Sediment model

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1   One-dimensional sediment model

This chapter describes the formulation of a one-dimensional sediment model. The formulations mainly refer to *Chikamoto and Yamanaka* (2005). In this chapter, I try to follow and reproduce the results obtained in *Chikamoto and Yamanaka* (2005).

1.1   Clay and Opal systems

1.1.1   No dissolution / No bioturbation

First, I deal with clay and opal systems. The governing equations are written as follows.

$$\frac{\partial S_{\text{Clay}}}{\partial t} = \frac{\partial}{\partial z}(wS_{\text{Clay}}),$$
$$\frac{\partial S_{\text{Opal}}}{\partial t} = \frac{\partial}{\partial z}(wS_{\text{Opal}}),$$
$$\frac{\partial w}{\partial z} = 0.$$

S_{Clay} and S_{Opal} mean the concentration of clay and opal. w means the sedimentation rate.

The units of S_{Clay} and S_{Opal} are (g/m^3) and (mmol/m^3), respectively.

Boundary conditions are imposed as follows.

$$w\big|_{z=0} = \text{(total) sedimentation rate } \left(= F_{\text{Clay}}/\rho_{\text{Clay}} + F_{\text{Opal}}/(\rho_{\text{Opal}} \cdot M_{\text{Opal}}^{-1})\right),$$
$$wS_{\text{Clay}}\big|_{z=0} = F_{\text{Clay}}, \ (\text{g m}^{-2} \text{ yr})$$
$$wS_{\text{Opal}}\big|_{z=0} = F_{\text{Opal}}. \ (\text{mmol m}^{-2} \text{ yr})$$

Here, the density of clay (g/cm^3), the density (g/cm^3) and the molar mass of opal (g/mol) are as follows.

$$\rho_{\text{Clay}} = 2.75,$$
$$\rho_{\text{Opal}} = 2.20,$$
$$M_{\text{Opal}} = 60.$$

The depth of sediment layer sets to 100 cm. Each layer has a thickness of $\Delta z = 0.5$ cm. The time step Δt is 1 day. The dry weight percentage of clay and opal (%) are as follows.

$$P_{\text{Clay}} = \frac{S_{\text{Clay}}}{S_{\text{Clay}} + S_{\text{Opal}} \cdot M_{\text{Opal}}} \times 100,$$
$$P_{\text{Opal}} = \frac{S_{\text{Opal}}}{S_{\text{Clay}} + S_{\text{Opal}} \cdot M_{\text{Opal}}} \times 100.$$

Let us consider finite-difference methods of a one-dimensional advection equation for tracer.

$$\frac{\partial S}{\partial t} = \frac{\partial}{\partial z}(wS).$$

The above equation is written as follows.

$$\frac{S_k^{n+1} - S_k^n}{\Delta t} = \frac{w_k \cdot S_{\overline{k}}^n - w_{k+1} \cdot S_{\overline{k+1}}^n}{\Delta z}.$$

Where the position $\overline{k}$ locates between $k-1$ and k. For the up-wind scheme,

$$S_{\overline{k}} = \begin{cases} S_{k-1}, & (w_k > 0) \\ S_k. & (w_k < 0) \end{cases}$$

For the weighted up-wind scheme,

$$S_{\overline{k}} = \begin{cases} \alpha \cdot S_{k-1} + (1-\alpha) \cdot S_k, & (if \ w_k > 0) \\ (1-\alpha) \cdot S_k + \alpha \cdot S_k. & (if \ w_k < 0) \end{cases}$$
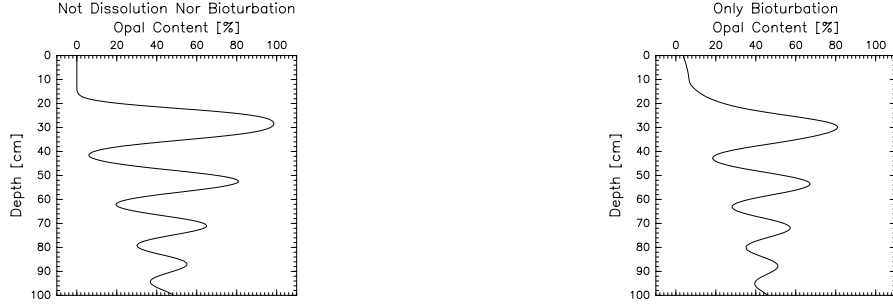
1.1: Not Dissolution Nor Bioturbation. Only Bioturbation. This is the same experiment as depicted in Figure 1 of *Chikamoto and Yamanaka* (2005).

Boundary conditions are imposed as follows.

$$w_1 \cdot S_{\bar{1}} = F_{\text{Clay or Opal}} \begin{cases} 9075 & \mu\text{g/cm}^2 \cdot \text{yr} \\ 120 & \mu\text{mol/cm}^2 \cdot \text{yr} \end{cases}$$

Also, because the equation of continuity

$$\frac{\partial w}{\partial z} = 0,$$

$w_{k+1} = w_k$. From boundary conditions,

$$w_1 = \text{sedimentation rate.}$$
$$\left(= F_{\text{Clay}}/\rho_{\text{Clay}} + F_{\text{Opal}}/(\rho_{\text{Opal}} \cdot M_{\text{Opal}}^{-1}) \right)$$
$$\left(= 3.3 \times 10^{-3} \text{ cm/yr} \right)$$

1.1.2   No dissolution

In this subsection, I consider the vertical diffusion due to bioturbation. Here, I introduce porosity ϕ, which is the fraction of the pore-water in the sediment layer.

$$\frac{\partial}{\partial t}\{(1-\phi)S_{\text{Clay}}\} = \frac{\partial}{\partial z}\left\{(1-\phi)wS_{\text{Clay}}\right\} + \frac{\partial}{\partial z}\left\{(1-\phi)D_B\frac{\partial S_{\text{Clay}}}{\partial z}\right\},$$
$$\frac{\partial}{\partial t}\{(1-\phi)S_{\text{Opal}}\} = \frac{\partial}{\partial z}\left\{(1-\phi)wS_{\text{Opal}}\right\} + \frac{\partial}{\partial z}\left\{(1-\phi)D_B\frac{\partial S_{\text{Opal}}}{\partial z}\right\},$$
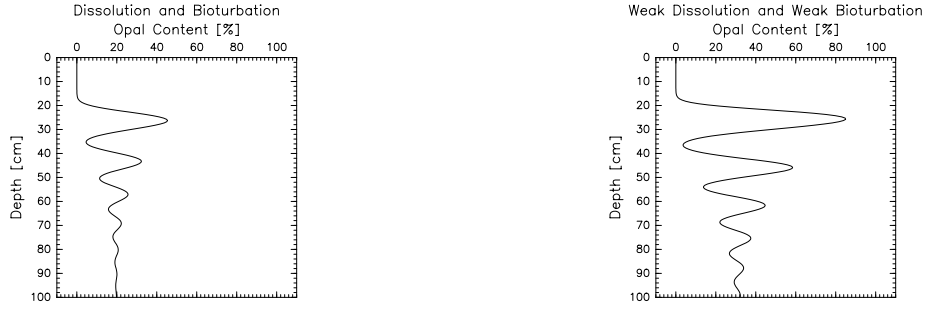$$\frac{\partial}{\partial z}\{(1-\phi)w\} = 0.$$

1.2: Dissolution and Bioturbation. Weak Dissolution and Weak Bioturbation. This is the same experiment as depicted in Figure 2 of *Chikamoto and Yamanaka* (2005).

The vertical distribution of ϕ is given as follows.

$$\phi = \phi_0 \cdot \exp\left(-\frac{z}{z_0}\right). \ \left(\phi_0 = 0.9, \ z_0 = 182.3 \text{ cm}\right)$$

D_B is a mixing coefficient of bioturbation. The vertical distribution of D_B is given as follows (*Berner*, 1980).

$$D_B(z) = \frac{D_B^0}{1 + \exp\left\{2(z - z_B)\right\}}. \ \left(D_B^0 = 0.3 \text{ cm}^2/\text{yr}, \ z_B = 10 \text{ cm}\right)$$

Boundary conditions are imposed as follows.

$$(1 - \phi)w\big|_{z=0} = \text{(total) sedimentation rate.}$$
$$= \left(F_{\text{Clay}}/\rho_{\text{Clay}} + F_{\text{Opal}}/(\rho_{\text{Opal}} \cdot M_{\text{Opal}}^{-1})\right)$$
$$(1 - \phi)wS_{\text{Clay}}\big|_{z=0} = F_{\text{Clay}},$$
$$(1 - \phi)wS_{\text{Opal}}\big|_{z=0} = F_{\text{Opal}}.$$

1.1.3 Bioturbation and Dissolution

In this subsection, I consider the vertical diffusion due to bioturbation and dissolution of opal.

$$\frac{\partial}{\partial t}\{(1-\phi)S_{\text{Clay}}\} = \frac{\partial}{\partial z}\left\{(1-\phi)wS_{\text{Clay}}\right\} + \frac{\partial}{\partial z}\left\{(1-\phi)D_B\frac{\partial S_{\text{Clay}}}{\partial z}\right\},$$

$$\frac{\partial}{\partial t}\{(1-\phi)S_{\text{Opal}}\} = \frac{\partial}{\partial z}\left\{(1-\phi)wS_{\text{Opal}}\right\} + \frac{\partial}{\partial z}\left\{(1-\phi)D_B\frac{\partial S_{\text{Opal}}}{\partial z}\right\} - (1-\phi)R_{\text{Opal}}S_{\text{Opal}},$$

$$\frac{\partial}{\partial x}\{(1-\phi)w\} = -(1-\phi)R_{\text{Opal}},$$

$$\frac{\partial}{\partial t}\{\phi C_{\text{Si(OH)4}}\} = \frac{\partial}{\partial z}\left\{\phi D_E\frac{\partial C_{\text{Si(OH)4}}}{\partial z}\right\} + (1-\phi)R_{\text{Opal}}S_{\text{Opal}}.$$

D_E is an effective molecular diffusivity

$$D_E = \phi^{n-1} \cdot D_{SW}.$$

$D_{SW} = 4.59 \times 10^{-6}$ cm^2/s, $n = 2.5$ (*Hensen et al.*, 1998; *Ridgwell et al.*, 2002).

Boundary conditions are imposed as follows.

$$(1-\phi)w\big|_{z=0} = \text{(total) sedimentation rate},$$
$$= \left(F_{\text{Clay}}/\rho_{\text{Clay}} + F_{\text{Opal}}/(\rho_{\text{Opal}} \cdot M_{\text{Opal}}^{-1})\right)$$
$$(1-\phi)wS_{rmClay}\big|_{z=0} = F_{\text{Clay}},$$
$$(1-\phi)wS_{\text{Opal}}\big|_{z=0} = F_{\text{Opal}},$$
$$C_{\text{Si(OH)4}}\big|_{z=0} = C_{WO},$$
$$\frac{\partial C_{\text{Si(OH)4}}}{\partial z}\bigg|_{z=z_{\text{Bottom}}} = 0.$$

C_{WO} is the seawater concentration of silicate.

When $w < 0$ at $z = z_{\text{Bottom}}$,

$$\frac{\partial S_{\text{Clay}}}{\partial z}\bigg|_{z=z_{\text{Bottom}}} = 0.$$

$$S_{\text{Opal}}\bigg|_{z=z_{\text{Bottom}}} = 0.$$

In other words, it is assumed that only clay exists at $z > z_{\text{Bottom}}$.

R_{Opal} is an opal dissolution rate (yr^{-1}), which is simplified as follows.

$$
R_{\mathrm{Opal}}(z) = \begin{cases} k_0 \cdot \left(\dfrac{[\mathrm{Si(OH)_4}]^{\mathrm{sat}}(z) - [\mathrm{Si(OH)_4}](z)}{[\mathrm{Si(OH)_4}]^{\mathrm{sat}}(z)} \right), & \left([\mathrm{Si(OH)_4}] < [\mathrm{Si(OH)_4}]^{\mathrm{sat}}\right) \\ 0. & \left([\mathrm{Si(OH)_4}] > [\mathrm{Si(OH)_4}]^{\mathrm{sat}}\right) \end{cases}
$$

$k_0 \sim 0.032 \ \mathrm{yr}^{-1}$, and $[\mathrm{Si(OH)_4}]_{\mathrm{sat}} \sim 1000 \ \mu\mathrm{mol} \ \mathrm{l}^{-1} = 1.0 \ \mu\mathrm{mol/cm}^3$. I also consider the dependency of temperature and pressure on $R_{\mathrm{Opal}}(z)$. First,

$$
u_{\mathrm{Opal}}(z) = \left(\frac{[\mathrm{Si(OH)_4}]^{\mathrm{sat}}(z) - [\mathrm{Si(OH)_4}](z)}{[\mathrm{Si(OH)_4}]^{\mathrm{sat}}(z)} \right).
$$

The presence of aluminium affects the solubility of opal as follows.

$$
\gamma_{\mathrm{Al}} = \begin{cases} 0.2, & \dfrac{P^{\mathrm{Detrial}}}{P^{\mathrm{Opal}}} > 15 \\ 1.0 - \left(0.045 \dfrac{P^{\mathrm{Detrial}}}{P^{\mathrm{Opal}}} \right)^{0.58}. & \dfrac{P^{\mathrm{Detrial}}}{P^{\mathrm{Opal}}} \le 15 \end{cases}
$$

$$
[\mathrm{Si(OH)_4}]^{\mathrm{sat}}(z) = \gamma_{\mathrm{Al}} 10^{\left(6.44 - \frac{968}{T(z)}\right)}.
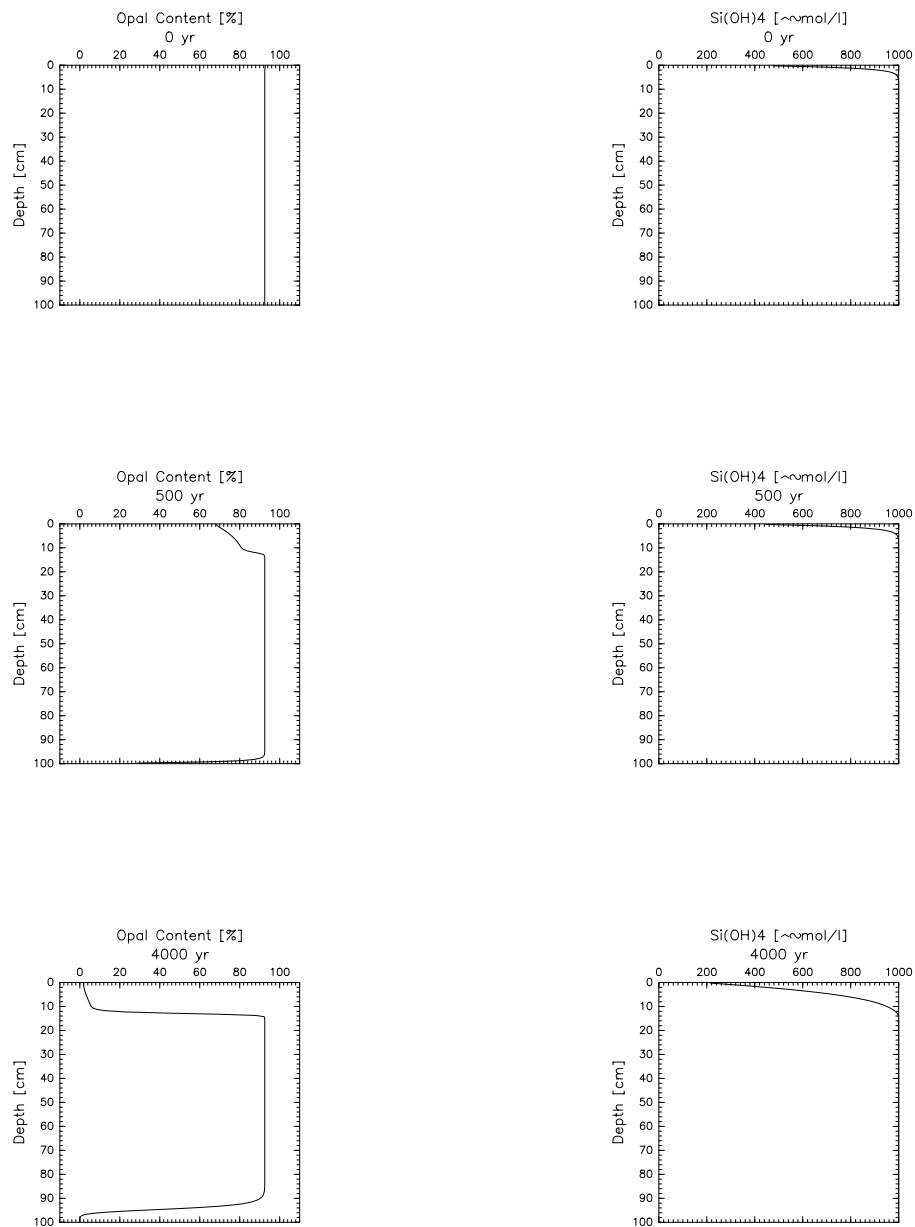$$

P^{Detrial} and P^{Opal} are the dry weight percentage of detrial material and opal (wt%). Next, I introduce the following parameters

$$
\eta_{1 \ \mathrm{Opal}}(z) = 0.225 \left(1 + \frac{T}{15} \right) u_{\mathrm{Opal}}(z) + 0.775 \left[\left(1 + \frac{T}{400} \right)^4 u_{\mathrm{Opal}}(z) \right]^{9.25},
$$

$$
\eta_{2 \ \mathrm{Opal}}(z) = 0.26 + 0.74 \ \mathrm{e}^{-\frac{z}{7.0}}.
$$

Finally, when $[\mathrm{Si(OH)_4}] < [\mathrm{Si(OH)_4}]^{\mathrm{sat}}$,

$$
R_{(z)}^{\mathrm{Opal}} = \eta_1(z) \eta_2(z) k_0 u(z).
$$

The above formulation refers to *Ridgwell et al.* (2002).

1.3: Dissolution and Bioturbation. Weak Dissolution and Weak Bioturbation. This is the same experiment as depicted in Figure 3 of *Chikamoto and Yamanaka* (2005).

Time Series of Total Dissolution Fluxes
after the Abrupt Rain Flux Change

Time Series of Total Dissolution Fluxes
after the Abrupt Rain Flux Change
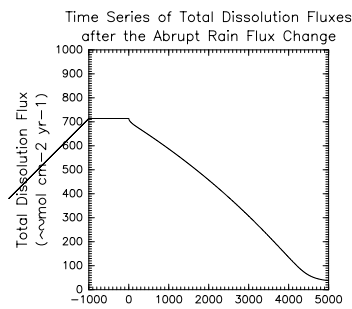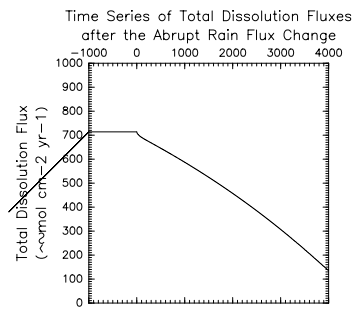
1.4: Time series of the total dissolution flux of biogenic silica. This is the same experiment as depicted in Figure 4 of *Chikamoto and Yamanaka* (2005).

Time Series of Total Dissolution Fluxes
after the Abrupt Rain Flux Change
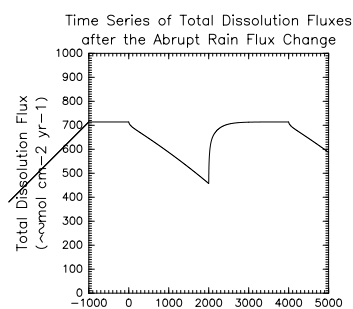
1.5: Time series of the total dissolution flux of biogenic silica. This is the same experiment as depicted in Figure 5 of *Chikamoto and Yamanaka* (2005).
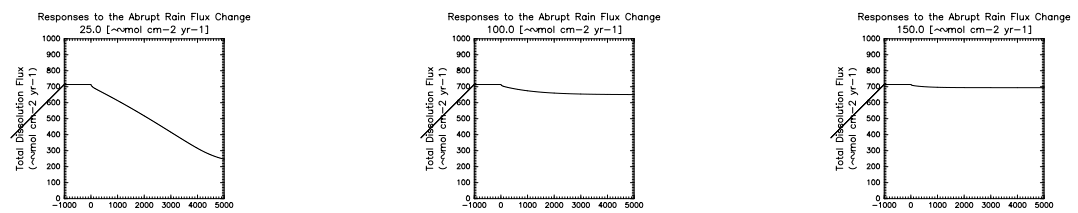
1.6: Time series of the total dissolution flux of biogenic silica. This is the same experiment as depicted in Figure 8 of *Chikamoto and Yamanaka* (2005).
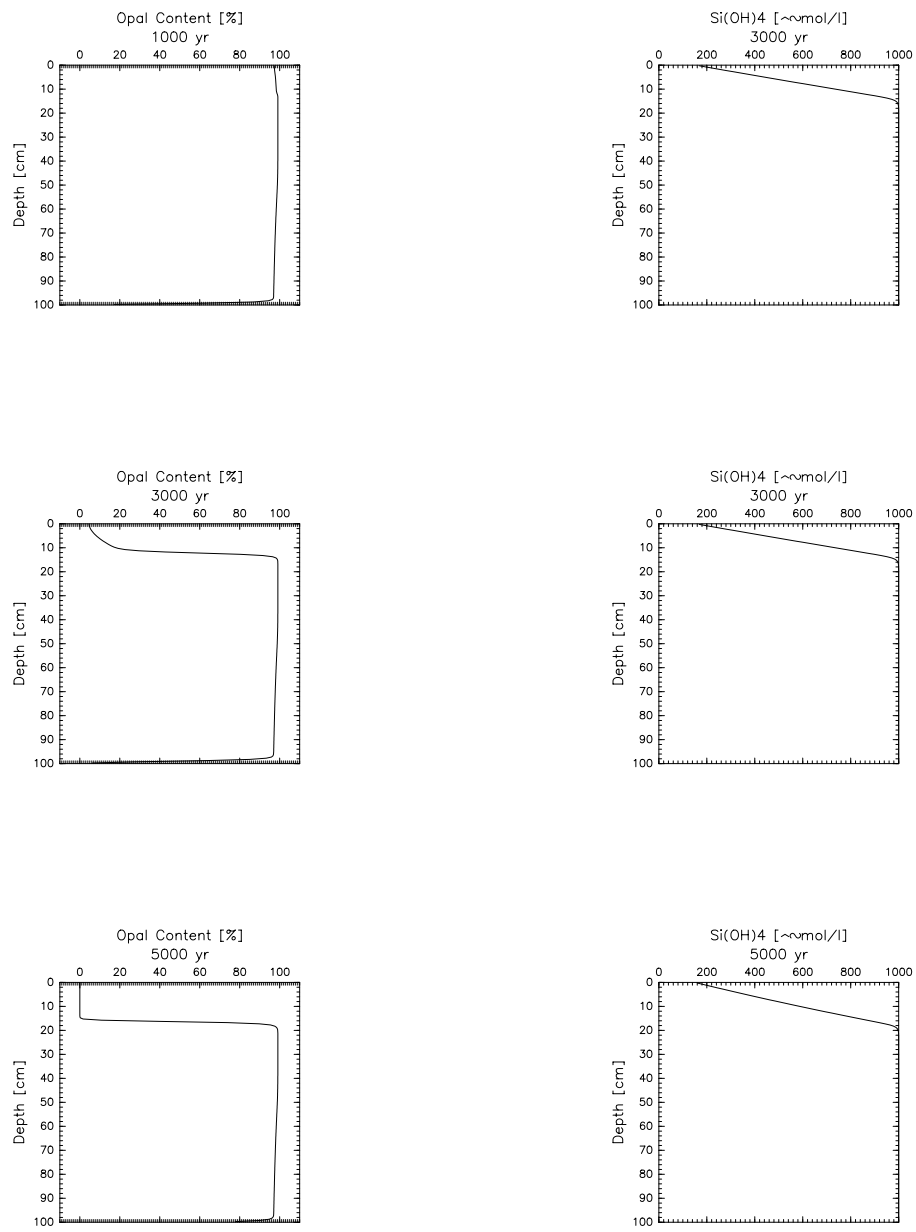
1.7: Time series of the total dissolution flux of biogenic silica. This is the same experiment as depicted in Figure 9 of *Chikamoto and Yamanaka* (2005).

2   Three-dimensional sediment model

This chapter describes the formulation of a three-dimensional sediment model. The formulations mainly refer to *Archer* (1991) and *Archer et al.* (2002).

2.1   Equations

The prognostic variables included in the sediment model are as follows.

- Solid particles: Clay, Particulate Organic Matter, Calcium carbonate, and Opal

- Dissolved substances: Phosphate, Dissolved inorganic carbon, Alkalinity, Dissolved Oxygen, and Silicate

The unit of solid particles is (g/m^3) for clay, and ($mmol/m^3$) for the others. The unit of dissolved substance are ($mmol/m^3$).

$$\frac{\partial}{\partial t}\{(1-\phi)S_{\text{Clay}}\} = \frac{\partial}{\partial z}\left\{(1-\phi)wS_{\text{Clay}}\right\} + \frac{\partial}{\partial z}\left\{(1-\phi)D_B\frac{\partial S_{\text{Clay}}}{\partial z}\right\},$$

$$\frac{\partial}{\partial t}\{(1-\phi)S_{\text{POM}}\} = \frac{\partial}{\partial z}\left\{(1-\phi)wS_{\text{POM}}\right\} + \frac{\partial}{\partial z}\left\{(1-\phi)D_B\frac{\partial S_{\text{POM}}}{\partial z}\right\} - (1-\phi)R_{\text{POM}}S_{\text{POM}},$$

$$\frac{\partial}{\partial t}\{(1-\phi)S_{\text{CaCO}_3}\} = \frac{\partial}{\partial z}\left\{(1-\phi)wS_{\text{CaCO}_3}\right\} + \frac{\partial}{\partial z}\left\{(1-\phi)D_B\frac{\partial S_{\text{CaCO}_3}}{\partial z}\right\} - (1-\phi)R_{\text{CaCO}_3}S_{\text{CaCO}_3},$$

$$\frac{\partial}{\partial t}\{(1-\phi)S_{\text{Opal}}\} = \frac{\partial}{\partial z}\left\{(1-\phi)wS_{\text{Opal}}\right\} + \frac{\partial}{\partial z}\left\{(1-\phi)D_B\frac{\partial S_{\text{Opal}}}{\partial z}\right\} - (1-\phi)R_{\text{Opal}}S_{\text{Opal}},$$

$$\frac{\partial\{(1-\phi)w\}}{\partial z} = -(1-\phi)(R_{\text{POM}}S_{\text{POM}} + R_{\text{CaCO}_3}S_{\text{CaCO}_3} + R_{\text{Opal}}S_{\text{Opal}}),$$

$$\frac{\partial\{\phi C_{\text{PO4}}\}}{\partial t} = \frac{\partial}{\partial z}\left\{\phi D_E\frac{\partial C_{\text{PO4}}}{\partial z}\right\} + \mathcal{R}_{PO_4}/\mathcal{R}_C \cdot (1-\phi)R_{\text{POM}}S_{\text{POM}},$$

$$\frac{\partial\{\phi C_{\text{DIC}}\}}{\partial t} = \frac{\partial}{\partial z}\left\{\phi D_E\frac{\partial C_{\text{DIC}}}{\partial z}\right\} + (1-\phi)R_{\text{POM}}S_{\text{POM}} + (1-\phi)R_{\text{CaCO}_3}S_{\text{CaCO}_3},$$

$$\frac{\partial\{\phi C_{\text{Alk}}\}}{\partial t} = \frac{\partial}{\partial z}\left\{\phi D_E\frac{\partial C_{\text{Alk}}}{\partial z}\right\} - (1-\phi)R_{\text{POM}}S_{\text{POM}} + 2 \cdot (1-\phi)R_{\text{CaCO}_3}S_{\text{CaCO}_3},$$

$$\frac{\partial\{\phi C_{\text{O2}}\}}{\partial t} = \frac{\partial}{\partial z}\left\{\phi D_E\frac{\partial C_{\text{O2}}}{\partial z}\right\} - \mathcal{R}_{O_2}/\mathcal{R}_C \cdot (1-\phi)R_{\text{POM}}S_{\text{POM}},$$

$$\frac{\partial\{\phi C_{\text{Si(OH)4}}\}}{\partial t} = \frac{\partial}{\partial z}\left\{\phi D_E\frac{\partial C_{\text{Si(OH)4}}}{\partial z}\right\} + (1-\phi)R_{\text{Opal}}S_{\text{Opal}}.$$

D_B is a mixing coefficient of bioturbation. The vertical distribution of D_B is given as follows (*Berner*, 1980).

$$D_B(z) = \frac{D_B^0}{1 + \exp\{2(z - z_B)\}}. \ \left(D_B^0 = 0.3 \text{ cm}^2/\text{yr}, \ z_B = 10 \text{ cm}\right)$$

D_E is an effective molecular diffusivity. The distribution introduced in *Hensen et al.* (1998) and *Ridgwell et al.* (2002) is as follows.

$$D_E = \phi^{n-1} \cdot D_{SW}.$$

$D_{SW} = 4.59 \times 10^{-6} \text{ cm}^2/\text{s}$, $n = 2.5$. Also, *Archer et al.* (2002) give $D_E = D_c/F$. D_c is the molecular diffusion coefficient of each dissolved substance shown in the table below. F is the formation factor.

$$F = \frac{1}{\phi^m}.$$

Archer et al. (2002) introduce $m = 3$ based on *Ullman and Aller* (1982). I choose the latter Archer's form.

2.1.1   Boundary conditions

$$
\begin{aligned}
(1 - \phi)w|_{z=0} &= \text{(total) sedimentation rate,} \\
(1 - \phi)wS_{\text{Clay}}|_{z=0} &= F_{\text{Clay}}, \\
(1 - \phi)wS|_{z=0} &= F \ (\text{POM}, \text{CaCO}_3, \text{Opal}), \\
C\big|_{z=0} &= C_W \ (\text{PO}_4, \text{DIC}, \text{Alk}, \text{O}_2, \text{Si(OH)}_4), \\
\frac{\partial C}{\partial z}\bigg|_{z=z_{\text{Bottom}}} &= 0. \ (\text{PO}_4, \text{DIC}, \text{Alk}, \text{O}_2, \text{Si(OH)}_4)
\end{aligned}
$$

Where C_W is the bottom-water concentration of each dissolved substance.

When $w < 0$ at $z = z_{\text{Bottom}}$,

$$
\begin{aligned}
\frac{\partial S_{\text{Clay}}}{\partial z}\bigg|_{z=z_{\text{Bottom}}} &= 0, \\
S_{\text{POM}}\big|_{z=z_{\text{Bottom}}} &= 0, \\
S_{\text{CaCO}_3}\big|_{z=z_{\text{Bottom}}} &= 0, \\
S_{\text{Opal}}\big|_{z=z_{\text{Bottom}}} &= 0.
\end{aligned}
$$

In other words, it is assumed that only clay exists at $z > z_{\text{Bottom}}$.

2.1.2   Dissolution terms

R_{Opal} is an opal dissolution rate (s^{-1}), which is simplified as follows.

$$
R_{\text{Opal}} = \begin{cases} \eta_{1(z)}^{\text{Opal}} \eta_{2(z)}^{\text{Opal}} k_0 u_{(z)}^{\text{Opal}}, & ([\text{Si(OH)}_4] < [\text{Si(OH)}_4]^{\text{sat}}) \\ 0. & ([\text{Si(OH)}_4] > [\text{Si(OH)}_4]^{\text{sat}}) \end{cases}
$$

Otherwise, following *Archer et al.* (1993),

$$
R_{\text{Opal}} = \begin{cases} r_{\text{Opal}} \cdot \left([\text{Si(OH)}_4]^{\text{sat}} - [\text{Si(OH)}_4]\right), & ([\text{Si(OH)}_4] < [\text{Si(OH)}_4]^{\text{sat}}) \\ 0. & ([\text{Si(OH)}_4] = [\text{Si(OH)}_4]^{\text{sat}}) \end{cases}
$$

$r_{\text{Opal}} = 5.0 \times 10^{-6} \ \text{cm}^3\text{mol}^{-1}\text{s}^{-1}$. $[\text{Si(OH)}_4]^{\text{sat}}$ consider the existence of Al as

$$
\gamma_{\text{Al}} = \begin{cases} 0.2, & \frac{P^{\text{Detrial}}}{P^{\text{Opal}}} > 15 \\ 1.0 - \left(0.045\frac{P^{\text{Detrial}}}{P^{\text{Opal}}}\right)^{0.58} \cdot & \frac{P^{\text{Detrial}}}{P^{\text{Opal}}} \leq 15 \end{cases}
$$

$$[\mathrm{Si(OH)_4}]^{\mathrm{sat}}(z) = \gamma_{\mathrm{Al}}10^{\left(6.44 - \frac{968}{T(z)}\right)}.$$

R_{POM} is a POM dissolution rate (s^{-1}), which is simplified as follows.

$$R_{\mathrm{POM}} = \begin{cases} k_{\mathrm{OX}}, & (C_{\mathrm{O_2}} > 0) \\ k_{\mathrm{AX}}. & (C_{\mathrm{O_2}} = 0) \end{cases}$$

$k_{\mathrm{OX}} = 2 \times 10^{-9}$ s^{-1} (*Archer*, 1991), and $k_{\mathrm{AX}} = 7.9 \times 10^{-11}$ s^{-1} (*Berner*, 1980) as shown in *Chikamoto et al.* (2009).

$R_{\mathrm{CaCO_3}}$ is a CaCO$_3$ dissolution rate (s^{-1}), which is simplified as follows.

$$R_{\mathrm{CaCO_3}} = \begin{cases} r_{\mathrm{CaCO_3}} \cdot \left(\dfrac{[\mathrm{CO_3^{2-}}]^{\mathrm{sat}} - [\mathrm{CO_3^{2-}}]}{[\mathrm{CO_3^{2-}}]^{\mathrm{sat}}} \right)^n, & ([\mathrm{CO_3^{2-}}] < [\mathrm{CO_3^{2-}}]^{\mathrm{sat}}) \\ 0. & ([\mathrm{CO_3^{2-}}] = [\mathrm{CO_3^{2-}}]^{\mathrm{sat}}) \end{cases}$$

$r_{\mathrm{CaCO_3}} = 1.0$ day^{-1} (*Archer*, 1991), and $n = 4.5$ (*Keir*, 1980) as shown in *Chikamoto et al.* (2009). The pore-water concentration of carbonate ion $[\mathrm{CO_3^{2-}}]$ is calculated from the bottom-water temperature and salinity and the pore-water concentration of DIC and Alk.

Parameter settings used in the sediment model is shown as below.

2.1: Parameters and References

Symbol	Parameter	Value	Reference
ρ	Density of solid sediment components	2.6 g cm^{-3}	(*Heinze*, 1999)
M_{POM}	Molar weight of POM	32.74 g mol^{-1}	(*Heinze*, 1999)
$M_{\mathrm{CaCO_3}}$	Molar weight of CaCO$_3$	100.0 g mol^{-1}	(*Heinze*, 1999)
M_{Opal}	Molar weight of Opal	67.2 g mol^{-1}	(*Heinze*, 1999)
	for porewater silicic acid		
$\phi\big|_{z=0}$	Porosity ($z=0$)	0.9	(*Berner*, 1980)
z_0	Porosity e-folding depth	182.3 cm	(*Berner*, 1980)
$D_B\big|_{z=0}$	Bioturbation diffusion coefficient ($z=0$)	3×10^{-1} cm^2 yr^{-1}	(*Berner*, 1980)
z_B	Bioturbation diffusion e-folding depth	10.0 cm	(*Berner*, 1980)
$D_c^{\mathrm{PO_4}}$	Pore water diffusion coefficient	5.00×10^{-10} cm^2 s^{-1}	(*Archer et al.*, 2002)
D_c^{DIC}	Pore water diffusion coefficient	6.40×10^{-10} cm^2 s^{-1}	(*Archer et al.*, 2002)
D_c^{Alk}	Pore water diffusion coefficient	6.40×10^{-10} cm^2 s^{-1}	(*Archer et al.*, 2002)
$D_c^{\mathrm{O_2}}$	Pore water diffusion coefficient	1.20×10^{-9} cm^2 s^{-1}	(*Archer et al.*, 2002)
$D_c^{\mathrm{Si(OH)_4}}$	Pore water diffusion coefficient	5.00×10^{-10} cm^2 s^{-1}	(*Archer et al.*, 2002)
D_{SW}	Pore water diffusion coefficient	4.59×10^{-6} cm^2 s^{-1}	(*Ridgwell et al.*, 2002)
N	Pore water diffusion coefficient	2.5	(*Ridgwell et al.*, 2002)
r_{Opal}	Rate constant for Opal redissolution	5.0×10^{-6} cm^{3}mol^{-1}s^{-1}	(*Archer et al.*, 1993)
r_{POM}	Rate constant for POM redissolution	2.0×10^{-9} s^{-1}	(*Archer*, 1991)
r_{POM}	Rate constant for POM redissolution	7.9×10^{-11} s^{-1}	(*Berner*, 1980)
$r_{\mathrm{CaCO_3}}$	Rate constant for CaCO$_3$ redissolution	1.0 day^{-1}	(*Archer*, 1991)
$\mathcal{R}_{\mathrm{PO_4}}$	Redfield coefficient for phosphate	1	(*Anderson and Sarmiento*, 1995)
$\mathcal{R}_{\mathrm{O_2}}$	Redfield coefficient for oxygen	170	(*Anderson and Sarmiento*, 1995)
$\mathcal{R}_{\mathrm{C}}$	Redfield coefficient for carbon	16	(*Anderson and Sarmiento*, 1995)

2.2 Finite-difference methods

For solid particles, the diffusion term due to bioturbation is solved implicitly. The advection and dissolution terms are solved explicitly. For the dissolved substances, the diffusion term due to molecular diffusion is solved implicitly. The dissolution term is solved explicitly.

Solid Particles

The governing equation is as follows.

$$\frac{\partial}{\partial t}\{(1-\phi)S\} = \frac{\partial}{\partial z}\Big\{(1-\phi)wS\Big\} + \frac{\partial}{\partial z}\Big\{(1-\phi)D\frac{\partial S}{\partial z}\Big\} - DIS.$$

First, the advection term is differentiated using the QUICKEST scheme, and the interlayer flux is calculated.

$$\frac{(1-\phi_k)(S_k^{n+1}-S_k^n)}{\Delta t} = \frac{(1-\phi_{k-1/2})w_{k-1/2}S_{k-1/2}^n - (1-\phi_{k+1/2})w_{k+1/2}S_{k+1/2}^n}{\Delta z_k} + \alpha.$$

$$S_{k-1/2}^n = c_0 - c_1\frac{w\Delta t}{2} + c_2\Big(\frac{w^2\Delta t^2}{3} - \frac{\Delta z^2}{12}\Big).$$

c_0, c_1, and c_2 is obtained as follows.

$$c_0 = \frac{\Delta z_k \times S_{k-1}^n + \Delta z_{k-1} \times S_k^n}{2 \times \Delta_{k-1/2}} - \frac{\Delta z_{k-1} \times \Delta z_k}{4} \times c_2,$$

$$c_1 = \frac{S_k^n - S_{k-1}^n}{\Delta z_{k-1/2}} + \frac{\Delta z_{k-1} - \Delta z_k}{2} \times c_2,$$

$$c_2 = \frac{1}{\Delta z_{k-3/2} + \Delta z_{k-1/2}} \times \Big\{\frac{S_{k-2}^n - S_{k-1}^n}{\Delta z_{k-3/2}} - \frac{S_{k-1}^n - S_k^n}{\Delta z_{k-1/2}}\Big\}, \qquad (w_{k-1/2} > 0)$$

$$c_2 = \frac{1}{\Delta z_{k-1/2} + \Delta z_{k+1/2}} \times \Big\{\frac{S_{k-1}^n - S_k^n}{\Delta z_{k-1/2}} - \frac{S_k^n - S_{k+1}^n}{\Delta z_{k+1/2}}\Big\}. \qquad (w_{k-1/2} < 0)$$

Here, since $S_{k-1/2}^{n+1}$ may be smaller or larger than S_{k-1}^n and S_k^n, a flux limiter is applied. When $w_{k-1/2} > 0$,

$$\delta = S_k^n - S_{k-2}^n,$$

$$\gamma = \frac{S_k^n - S_{k-1}^n}{\Delta z_{k-1/2}} - \frac{S_{k-1}^n - S_{k-2}^n}{\Delta z_{k-3/2}}.$$

The limiter is applied in the case as follows.

$$S_{k-1/2}^{n+1} = S_{k-1}^n. \quad (|\gamma\Delta z_{k-1}| > |\delta|),$$

$$S_{k-1}^n \leq S_{k-1/2}^{n+1} \leq \min\Big(S_{k-2}^n + \frac{S_{k-1}^n - S_{k-2}^n}{w_{k-1/2}}\Delta z_{k-1/2}, S_k^n\Big), \quad (|\gamma\Delta z_{k-1}| < |\delta|, \delta > 0)$$

$$\max\Big(S_{k-2}^n + \frac{S_{k-1}^n - S_{k-2}^n}{w_{k-1/2}}\Delta z_{k-1/2}, S_k^n\Big) \leq S_{k-1/2}^{n+1} \leq S_{k-1}^n. \quad (|\gamma\Delta z_{k-1}| < |\delta|, \delta < 0)$$

Also, when $w_{k-1/2} < 0$,

$$\delta = S_{k-1}^n - S_{k+1}^n,$$

$$\gamma = \frac{S_{k-1}^n - S_k^n}{\Delta z_{k-1/2}} - \frac{S_k^n - S_{k+1}^n}{\Delta z_{k+1/2}}.$$

The limiter is applied in the case as follows.

$$S_{k-1/2}^{n+1} = S_k^n, \quad (|\gamma \Delta z_k| > |\delta|)$$

$$S_k^n \leq S_{k-1/2}^{n+1} \leq \min\left(S_{k+1}^n + \frac{S_k^n - S_{k+1}^n}{|w_{k-1/2}|} \Delta z_{k-1/2}, S_{k-1}^n \right), \quad (|\gamma \Delta z_k| < |\delta|, \delta > 0)$$

$$\max\left(S_{k+1}^n + \frac{S_k^n - S_{k+1}^n}{|w_{k-1/2}|} \Delta z_{k-1/2}, S_{k-1}^n \right) \leq S_{k-1/2}^{n+1} \leq S_k^n. \quad (|\gamma \Delta z_k| < |\delta|, \delta < 0)$$

The advection flux is described as follows:

$$F_k^{adv} = (1 - \phi_k) w_k S_k.$$

Differentiating with the implicit method,

$$\frac{(1 - \phi_k)(S_k^{n+1} - S_k^n)}{\Delta t}$$

$$= \frac{1}{\Delta z_k} \left\{ \left[(1 - \phi_{k-1/2}) D_{k-1/2} \frac{\partial S}{\partial z} \Big|_{k-1/2} \right] - \left[(1 - \phi_{k+1/2}) D_{k+1/2} \frac{\partial S}{\partial z} \Big|_{k+1/2} \right] \right\}$$

$$- (1 - \phi_k) R_k^n S_k^n + (F_{k-1/2}^{adv} - F_{k+1/2}^{adv})$$

$$= \frac{1}{\Delta z_k} \left\{ \left[(1 - \phi_{k-1/2}) D_{k-1/2} \frac{S_{k-1} - S_k}{\Delta z_{k-1/2}} \right] - \left[(1 - \phi_{k+1/2}) D_{k+1/2} \frac{S_k - S_{k+1}}{\Delta z_{k+1/2}} \right] \right\}$$

$$- (1 - \phi_k) R_k^n S_k^n + \frac{F_{k-1/2}^{adv} - F_{k+1/2}^{adv}}{\Delta z_k}$$

$$\frac{(1-\phi_k)}{\Delta t}\{S_k^{n+1} - S_k^n\}$$

$$= \left(\frac{(1-\phi_{k-1/2})D_{k-1/2}}{\Delta z_k \Delta z_{k-1/2}}\right)S_{k-1} - \left(\frac{(1-\phi_{k-1/2})D_{k-1/2}}{\Delta z_k \Delta z_{k-1/2}}\right)S_k$$

$$- \left(\frac{(1-\phi_{k+1/2})D_{k+1/2}}{\Delta z_k \Delta z_{k+1/2}}\right)S_k + \left(\frac{(1-\phi_{k+1/2})D_{k+1/2}}{\Delta z_k \Delta z_{k+1/2}}\right)S_{k+1}$$

$$- (1-\phi_k)R_k^n S_k^n + \frac{F_{k-1/2}^{adv} - F_{k+1/2}^{adv}}{\Delta z_k}$$

$$= \left(\frac{(1-\phi_{k-1/2})D_{k-1/2}}{\Delta z_k \Delta z_{k-1/2}}\right)S_{k-1}^{n+1} - \left(\frac{(1-\phi_{k-1/2})D_{k-1/2}}{\Delta z_k \Delta z_{k-1/2}}\right)S_k^{n+1}$$

$$- \left(\frac{(1-\phi_{k+1/2})D_{k+1/2}}{\Delta z_k \Delta z_{k+1/2}}\right)S_k^{n+1} + \left(\frac{(1-\phi_{k+1/2})D_{k+1/2}}{\Delta z_k \Delta z_{k+1/2}}\right)S_{k+1}^{n+1}$$

$$- (1-\phi_k)R_k^n S_k^n + \frac{F_{k-1/2}^{adv} - F_{k+1/2}^{adv}}{\Delta z_k}.$$

I set α, β, and γ as follows.

$$\alpha = \frac{(1-\phi_k)}{\Delta t},$$
$$\beta = \frac{(1-\phi_{k-1/2})D_{k-1/2}}{\Delta z_k \Delta z_{k-1/2}},$$
$$\gamma = \frac{(1-\phi_{k+1/2})D_{k+1/2}}{\Delta z_k \Delta z_{k+1/2}}.$$

Then,

$$-\beta S_{k-1}^{n+1} + (\alpha + \beta + \gamma)S_k^{n+1} - \gamma S_{k+1}^{n+1}$$

$$= \alpha S_k^n - (1-\phi_k)R_k^n S_k^n + \frac{F_{k-1/2}^{adv} - F_{k+1/2}^{adv}}{\Delta z_k}.$$

Therefore,

$$\begin{bmatrix} \alpha+\beta+\gamma & -\gamma & & & & \\ -\beta & \alpha+\beta+\gamma & -\gamma & & & \\ & & \cdots & & & \\ & & & \cdots & & \\ & & & -\beta & \alpha+\beta+\gamma & -\gamma \\ & & & & -\beta & \alpha+\beta+\gamma \end{bmatrix} \begin{bmatrix} S_1^{n+1} \\ S_2^{n+1} \\ \cdots \\ \cdots \\ S_{N-1}^{n+1} \\ S_N^{n+1} \end{bmatrix} = \begin{bmatrix} \chi_1^n \\ \chi_2^n \\ \cdots \\ \cdots \\ \chi_{N-1}^n \\ \chi_N^n \end{bmatrix}$$

Here,

$$\chi_k^n = \alpha S_k^n - (1-\phi_k)R_k^n S_k^n + \frac{F_{k-1/2}^{adv} - F_{k+1/2}^{adv}}{\Delta z_k}.$$

Dissolved substances

The governing equation is as follows.

$$\frac{\partial}{\partial t}\{\phi C\} = \frac{\partial}{\partial z}\left\{\phi D \frac{\partial C}{\partial z}\right\} + DIS.$$

Differentiating with the implicit method, I set α, β, and γ as follows.

$$\alpha = \frac{\phi_k}{\Delta t},$$
$$\beta = \frac{\phi_{k-1/2} D_{k-1/2}}{\Delta z_k \Delta z_{k-1/2}},$$
$$\gamma = \frac{\phi_{k+1/2} D_{k+1/2}}{\Delta z_k \Delta z_{k+1/2}}.$$

Then,

$$-\beta C_{k-1}^{n+1} + (\alpha + \beta + \gamma) C_k^{n+1} - \gamma C_{k+1}^{n+1} = \alpha C_k^n + DIS_k^n.$$

Therefore,

$$\begin{bmatrix} \alpha+\beta+\gamma & -\gamma & & & & \\ -\beta & \alpha+\beta+\gamma & -\gamma & & & \\ & & \cdots & & & \\ & & & \cdots & & \\ & & & -\beta & \alpha+\beta+\gamma & -\gamma \\ & & & & -\beta & \alpha+\beta+\gamma \end{bmatrix} \begin{bmatrix} C_1^{n+1} \\ C_2^{n+1} \\ \cdots \\ \cdots \\ C_{N-1}^{n+1} \\ C_N^{n+1} \end{bmatrix} = \begin{bmatrix} \chi_1^n \\ \chi_2^n \\ \cdots \\ \cdots \\ \chi_{N-1}^n \\ \chi_N^n \end{bmatrix}$$

Here,

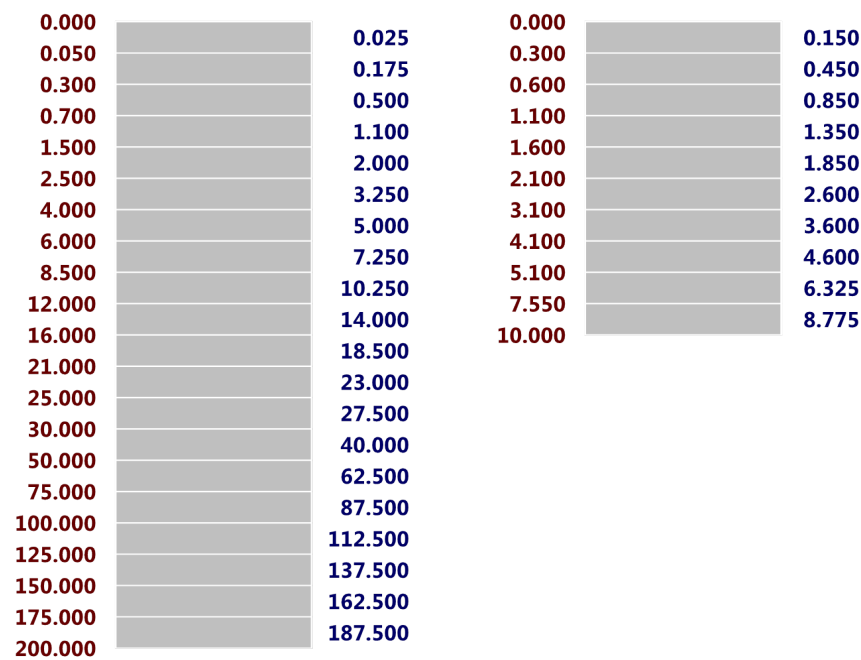$$\chi_k^n = \alpha C_k^n + DIS_k^n.$$

0.000	
0.050	**0.025**
0.300	**0.175**
0.700	**0.500**
1.500	**1.100**
2.500	**2.000**
4.000	**3.250**
6.000	**5.000**
8.500	**7.250**
12.000	**10.250**
16.000	**14.000**
21.000	**18.500**
25.000	**23.000**
30.000	**27.500**
50.000	**40.000**
75.000	**62.500**
100.000	**87.500**
125.000	**112.500**
150.000	**137.500**
175.000	**162.500**
200.000	**187.500**

0.000	
0.300	**0.150**
0.600	**0.450**
1.100	**0.850**
1.600	**1.350**
2.100	**1.850**
3.100	**2.600**
4.100	**3.600**
5.100	**4.600**
7.550	**6.325**
10.000	**8.775**

2.1: The position of vertical grid points as shown in *Archer* (2003) and *Heinze* (1999). The unit is cm.

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