$F_{BIO,i}$	Microbial biomasses
$F_{TEA,i}$	Terminal electron acceptor
$F_{IN,i}$	Inhibition by other TEA
$F_{T,i}$	bioenergetic limitation (Gibbs energy)

According to complexity, several factors are empirically included in k

Organic Matter Lability II



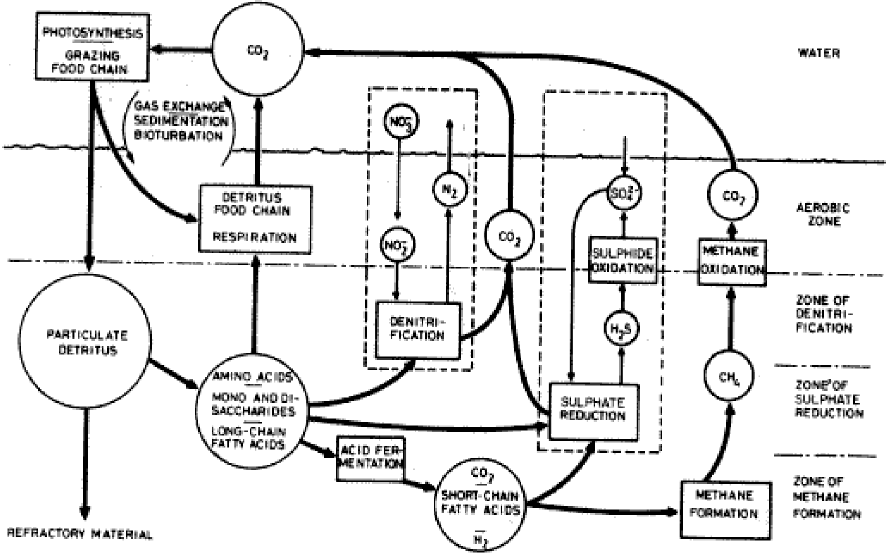
Single G neglects

- Various organic compounds in OM source :
- Refractory OM formed during bacterial remin.

Arndt,2013 (review) :

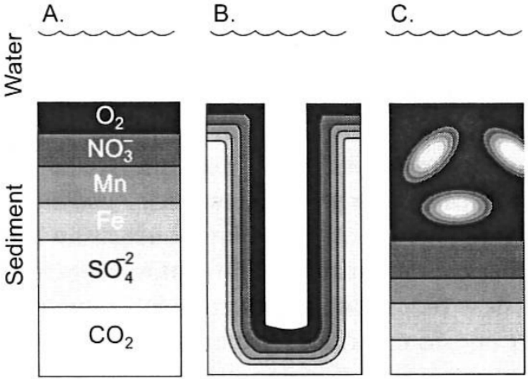
- Multi-G model
  $R_G = \sum_i k_i G_i$
- Continuous lability spectrum models
  $$R_G = -\int_0^\infty k g(k) dk$$
- OM degradation explicitely driven by ecosytem dynamics (incl. bact.)

Redox zonation I



Redox zonation II

Microscales



N cycling

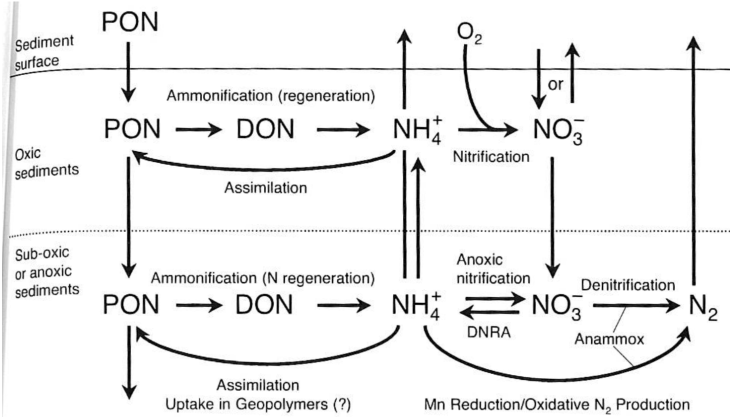
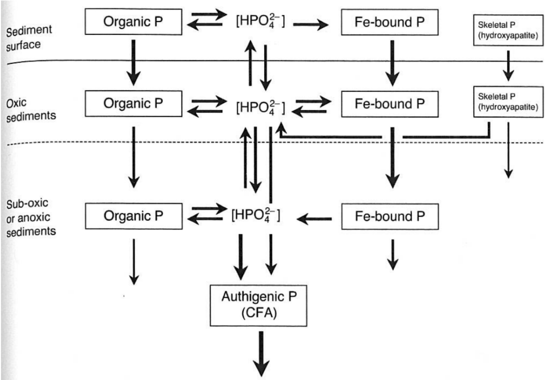


Figure 16.2 A conceptual model illustrating the processes associated with nitrogen cycling in marine sediments (based on information from several sources).

Phosphorus cycling I



Slomp et al, 2007

Case Study : Oxygen diffusion

- We consider dissolved Oxygen (only liquid phase).
- Non-permeable sediments $\rightarrow$ No liquid flow, no advection.
- Constant oxygen consumption rate above a certain depth, 0 below.

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$$\gamma(z) = \gamma_0 \cdot \frac{O_2(z)}{O_2(z) + k_s} \tag{3}$$

- Boundary conditions:
  $O_2|_{z=0} = O_{2\ b.w.}$; $\frac{\partial O_2}{\partial z}|_{z=\infty} = 0$
- Steady-state solution : $\frac{\partial O_2}{\partial t} = 0$

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ϕ	Porosity
D	Diffusion coeficient
γ_0	Respiration rate
k_s	"*Oxygen Limitation*"
$O_{2\ b.w.}$	$[O_2]$ bottom waters

Case Study : Oxygen diffusion

- Describe model implementation in R (using the Reactran framework)
- Compare with oxygen profile from the mud sediment core
- Infer diffusive flux at the Sediment-Water interface
- Extend the model :
  - Include Solid phase for organic carbon
  - Include Bioirrigation
  - Include Nitrogen Cycle

Why do we consider cohesive sediments ?

Sands
$\rightarrow$ Permeability
$\rightarrow$ Needs to resolve flows through the sediment matrix
$\rightarrow$ Needs higher dimensional context.