1D Diagenetic modelling - Porous Media

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Reaction-Transport Models

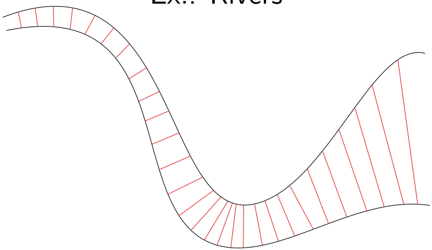
Transport Reaction Equation

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

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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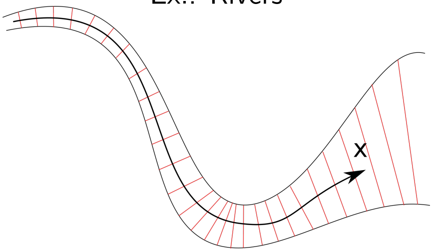
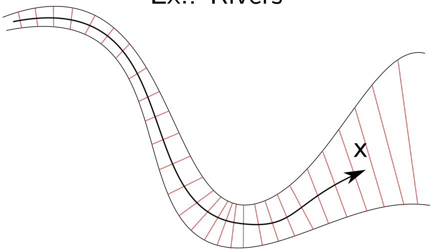


- $C : C(x, t)$
- x: main axis of spatial variability

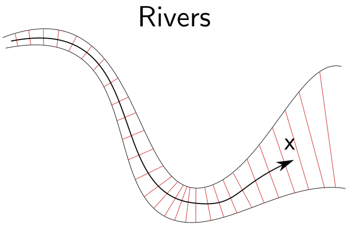
1D spatial contexts

Ex.: Rivers



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

1D spatial contexts



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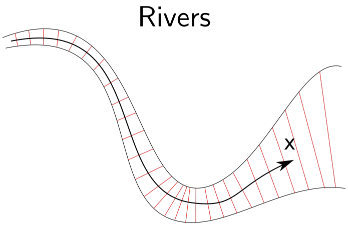

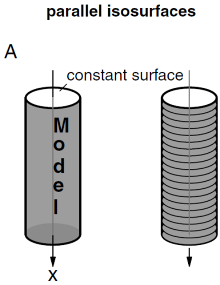

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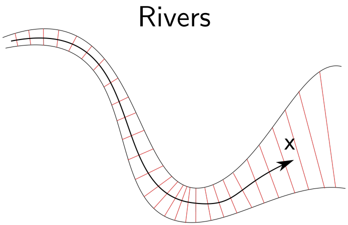
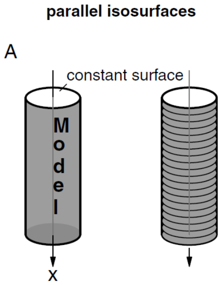
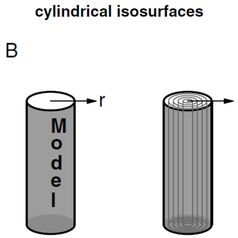
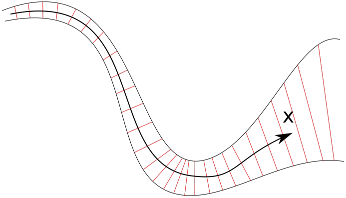






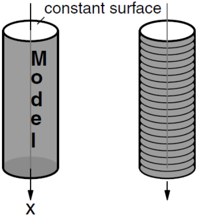
1D spatial contexts

Rivers



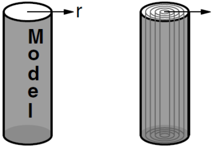
parallel isosurfaces

A



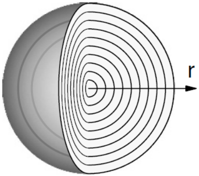
cylindrical isosurfaces

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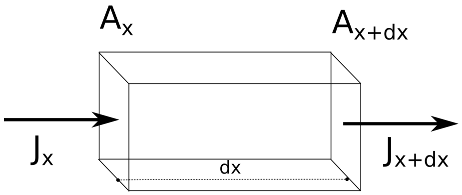
R	Reaction	mass/m^3/time
A_x	Surface	m^2
J	Flux	mass/m^2/time



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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

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

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

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

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

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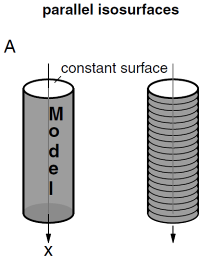

Spatial context

Horizontal homogeneity

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

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

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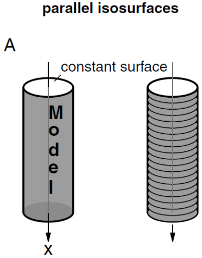

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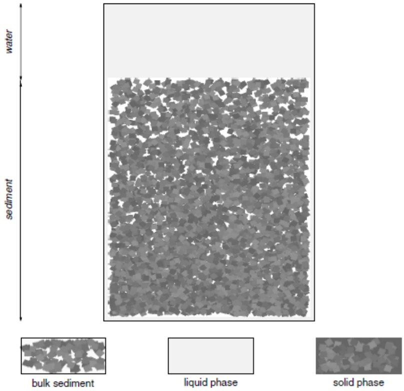
$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left[D\frac{\partial (C)}{\partial x} - vC\right] + R$$

Multiple phases !

Bulk Sediments = Solid + Liquid



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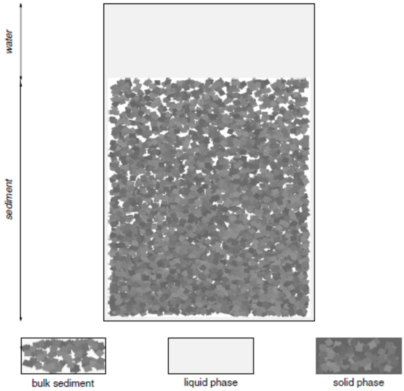
Until now :

- Concentrations
  Mass / Vol. of Bulk Sediments



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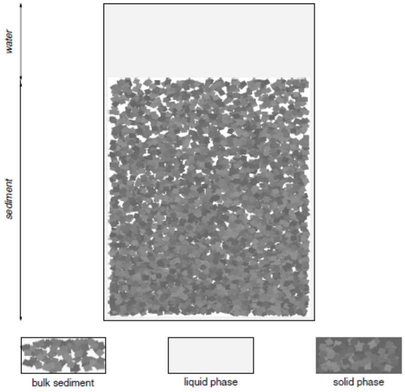
More convenient :

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



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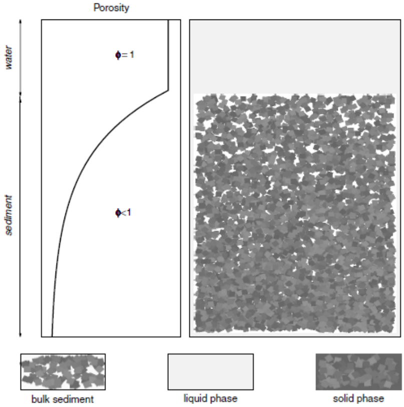


Useful for conversion: Porosity (ϕ)

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

Multiple phases : porosity

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

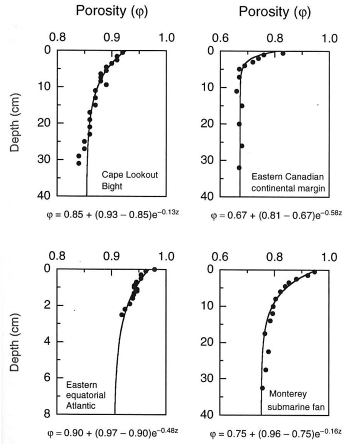


Figure 1: Examples of porosity profiles

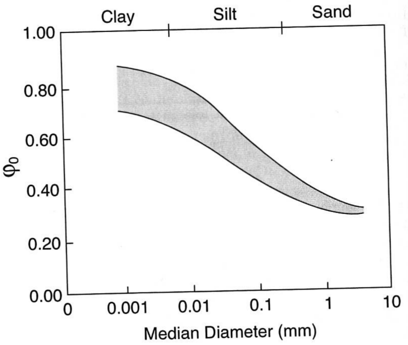


Figure 2: Upper porosity and grain size

Multiple phases : porosity

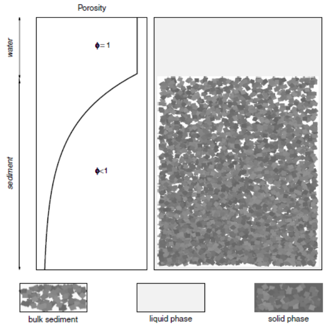
Porosity :

ϕ = Vol. Liquid / Vol. Bulk

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

Example : Solid Dissolution

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



Multiple phases : porosity

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

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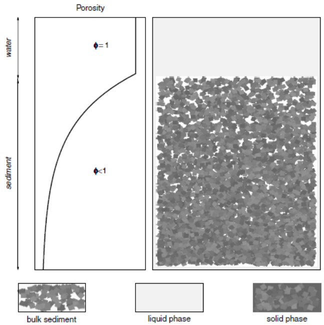
$\frac{\partial S}{\partial t} = -\gamma S$ (No Transport)

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



Multiple phases : porosity

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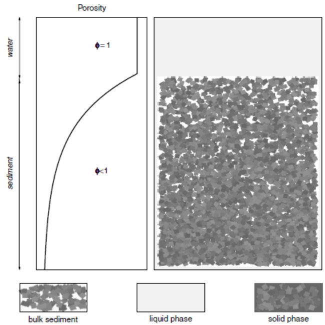
S	Conc. in solid	[mmol m^{-3}_{solid}]
γ	diss. rate	[d^{-1}]
C	Conc. in liquid	[mmol m^{-3}_{liquid}]

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.

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

Tortuosity

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

Boudreau, 1996

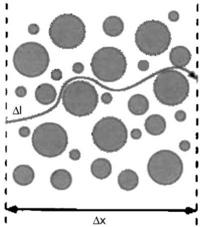


Fig. 1. Convolute diffusion path in a sediment from Boudreau (1996).

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.

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

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)

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

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

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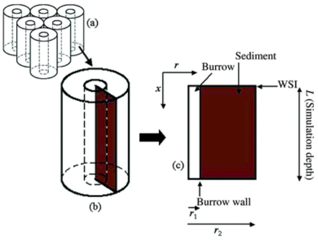
- 1D vertical set-up with non-local exchange of pore waters

$$
\begin{aligned}
\frac{\partial C}{\partial t} &= D_s \frac{\partial^2 C}{\partial z^2} + \frac{D_s}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) + \sum R \\
\frac{\partial \overline{C}}{\partial t} &= D_s \frac{\partial \overline{C}}{\partial z^2} - \alpha(\overline{C} - C_0) + \sum \overline{R} \\
\alpha &= \frac{2 D_s r_1}{(r_2^2 - r_1^2)(\overline{r} - r_1)}
\end{aligned}
\tag{3}
$$



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

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

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

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

Reactive Transport in Porous Media

Solutes

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

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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

Solutes

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

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

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 $(x = \infty)$
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Organic Matter Lability I

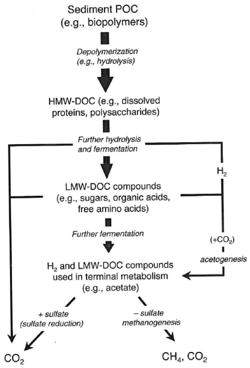


Figure 3: Example of (simplified) OM degradation (anoxic)

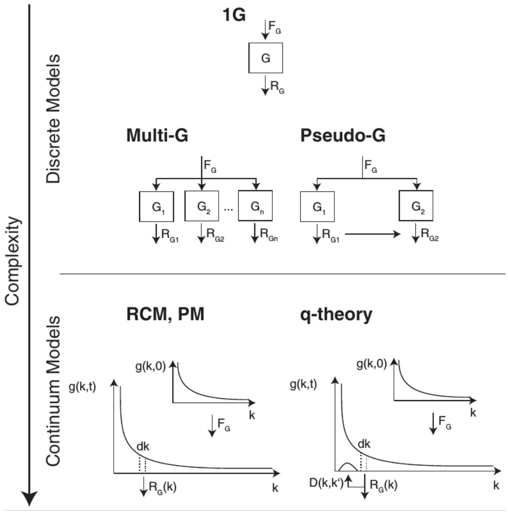
Large chain generally replaced by one step reaction $G \xrightarrow{R_G} DIC$

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

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



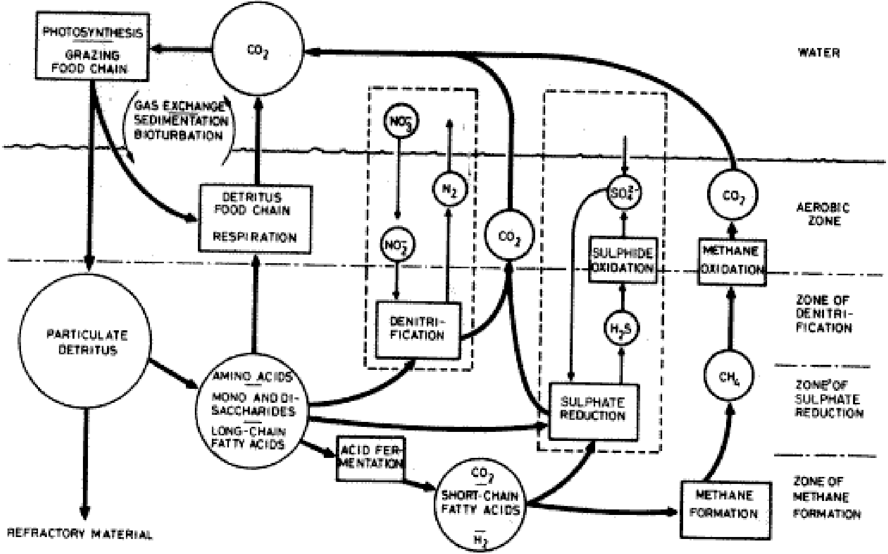
Single G neglects

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

Arndt,2013 (review) :

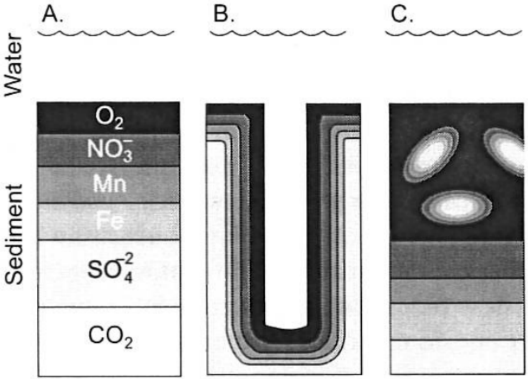
- Multi-G model
  $R_G = \sum_i k_i G_i$
- Continuous lability spectrum models
  $$R_G = -\int_0^\infty k g(k) dk$$
- OM degradation explicitely driven by ecosytem dynamics (incl. bact.)

Redox zonation I



Redox zonation II

Microscales



N cycling

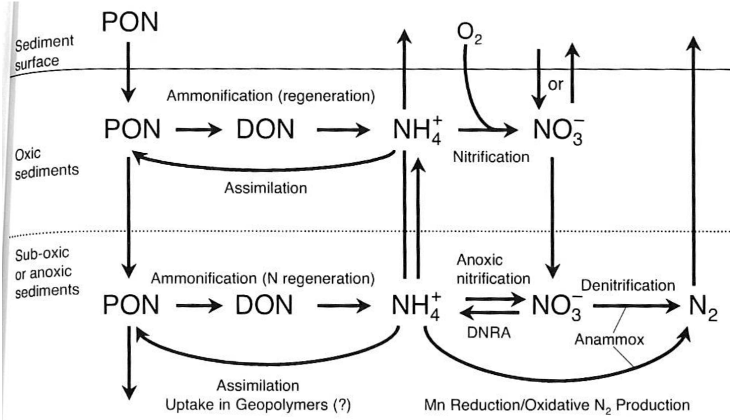
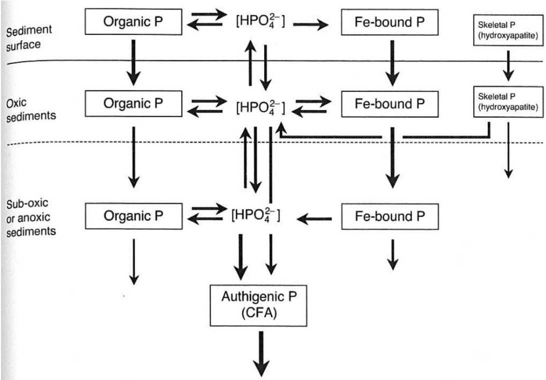


Figure 16.2 A conceptual model illustrating the processes associated with nitrogen cycling in marine sediments (based on information from several sources).

Phosphorus cycling I



Slomp et al, 2007

Phosphorus cycling II

Table 2. The differential equations for each P reservoir in the (I) oxidized surface zone ($0 \leq x \leq L_1$) and (II) reduced sediment zone ($x > L_1$).

Porewater PO_4 (C)

$$[\overbrace{D_b(\underbrace{1+K_{eq1}}_{\text{Eq. Ads.}})+D_s}^{\text{Diff.}}]\frac{d^2C_I}{dx^2} - \underbrace{\omega(1+K_{eq1})\frac{dC_I}{dx}}_{\text{Adv.}} + \overbrace{k_g\vartheta(G_I-G_\infty)}^{\text{Remin.}} - \underbrace{\alpha(C_I-C_o)}_{\text{Bioirrig.}} - \overbrace{k_s(C_I-C_s)}^{\text{Kin. ads.}} = 0 \quad \text{(A1)}$$

$$[D_b(1+K_{eq2})+D_s]\frac{d^2C_{II}}{dx^2} - \omega(1+K_{eq2})\frac{dC_{II}}{dx} + k_g\vartheta(G_{II}-G_\infty) - \alpha(C_{II}-C_o) - \underbrace{k_a(C_{II}-C_a)}_{\text{Dissolution Fe-bound P}} + \overbrace{k_m\vartheta(M_{II}-M_\infty)}^{\text{Apathite precipitation}} = 0 \quad \text{(A2)}$$

Organic P (G)

$$D_b\frac{d^2G_I}{dx^2} - \omega\frac{dG_I}{dx} - k_g(G_I-G_\infty) = 0 \quad \text{(A3)}$$

$$D_b\frac{d^2G_{II}}{dx^2} - \omega\frac{dG_{II}}{dx} - k_g(G_{II}-G_\infty) = 0 \quad \text{(A4)}$$

Fe-bound P (M)

$$D_b\frac{d^2M_I}{dx^2} - \omega\frac{dM_I}{dx} + \frac{k_s}{\vartheta}(C_I-C_s) = 0 \quad \text{(A5)}$$

$$D_b\frac{d^2M_{II}}{dx^2} - \omega\frac{dM_{II}}{dx} - k_m(M_{II}-M_\infty) = 0 \quad \text{(A6)}$$

Authigenic P (A)

$$D_b\frac{d^2A_I}{dx^2} - \omega\frac{dA_I}{dx} = 0 \quad \text{(A7)}$$

$$D_b\frac{d^2A_{II}}{dx^2} - \omega\frac{dA_{II}}{dx} + \frac{k_a}{\vartheta}(C_{II}-C_a) = 0 \quad \text{(A8)}$$

Instantaneous, reversible linear equilibrium adsorption gives

Adsorbed P (S)

$$S_I = \frac{K_{eq1}}{\vartheta}C_I \quad \text{(A9)}$$

$$S_{II} = \frac{K_{eq2}}{\vartheta}C_{II} \quad \text{(A10)}$$

1. Reaction-Transport Models in 1D

2. Porous Media

3. Reaction-Transport in Porous Media

4. Case Study : Oxygen diffusion

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- We consider dissolved Oxygen (only liquid phase).
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ϕ	Porosity
D	Diffusion coeficient
γ_0	Respiration rate
L	"*Respiration Depth*"
$O_{2\ b.w.}$	$[O_2]$ bottom waters

Why do we consider cohesive sediments ?

Sands

$\rightarrow$ Permeability

$\rightarrow$ Needs to resolve flows through the sediment matrix

$\rightarrow$ Needs higher dimensional context.