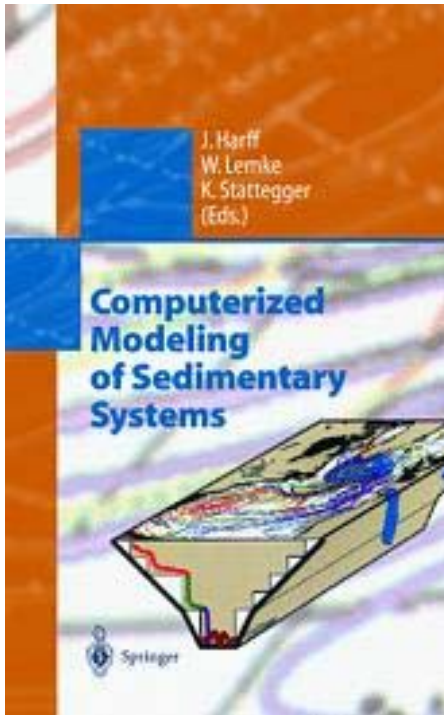


Haupt, B.J., D. Seidov, and K. Stattegger, Numerical study of glacial and meltwater global ocean. in *Computerized Modeling of Sedimentary Systems*, edited by Harff, J., J. Lemke and K. Stattegger, pp. 115-147, Springer, New York, 1999.



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Computerized Modeling of Sedimentary Systems

Computerized modeling is a powerful tool to describe the complex interrelations between measured data and the dynamics of sedimentary systems. Complex interaction of environmental factors with natural variations and increasing anthropogenic intervention is reflected in the sedimentary record at varying scales. The understanding of these processes gives way to the reconstruction of the past and is a key to the prediction of future trends. Especially in cases where observations are limited and/or expensive, computer simulations may substitute for the lack of data. State-of-the-art research work requires a thorough knowledge of processes at the interfaces between atmosphere, hydrosphere, biosphere, and lithosphere, and is therefore an interdisciplinary approach.

Keywords: sedimentology, oceanography, mathematical geology prediction, modeling

Fields: Computer Applications in Geosciences; Math. Applications in Geosciences; Sedimentology

Written for: Graduate students and professionals engaged in the field of sedimentary basin analysis and sedimentary modeling in general

Table of Contents

Contents: From the contents: Climatic, oceanographic and biological forcing of sedimentary systems.- Trends and periodicity in the sedimentary record as a response to environmental changes.- Space-time models of the basin fill.

1998 . Approx. 480 pp. 212 figs. 57 in color, 37 tabs.

ISBN 3-540-64109-2

Hardcover

DM 198,- /US\$ 129,-

Publication date: October, 1998

Book category: Proceedings

Publication language English

SEDLOB and PATLOB: Two numerical tools for modeling climatically–forced sediment and water volume transport in large ocean basins.

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Abstract

Two new three–dimensional (3–D) numerical prognostic sedimentation and water transport models, SEDLOB (SEDimentation in Large Ocean Basins) and PATLOB (PArTicle Tracing in Large Ocean Basins), were developed for large ocean basins and tested for the North Atlantic. SEDLOB consists of a 3–D submodel for the water column and a coupled 2–D submodel for the bottom layer. The semi–Lagrangian PATLOB is similarly designed. The models are driven by steady thermohaline circulation which can be taken from any 3–D–ocean general circulation model (OGCM) (temperature, salinity, velocity, and convection depths). Using these 3–D models, we show the drifting routes of water masses and sediment transport corresponding to the ocean circulation during a time interval covering several hundreds to thousands of years.

Introduction

The processes of sediment erosion, transport and deposition in large ocean basins depend strongly on sediment input from various sources and on oceanic circulation patterns. Most sedimentation models developed during the last decade are designed for small basins and specific sediment input simulating alluvial or deltaic basin fill (cf. *Bitzer and Pflug*, 1989; *Cao and Lerche*, 1994; *Paola et al.*, 1992; *Slingerland et al.*, 1994; *Syvitzki and Daughney*, 1992; *Tetzlaff and Harbaugh*, 1989). In order to simulate large basins we need to couple an ocean general circulation model (OGCM) with an sedimentation model.

Oceanic thermohaline circulation is controlled mainly by the morphology of a basin and by climate. Given a specific steady state oceanic circulation pattern from an OGCM with its temperature-, salinity-, velocity-fields and convection depths, one can add sediment characterized by its physical properties to the circulating water volumes. The proper representation of important topographic features depends on the spatial resolution of the model-basin.

With respect to sediments, a numerical model should allow to simulate

- (i) sediment distribution patterns on the sea floor, especially accumulation and erosion of sediments integrated over time intervals long enough to represent the stratigraphic architecture; and
- (ii) transport paths of water volumes and defined sediment particles from prescribed sources.

Two numerical models, SEDLOB (SEDimentation in large Ocean Basins) and PATLOB (PARTicle Tracing in Large Ocean Basins) were developed for this purpose. Especially PATLOB is a useful tool to address both sedimentation and deep ocean ventilation problems. In this paper, the structure and most important algorithms of these models are described and they are applied to the modern North Atlantic. Earlier versions of the models can be found in *Haupt* [1995] and *Haupt et al.*, [1994, 1995].

The sediment transport model SEDLOB

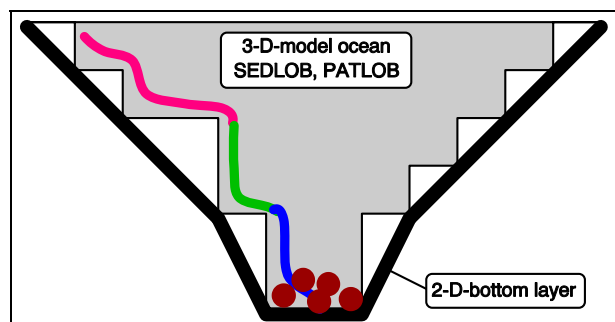


Figure 1: Coupling of the two submodels.

SEDLOB mainly consists of two coupled submodels which are linked with each other (Figure 1). The first submodel includes sediment transport in a 3-D water column [*Bitzer and Pflug, 1990; McCave and Gross, 1991; Zanke, 1977b*], and the second two-dimensional (2-D) submodel

simulates the near bottom processes in a one centimeter thick layer [*Puls, 1981; Sündermann and Klöcker, 1983; Zanke, 1978*]. This 2-D boundary layer is always parallel to the bottom and continuously follows the dynamic changes of the topography. Although

the model is used for the deep ocean, the one centimeter thickness is chosen for the bottom layer on the basis of experimental studies of flows in channels. These studies provide detailed information concerning the interdependence between temperature, salinity, viscosity, and velocity. Additionally, the bed and suspension transport are well documented in a set of equations for this one centimeter thick layer.

Three-dimensional submodel of SEDLOB

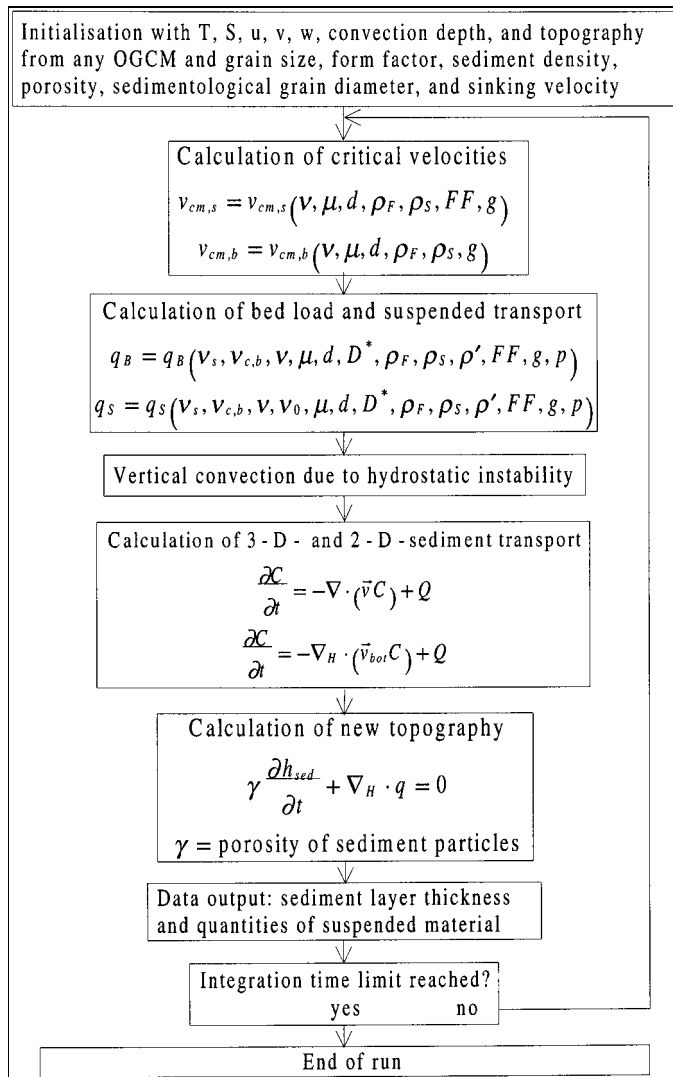


Figure 2: Flow chart of SEDLOB

Two-dimensional submodel of SEDLOB

The 2-D submodel of SEDLOB simulates the exchange of sediment between the water column and the ocean bottom. Within this layer, which follows the bottom topography,

The upper 3-D submodel simulates the lateral inflow and outflow of particles from coastal sources as well as the inputs of eolian dust (worldwide approximately 60 – 360 million tons per year), and melting icebergs (worldwide approximately 100 million tons per year including glaciers) [Allen, 1985; Goldschmidt et al., 1992; Möller, 1986; Pickard and Emery, 1988]. Moreover, several biological processes such as dying plankton and fecal pellet production can act as sediment sources.

erosion, transport (sliding, rolling, and skipping), and deposition of sediment is calculated based on the critical shear velocities of the bed load and the suspension load, the bottom slope, and bottom roughness (bottom friction) [Anderson and Humphrey, 1989; Bogárdi, 1974; Garde and Ranga Raju, 1977; Hsü, 1989; Puls, 1981; Sündermann and Klöcker, 1983; Zanke, 1976; 1977a; 1978; 1982]. The change of the bottom topography is calculated from the changing sediment content in the 1 cm thick bottom layer [Krohn, 1975; Sündermann and Klöcker, 1983].

Modeled processes depending on scales

Since our knowledge about many geological and biological processes is very limited, we assume a medium grain size homogenous mixture of sediment [Bitzer and Pflug, 1989; Sündermann and Klöcker, 1983] and that suspended particles in the water column are transported by currents [Bitzer and Pflug, 1989]. In order to calculate the vertical transport, one should take into account not only the vertical velocity w , but also the settling velocity w_s of suspended material. In addition to the vertical transport by upwelling/sinking water, the settling velocity relative to the water motion is superimposed on the water motion to obtain the true particles transport. The settling velocity depends on grain size, density and kinematic viscosity from the surrounding water as well as particle density, form factor and sedimentological grain diameter, and gravitational acceleration [Gibbs et al., 1971; Gibbs, 1985; McCave and Gross, 1991; Zanke, 1977b]. It must be emphasized that the vertical

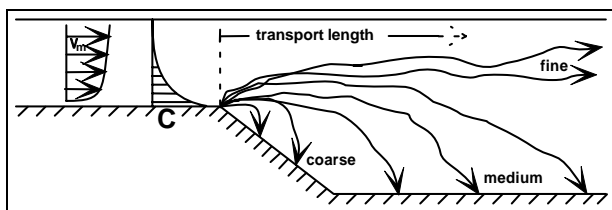


Figure 3: Sketch about different transport length due to different grain size, and different settling velocity w_s ; modified after Middleton and Southland [1984].

velocities are spatially variable, and are not preset fixed values as in many other models. This is significant, considering that transport and deposition mainly depend on the settling velocity w_s which normally exceeds the vertical velocity of the surrounding water (Figure 3) [McCave,

1984]. The movement of sediment is based on mechanical processes [Dietrich et al., 1975; Miller et al., 1977; Zanke, 1982].

Tectonic processes are not considered here because our sedimentation reconstructions cover only geologically short time periods lasting from several hundreds to several thousands of years. During such time intervals, the overall ocean geometry may be considered stationary for the North Atlantic [Wold, 1992]. Tectonic subsidence or uplift is much slower than the expected sedimentation rate within a range from a few millimeters to several meters over a 1000 year timespan [Shaw and Hay, 1989]. As a consequence, tectonic movements and their effects on topography are negligible [Stephenson, 1989].

Model equations of SEDLOB

In the following section, the equations of the 3–D and 2–D submodels are listed separately. The symbols and units used are listed in the Appendix. For the sake of clarity, all equations are shown in cartesian coordinates.

The three–dimensional submodel of SEDLOB

The 3–D submodel of SEDLOB consists of a transport equation with a source term Q [Bryan, 1969; Dietrich et al., 1975; Eppel, 1977/78; Fahrbach et al., 1989; Gerdes, 1988; Struve, 1978; Tetzlaff and Harbaugh, 1989]

$$\frac{\partial C}{\partial t} = -\nabla \cdot (\vec{v} C) + Q \quad (1)$$

and a continuity equation (conservation of mass) for an incompressible medium ($d\rho_F/dt = 0$) [Apel, 1987; Bryan, 1969; Fahrbach et al., 1989; Kurz, 1977; Krauß, 1973; LeBlond and Mysak, 1978; Pond and Pickard, 1986; Tetzlaff and Harbaugh, 1989]:

$$\nabla \cdot \vec{v} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \quad (2)$$

The hydrostatic equation gives the local pressure p [Bryan, 1969; Cox, 1984; Haupt, 1990]:

$$p(z) = p_{surf} + g \int_z^0 \rho_F dz \quad (3)$$

The nonlinear equation of state is given by the UNESCO formula [UNESCO, 1981; see also Millero and Poisson, 1981]

$$\rho_F = \rho_F(T, S, p) \quad (4)$$

The settling velocity w_s of a single particle is calculated using the approximation given in *Zanke* [1977b]

$$w_s = w_s(v, \mu, d, \rho_F, \varphi_S, FF, g)$$

$$= \frac{12v}{d(2.7 - 2.3FF)} \left(\sqrt{1 + \left(0.21 \left(\frac{(\rho_S - \rho_F)g}{v^2} \right)^{\frac{1}{3}} \right)^3} (2.7 - 2.3FF) - 1 \right) \quad (5)$$

The equation for dynamic viscosity μ

$$\mu = \mu(T, S, p) \quad (6)$$

is approximated by a polynom [*Matthäus*, 1972]. The total vertical velocity of w_g is the sum of the water velocity and the particle settling velocity:

$$w_g = w + w_s \quad (7)$$

At the surface, the „rigid–lid“ approximation is used:

$$w_{surf} = 0 \quad \text{for} \quad z = 0 \quad (8)$$

The „rigid–lid“ approximation eliminates external gravity waves and allows for a longer time step (Δt) [*Cox*, 1984; *Haupt*, 1990; *LeBlond and Mysak*, 1978]. At lateral boundaries „no–flux“ and „no–slip“ boundary conditions are used:

$$u, v, C_n = 0 \quad (9)$$

No bottom friction is used, but rather a „free–slip“ boundary condition is employed at the bottom:

$$\frac{\partial u}{\partial z}, \frac{\partial v}{\partial z} = 0 \quad (10)$$

The fluxes through the bottom and lateral boundaries are set to zero:

$$\frac{\partial T}{\partial n}, \frac{\partial S}{\partial n}, \frac{\partial C}{\partial n} = 0 \quad (11)$$

The vertical velocity w at the bottom is calculated using the continuity equation

$$w = - \left(u \frac{\partial H}{\partial x} + v \frac{\partial H}{\partial y} \right) \quad (12)$$

The two–dimensional submodel of SEDLOB

In many aspects, the 2–D submodel of SEDLOB is similar to the 3–D submodel. The sediment transport at the bottom has the form

$$\frac{\partial C}{\partial t} = -\nabla_H \cdot (\vec{v}_{bot} C) + Q \quad (13)$$

The submodel uses the same hydrostatic equation for the local pressure p (compare with Equation 3), the same set of nonlinear equations for density (compare with Equation 4) and viscosity (compare with Equation 6). Similarly, the total vertical velocity w_g is the sum of the vertical velocity w (compare with Equation 2) and the settling velocity w_s of a single particle (compare with Equation 5). Even though the 1 centimeter bottom boundary layer is quasi–2–D, this vertical velocity is needed for coupling both submodels.

The critical velocities for sediment transport are approximated by polynomial equations given in *Zanke* (1977a) (Figure 4 and 5). One has to take into account

(i) the critical velocities for starting bed load transport

$$v_{cm,b} = v_{cm,b}(v, \mu, d, \rho_F, \rho_S, g) = 2.8 \left(\left(\frac{\rho_S - \rho_F}{\rho_F} \right) g d \right)^{0.5} + 14.7 \frac{v}{d} c \quad \text{where } c = 1; \quad (14)$$

(ii) the critical velocities for initiating of suspension load transport

$$\begin{aligned} v_{cm,s} &= v_{cm,s}(v, \mu, d, \rho_F, \rho_S, FF, g) \\ &= 8.4 \frac{12v}{d(2.7 - 2.3FF)} \left(\sqrt{1 + \left(0.21 \left(\frac{(\rho_S - \rho_F)}{\rho_F} g \right)^{\frac{1}{3}} \right)^3} (2.7 - 2.3FF) - 1 \right); \end{aligned} \quad (15)$$

and (iii) the critical velocity for deposition

$$\begin{aligned} v_{cm,d} &= v_{cm,d}(v, \mu, d, \rho_F, \rho_S, FF, g) \\ &= 3.93 \frac{12v}{d(2.7 - 2.3FF)} \left(\sqrt{1 + \left(0.21 \left(\frac{(\rho_S - \rho_F)}{\rho_F} g \right)^{\frac{1}{3}} \right)^3} (2.7 - 2.3FF) - 1 \right). \end{aligned} \quad (16)$$

The bed load transport and the suspended load transport are calculated using their dependence on the reduced bottom velocity \vec{v}_{bot} in the 1 cm thick bottom layer, also called *Prandtl's* boundary layer [*Sündermann and Klöcker*, 1983; *Zanke*, 1978]. The formula for calculating the bed load transport is

$$\begin{aligned}
q_B &= q_B(v_s, v_{c,b}, v, \mu, d, D^*, \rho_F, \rho_S, \rho', FF, g, p) \\
&= \frac{1}{p} 10^{-7} \left(\frac{v_s^2 - v_{c,b}^2}{w_s^2} D^{*2} \right)^2 v \quad \text{where } D^* = \left(\frac{\rho' g}{v^2} \right)^{\frac{1}{3}} d \quad \text{and } p \approx 0.7 \quad (17)
\end{aligned}$$

and for calculating the suspension transport is

$$\begin{aligned}
q_S &= q_S(v_s, v_{c,b}, v_{c,s}, v, v_0, \mu, d, D^*, \rho_F, \rho_S, \rho', FF, g, p) \\
&= 10^{-8} \frac{H}{h_1} \frac{(v_s^2 - v_{c,b}^2)(v_s^2 - v_{c,s}^2)}{w_s^4} D^{*4} \frac{1}{p} \left(\frac{v}{v_0 - v} \right)^{\frac{1}{4}} \quad (18)
\end{aligned}$$

The total sediment transport is computed by summing equations 17 and 18:

$$q = q_B + q_S \quad (19)$$

The relationship of critical velocities and sediment transport is summarized in Figure 4.

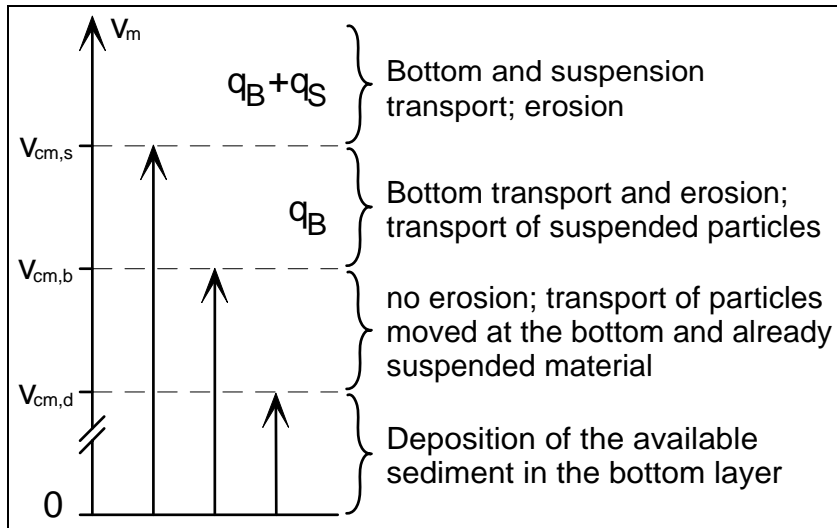


Figure 4: Critical velocities for initiating bed load and suspension load transport (confer Figure 5).

A diagram of critical velocities versus grain size is displayed in Figure 5.

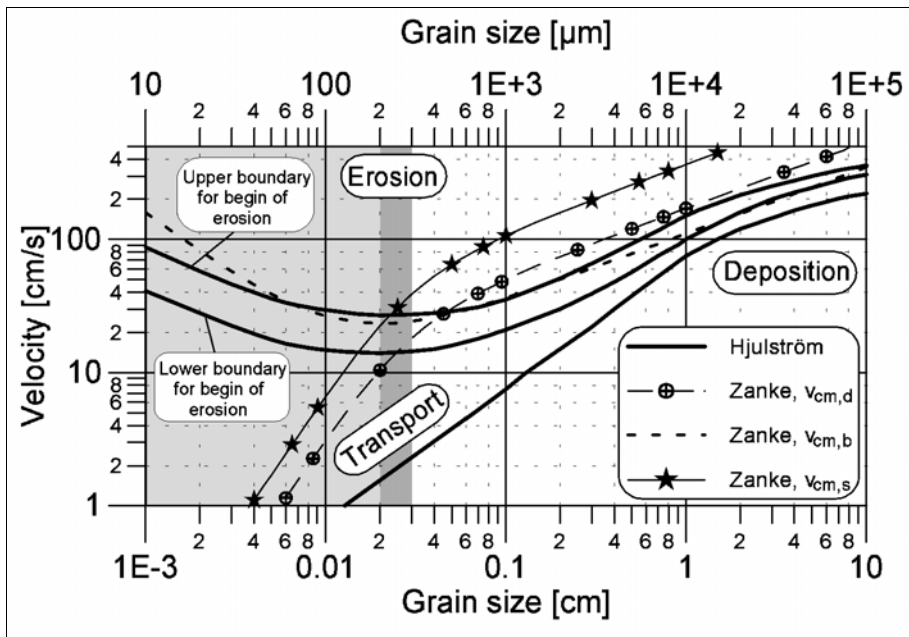


Figure 5: Critical velocities for beginning bed load transport and suspension load transport. The well known *Hjulström* [1935] curve is given as reference.

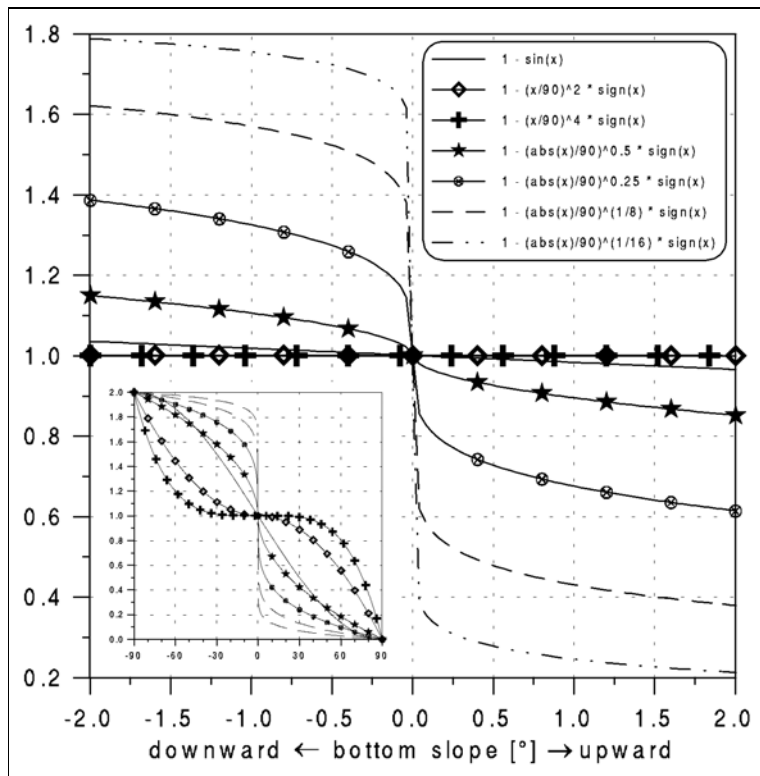


Figure 6: Modification of sediment transport and critical velocities. The main Figure shows the used functions in a range from -2 up to 2 degrees, while the lower left Figure shows the range from -90 up to 90 degrees, and the upper right box gives the functions embedded in the model.

The set of equations dealing with the critical velocities and the sediment transport are modified by the bottom slope. A downward flow leads to an increase of the transport capacities and a decrease of the critical velocities described above and vice versa. This modification is achieved by multiplying the transport velocities by an empirical function dependent on the bottom slope [Haupt, 1995] (Figure 6).

The change of the bottom topography due to erosion and deposition is computed using the sediment continuity equation [Sündermann and Klöcker, 1983; Tetzlaff and Harbaugh, 1989]:

$$\gamma \frac{\partial h_{sed}}{\partial t} + \nabla_H \cdot q = 0 \quad (20)$$

Sediment can be eroded or deposited according to [Gross and Dade, 1991; Tetzlaff, 1989]

$$\begin{aligned} \frac{\partial h_{sed}}{\partial t} < 0 & \text{ erosion} \\ \frac{\partial h_{sed}}{\partial t} > 0 & \text{ deposition} \end{aligned} \quad (21)$$

This technique makes the simulation of the process of redistribution of the already deposited sediment possible [Frohlich and Matthews, 1991]. Sediment is neither eroded, nor deposited when an equilibrium between the sediment transport and the sediment load exists. The equilibrium is checked at every time step in our model.

Coupling of SEDLOB's submodels

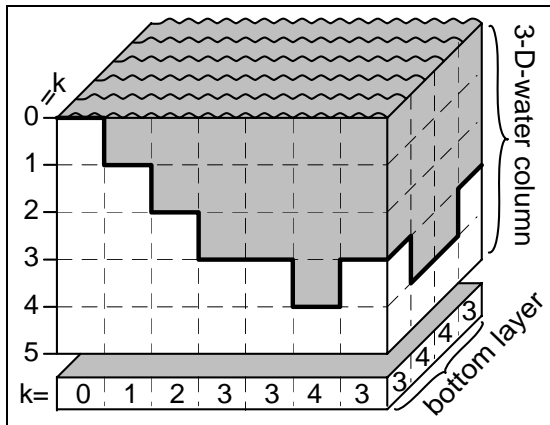


Figure 7: Projection and coupling of both submodel

The coupling of both submodels facilitates the sediment exchange between suspension load in the 3-D water column and the bottom layer (Figure 7). The 2-D bottom layer is initialized at every grid point (i, j) with the data of the 3-D submodel of SEDLOB. This is achieved by projecting the deepest „water grid point“ of the 3-D submodel onto the bottom. Since the projected velocity may belong to different

layers, the resulting 2-D velocity field is very inhomogeneous in areas where steep gradients in the bottom topography exist. To obtain a smoother flow, the velocity field is smoothed using a moving average technique. In a large set of numerical experiments, it was found that smoothing with 5 to 10 passes is sufficient to get an adequate velocity field in the bottom layer. The smoothed bottom velocity enables the model to run for more than 500 years without producing ripples and spikes of sediment transport capacity in the adjacent grid

points. Additional smoothing of other fields (bottom topography, sediment concentration near bottom, etc.) is therefore not required.

Numerical design

SEDLOB uses a staggered *Arakawa–B*-grid with a half grid distance's shift between T - S points and u - v points [Cox, 1984; Mesinger and Arakawa, 1976], and a cartesian coordinate system with the vertical axis directed downward. The time integration is carried out using an „upstream differencing“ scheme [Mesinger and Arakawa, 1976; Struve, 1978]. This scheme is known to be rather effective [Dube *et al.*, 1986], and may become essential for long-term integrations. It should be noted that this scheme, which is also called the „donor cell“, „upward,-, or „upwind“-scheme, is positive definite: Positive values, like concentration, always remain positive during integration („positivity“; $(C_i^o \geq 0 \text{ for all } i) \rightarrow (C_i^N \geq 0 \text{ for all } i \text{ and } N)$) [Eppel, 1977/78; Smolarkiewicz, 1983]. This is an important feature for mass transports, e.g., the transport of marine and eolian sediments, vapor, or gas in the atmosphere all are positive definite. Using second-order or higher-order-integration-accuracy schemes can introduce some difficulties because a negative solution of the equation results [Smolarkiewicz, 1983]. Furthermore, a given disturbance is transported in the direction of physical advection and not, as in other discretisation schemes, in the opposite direction [Mesinger and Arakawa, 1976; Struve, 1978]. Furthermore, the „upstream differencing“-scheme is mass conservative. All these requirements are only satisfied if the *Courant–Friedrichs–Levy* criterion is not violated [Eppel, 1977/78; Mesinger and Arakawa, 1976; Smolarkiewicz, 1983; Struve, 1978]:

$$c_x \geq u \frac{\Delta t}{\Delta x}, c_y \geq v \frac{\Delta t}{\Delta y}, c_z \geq w_g \frac{\Delta t}{\Delta z} \quad (22)$$

where c_x, c_y, c_z are Courant-numbers ($c_{x,y,z} \leq 1$). Thus, the maximum time step in the model is:

$$\Delta t \leq \min \left(\frac{dx_{i,j}}{|u_{i,j,k}|}, \frac{dy_{i,j}}{|v_{i,j,k}|}, \frac{dz_k}{|w_{g_{i,j,k}}|} \right) \quad (23)$$

Here $dx_{i,j}$, $dy_{i,j}$, dz_k denote the grid steps. The three velocity components are denoted by $u_{i,j,k}$, $v_{i,j,k}$, and $w_{g_{i,j,k}}$.

Because a normal „upwind“-scheme has a strong implicit diffusion, we modify it in the 2–D submodel. There are different schemes to overcome the deficiencies of the simple upwind formulation. For example, the self–adjusting hybrid scheme (SASH), or the flux correction technique (FCT) offer better functionality while retaining the advantages of the upward scheme. However, the usefulness of these schemes is rather limited because of excessive computer time required. In addition, a positive definite solution is not guaranteed. Yet any emerging negative values are small enough to be neglected [Smolarkiewicz, 1983; Struve, 1978]. An appropriate numerical scheme is essential for getting „sediment fronts“, produced by sediment slumps, or local sediment clouds, etc. Smolarkiewicz [1983] introduces an „antidiffusion“ with an „antidiffusion velocity“ to keep the fronts sharp in spite of the high artificial diffusion inherent to the upwind schemes.

The numerical advection scheme is illustrated below for one–dimensional advection only. In a normal upwind scheme, two terms are in balance: the local changes in time, and the advective term. Smolarkiewicz [1983] adds another term with a small implicit diffusion at a low computational cost:

$$\underbrace{\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(uC)}_{\text{normal "upwind"-scheme}} = \underbrace{\frac{\partial}{\partial x} \left(K_{impl} \frac{\partial C}{\partial x} \right)}_{\text{implicit diffusion}} \quad \text{where} \quad K_{impl} = 0.5(|u|\Delta x - \Delta t u^2) \quad (24)$$

Thus, for the normal „upwind“-scheme in the 3–D submodel the following discretisation on a staggered grid is chosen:

$$C_{n+1,i} = C_{n,i} - \left\{ F(C_{n,i}, C_{n,i+1}, u_{n,i+\frac{1}{2}}) - F(C_{n,i-1}, C_{n,i}, u_{n,i-\frac{1}{2}}) \right\} \quad (25)$$

where

$$F(C_i, C_{i+1}, u) = \left[(u + |u|)C_i + ((u - |u|)C_{i+1}) \right] \frac{\Delta t}{2\Delta x} \quad (26)$$

In the 2–D submodel we use the scheme of Smolarkiewicz [1983] with \tilde{u} as antidiffusion velocity. The function F has the same form as in equation 26.

$$C_i^* = C_{n,i} - \left\{ F(C_{n,i}, C_{n,i+1}, u_{n,i+\frac{1}{2}}) - F(C_{n,i-1}, C_{n,i}, u_{n,i-\frac{1}{2}}) \right\} \quad (27)$$

$$C_{n+1,i} = C_i^* - \left\{ F(C_i^*, C_{i+1}^*, \tilde{u}_{n,i+\frac{1}{2}}) - F(C_{i-1}^*, C_i^*, \tilde{u}_{n,i-\frac{1}{2}}) \right\} \quad (28)$$

where

$$\tilde{u}_{i+\frac{1}{2}} = \frac{\left(|u_{i+\frac{1}{2}}| \Delta x - \Delta t u_{i+\frac{1}{2}}^2 \right) (C_{i+1}^* - C_i^*)}{(C_i^* + C_{i+1}^* + \varepsilon) \Delta x} \quad (29)$$

ε is a small value (here 10^{-15}) to ensure $\tilde{u} = 0$ when $C_{i+1}^* = C_i^* = 0$.

A growth or decay of the initial signal can be obtained by scaling the antidiffusion velocity \tilde{u} by a factor Sc :

$$\tilde{u}_{scale} = Sc \tilde{u} \quad (30)$$

The best result was achieved using a scaling factor of $1 \leq Sc \leq 1.08$ after *Smolarkiewicz* [1983]. With $Sc = 0$ the above described scheme is identical to the normal upwind scheme without antidiffusion. Three experiments with different scaling factors are discussed below. These experiments were carried out to demonstrate how antidiffusion works and to check the program's overall performance. Starting from a given distribution of sediment in an anticyclone velocity field, the calculations are shown for one full rotation around the center (Figure 8). The first experiment (I) has been carried out without antidiffusion ($Sc = 0$), the second one (II) with a scaling factor $Sc = 1$, and the third one (III) with a factor $Sc = 1.08$ (Figure 9, 10). — With a scaling factor $Sc = 1$ we get results similar too those obtained by *Smolarkiewicz* [1983], i.e. best fit. The horizontal extent and intensity of the initial perturbation was preserved with good accuracy.

Without antidiffusion (experiment I) the experiment suffers from strong diffusion, which results in the signal being flattened and expanded horizontally. When the antidiffusion was overestimated, the initial perturbation was deformed and new maxima appeared (experiment III). It should be stressed that mass was conserved in all experiments.

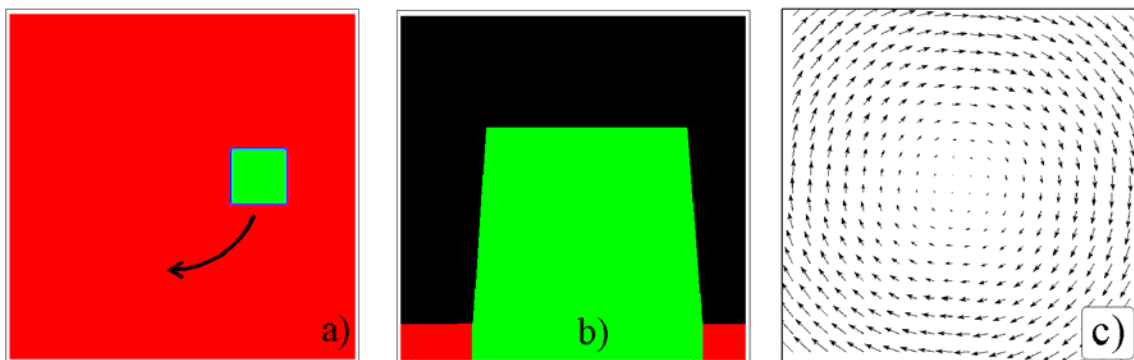


Figure 8: Sediment distribution of the three experiments I, II, and III as a map view (a) and as a sectional view (b). The velocity field is circular (c).

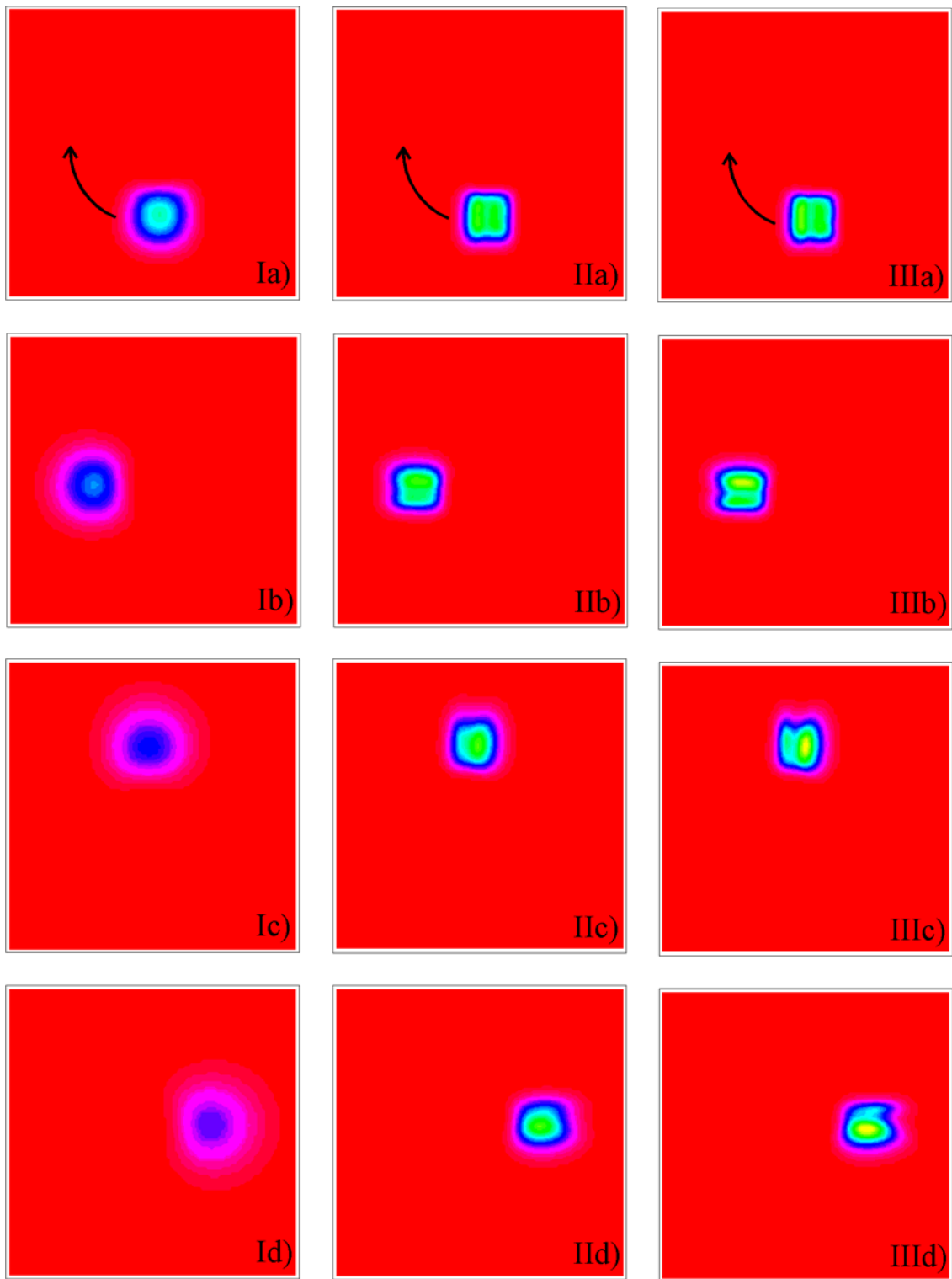


Figure 9: Sediment distribution of the three experiments I, II, and III as a map view. Experiment I is calculated without antidiffusion ($Sc = 0$), the experiments II ($Sc = 1$), and III ($Sc = 1.08$) are calculated with antidiffusion [Smolarkiewicz, 1983].

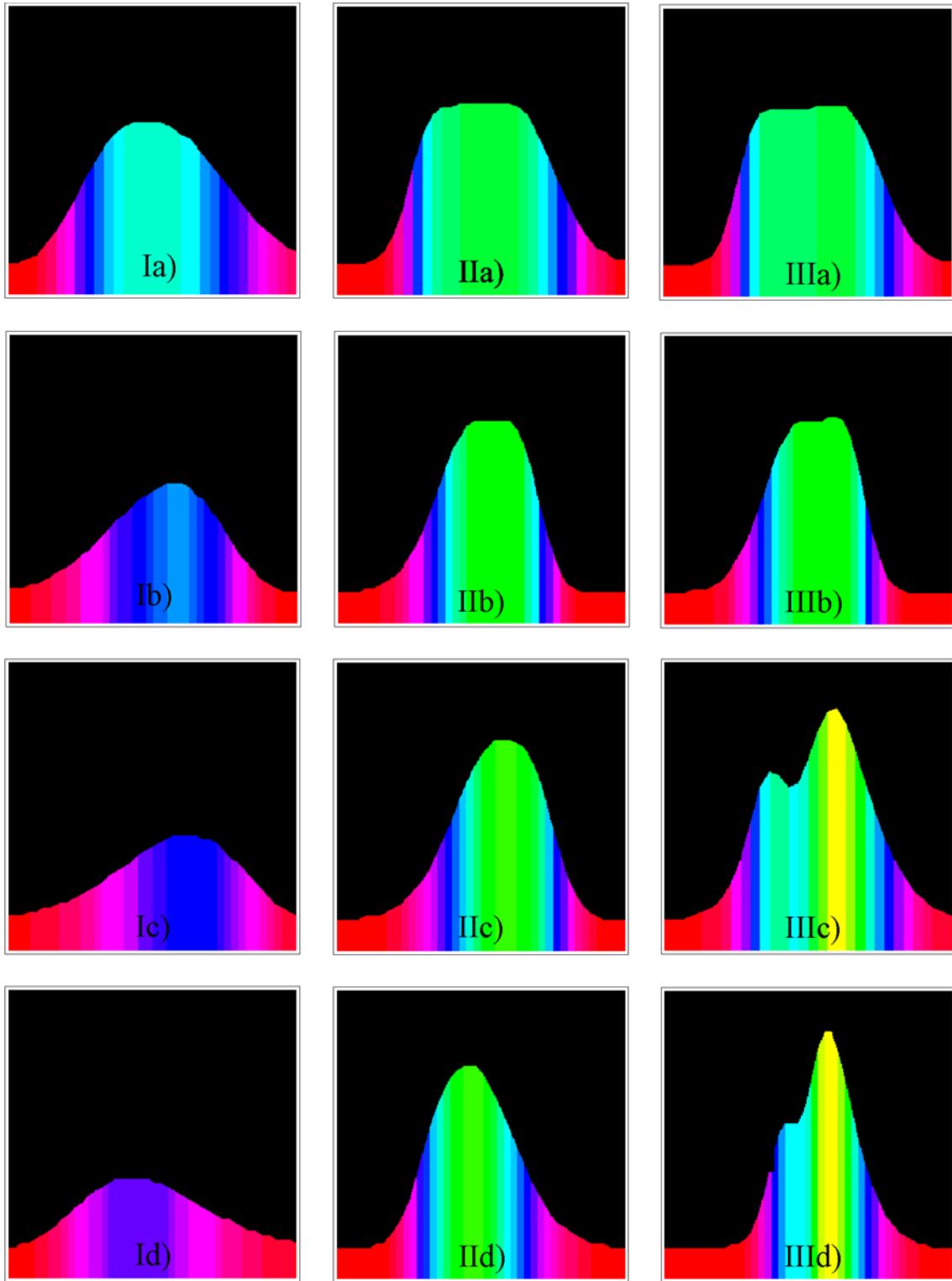


Figure 10: Sediment distribution of the three experiments I, II, and III as a sectional view. Experiment I is calculated without antidiffusion ($Sc = 0$), the experiments II ($Sc = 1$), and III ($Sc = 1.08$) are calculated with antidiffusion [Smolarkiewicz, 1983].

The particle–tracing model PATLOB

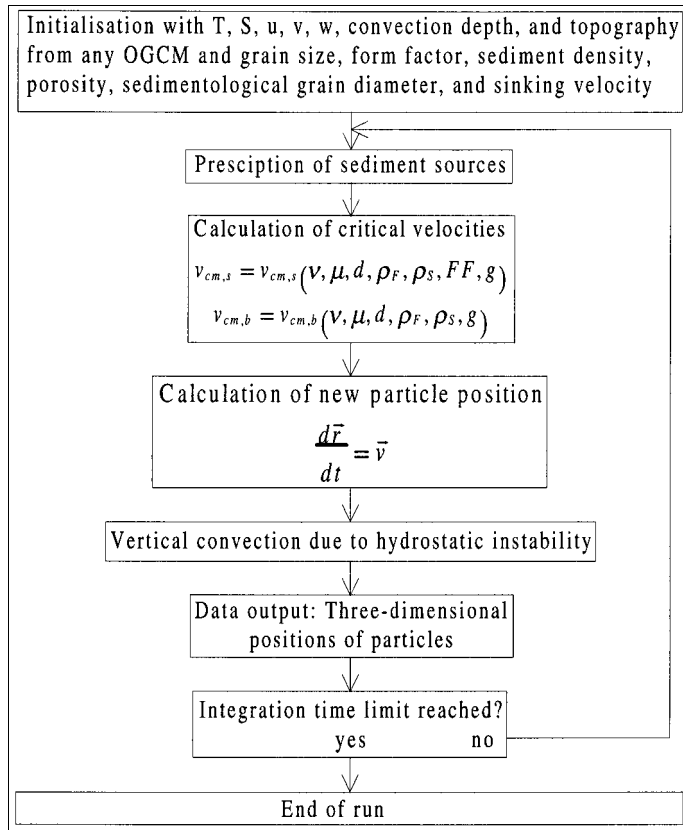


Figure 11: Flow chart of PATLOB

The semi–Lagrangian (hybrid Eulerian–Lagrangian approach) model PATLOB traces material parcels, e.g., water parcels, sediments, pollutants, natural or artificial organic material, etc. from their source area/origin until they are dissolved or deposited. This model is a useful tool to address both sedimentation and deep ocean ventilation problems. PATLOB was developed in order to use semi–Lagrangian calculations in combination with SEDLOB, which uses the output of the OGCM. Thus,

the assumptions made for PATLOB

are similar to those made for SEDLOB. Like SEDLOB, PATLOB mainly consists of two coupled submodels which are linked together. Hence, data flow between two submodels and the projection of data onto the 2–D 1 cm thick bottom layer works identically in SEDLOB and PATLOB. Additionally, PATLOB takes the change of the bottom topography into account, which is calculated with SEDLOB. This is also relevant to particles which have a settling velocity.

Formulation of PATLOB

PATLOB uses the same approximation for the settling velocity w_s , the critical shear velocities of bed load ($v_{cm,b}$) and suspension load ($v_{cm,s}$), and the critical velocity $v_{cm,d}$ for a final deposition of the parcels found in SEDLOB. Furthermore, the critical velocities are updated by the bottom slope.

The new location of every particle is calculated from the old position [Goldstein, 1985; Kurz, 1977]:

$$\frac{d\vec{r}}{dt} = \vec{v} . \quad (31)$$

For the 3–D submodel the equation above is written in cartesian coordinates as

$$\begin{aligned} r_{x,n+1} &= r_{x,n} + u_r \Delta t \\ r_{y,n+1} &= r_{y,n} + v_r \Delta t \\ r_{z,n+1} &= r_{z,n} + w_{g_r} \Delta t \end{aligned} \quad (32)$$

and for the 2–D submodel as

$$\begin{aligned} r_{bot,x,n+1} &= r_{bot,x,n} + u_{bot,r} \Delta t \\ r_{bot,y,n+1} &= r_{bot,y,n} + v_{bot,r} \Delta t \end{aligned} \quad (33)$$

where r is used for the location interpolated inside of the numerical grid and n for the time step. This means that the velocity components provided by the OGCM are interpolated to the current position of the Lagrangian particle from nearby points on the Eulerian numerical grid.

The vertical convection in SEDLOB and PATLOB

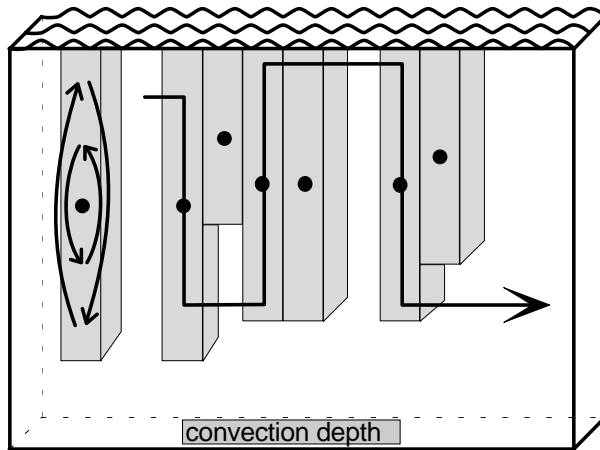


Figure 12: Sketch of two particles entering an „turbulent“ water columns or ‘chimneys’ area with different vertical convection depths [Seidov and Haupt; 1997].

SEDLOB and PATLOB take into account vertical convection. This is an important feature because convection does not transport water and sediment in the same way as advection does. Tracers are advected by currents, whereas convection due to hydrostatic instability mixes water, sediments, and the tracers vertically in

hydrostatic instability determines the depth of vertical mixing in the ocean. In the model, the convection depth indicates how many layers participate in mixing, that is to which layer a particle entering such a „turbulent“ water column is propelled within the chimney. We use different techniques to introduce this

mixing into the two models. In SEDLOB, the sediment concentrations of vertical grid boxes affected by the convection depth are mixed to get a homogenous sediment distribution in every time step. In PATLOB, a parcel entering a chimney at the top is propelled downward to the base of the chimney and vice versa. This is equivalent to the reflection of every particle around the middle depth of a convection site. If a particle enters a convection site, it is only mixed once. The vertical position remains unchanged if the particle enters an adjacent convection column having the same convection depth; in a case where the convection is deeper, the particle is brought to its new depth, either upward, or downward (Figure 12). Additional details of this technique for incorporating convection into SEDLOB and PATLOB are given in *Seidov and Haupt* [1997].

Validation of SEDLOB and PATLOB

The models were originally developed and designed to study sedimentation processes in the North Atlantic and to be integrated with paleoceanographic modeling [Haupt, 1995; Haupt et al., 1994, 1995]. Therefore, the control experiments presented here concentrate on the modern North Atlantic. We review the results based on model runs with a $0.5^\circ \times 0.5^\circ$ horizontal resolution (95 grid points in both horizontal directions). For calculating the sediment transport through gateways and cross-sections, e.g. the Denmark Strait, the Iceland–Faeroe–Scotland–Ridge, or Barents Sea inflow and outflow, it is important to use a high vertical resolution which represents the topography in a realistic manner. Therefore, we use a model topography derived from the *ETOPO5* [1986] data set (Figure 13) with 17 vertical layers which are 50, 50, 50, 50, 100, 100, 100, 250, 250, 250, 250, 500, 500, 500, 500, 500, and 1000 meters thick. The maximum bottom slope in the direction of flow is less than 2.65° . The staircase-type bottom topography must never exceed 5° [Puls, 1981], otherwise the turbulent bottom flow will detach from the seabed and the equation for sediment transport (Equation 20) will no longer be valid (Figure 14). We use a spherical coordinate system in which the equator has been rotated up to 60°N along zero meridian in order to minimize the convergence of meridians in high latitudes.

Furthermore, a high resolution bottom topography is required for the better understanding of the influence that the additional sediment sources near Iceland and in the Greenland–Iceland–Norwegian Seas have on the sedimentation patterns in the northern North Atlantic.

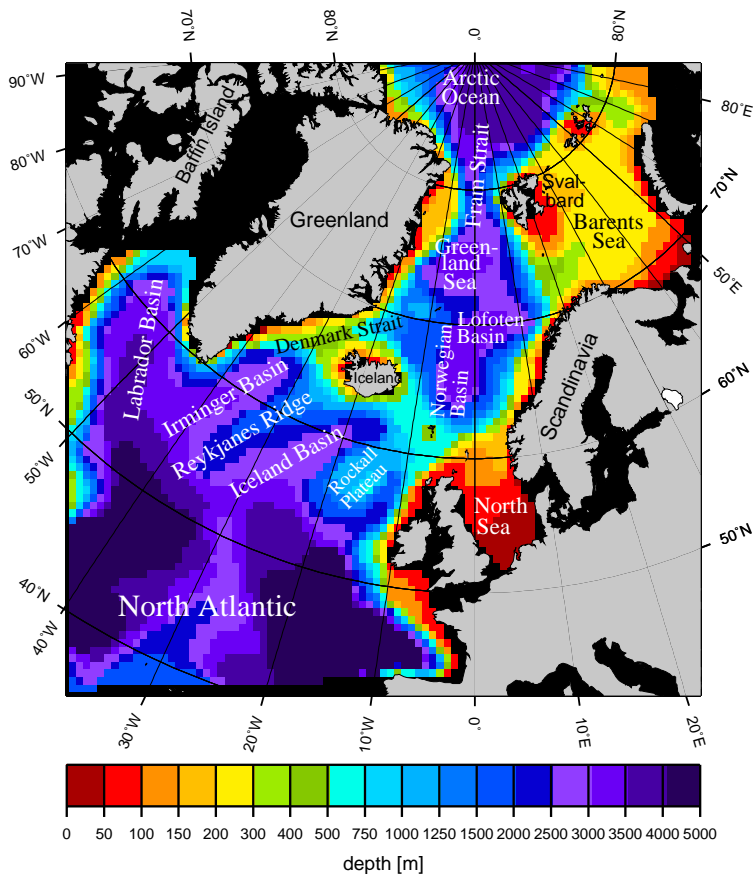


Figure 13: Modern model bottom topography of the northern North Atlantic on a $0.5^\circ \times 0.5^\circ$ grid with 17 unevenly spaced vertical layers.

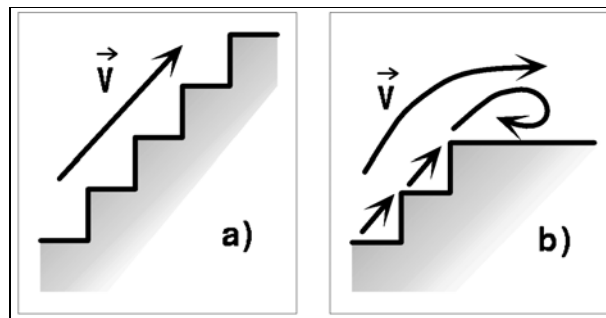


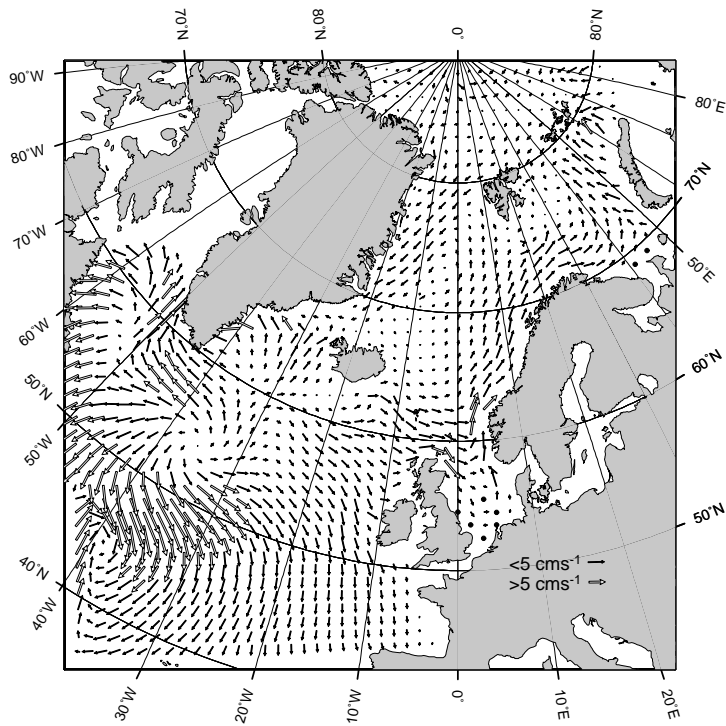
Figure 14: Sketch of currents at the staircase bottom topography without a detached sediment transport (a). In case of a detachment the bottom transport is in opposite direction [*Puls*, 1981].

Model initialization

As outlined above, in order to run the two models, one needs the output of an OGCM: temperature, salinity, velocity, and convection depths. A detailed description of the data fields is given in *Haupt* [1995]. Here, we present two examples of the circulation pattern:

the first one shows the circulation of the northern North Atlantic at 25 meters depth (Figure 15a), and the second one the bottom circulation resulting from the projection of the 3-D velocity field onto the bottom (Figure 15b). The bottom velocity is smoothed with a 10 pass sliding average. Although this experiment uses the closed boundary conditions with artificial walls at about 40°N, the model output from the OGCM shows the major currents around Iceland and in the Norwegian–Greenland Seas. These are mainly the West–Greenland Current, the East–Greenland Current, the outflow through the Denmark Strait, the Irminger Current, the North Atlantic Current, the Norwegian Current parallel to the Norwegian Coastal Current which enters the Barents Sea, and the West–Svalbard Current, or the Transpolar Drift (Figure 16).

a)



b)

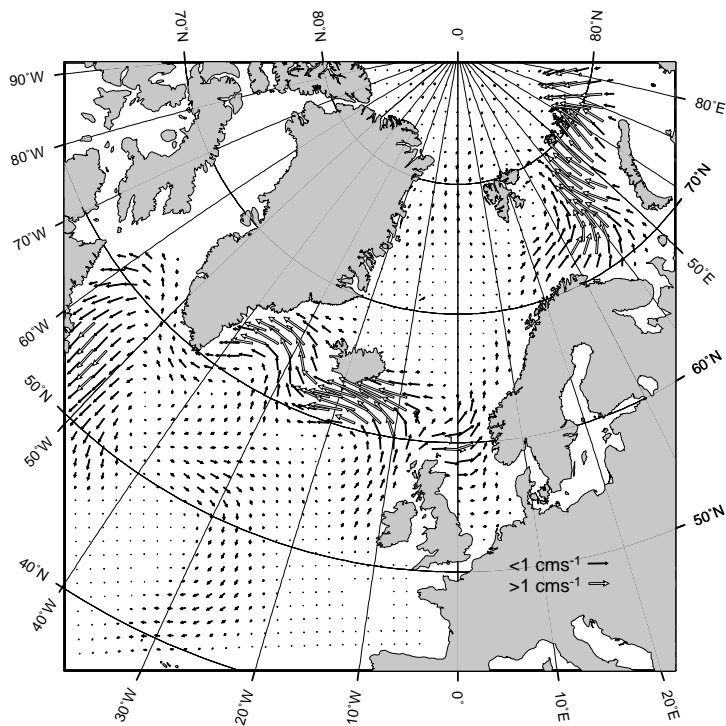


Figure 15: Modern velocity (a) at $z=25$ meter and (b) at the bottom. The bottom velocity in the 1 cm thick bottom is smoothed with a sliding average with 10 passes.

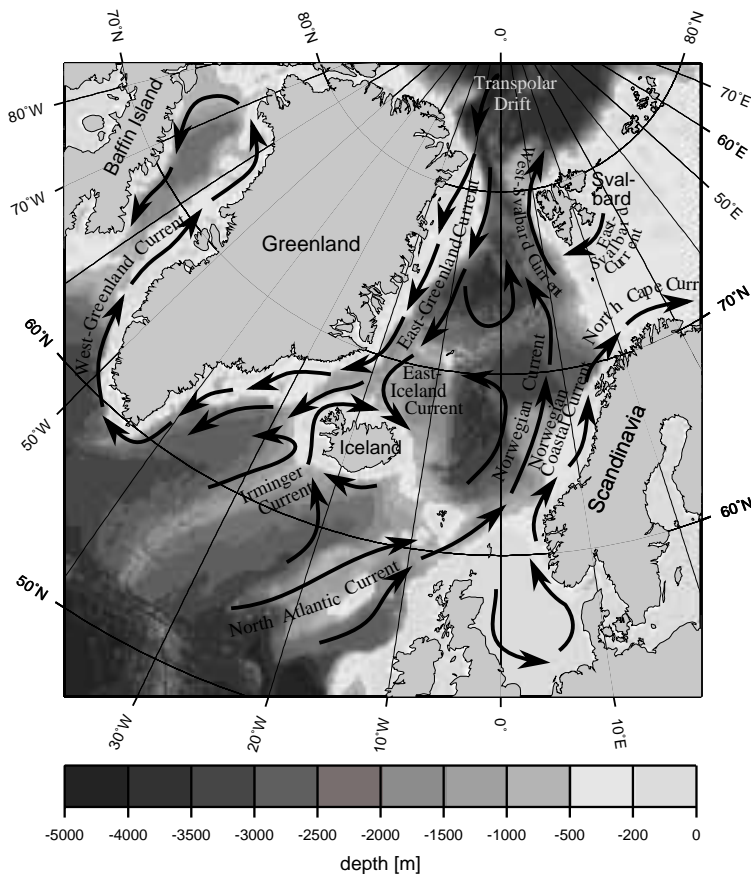


Figure 16: The North Atlantic upper ocean circulation pattern.

The sediment content of the 3-D water column in SEDLOB can be controlled in two different ways: sediment can be manually added to or taken from the water by sources and sinks, or alternatively, the exchange of sediment between the 3-D and the 2-D submodels is calculated automatically. Here, the external source of sediment is prescribed. Sediment sources and quantities inferred from the lateral river input and melting ice sheets are taken from Table 1 (Figure 17). The lateral river sediment input is restricted to the grid points adjacent to the coastline. To limit the simulations to the case where sediment sources are only known at the lateral boundary, internal sources such as sediment derived from submarine fan deposition or from icebergs and fjords are not considered.

Table 1: Survey of used sediment sources. In case of conversions the sediment density $\rho_s = 2.6 \text{ g/cm}^3$ and the porosity $\gamma = 0.75$ were used [Zanke, 1982]. The lower sediment input is used in case of a given range (Figure 17).

Region	Area [$\times 10^6 \text{ km}^2$]	Sediment input [$t/\text{km}^2 \text{ yr}$]	Reference
northern North Atlantic	n. a.	3.156×10^{-2}	<i>Honjo, 1990 / Miller et al., 1977</i>
East-Greenland	n. a.	6.96×10^{-2}	<i>Enos, 1991</i>
Iceland	n. a.	$6.1 \times 10^{-2} - 1.085 \times 10^{-1}$	<i>Enos, 1991</i>
Norwegian coast	n. a.	$6.06 \times 10^{-2} - 6.93 \times 10^{-2}$	<i>Enos, 1991</i>
Elbe	0.13	84	<i>Milliman / Syvitski, 1992</i>
Weser	0.038	33	<i>Milliman / Syvitski, 1992</i>
Seine	0.065	114.2	<i>Milliman / Syvitski, 1992</i>
Loire	0.155	150	<i>Milliman / Syvitski, 1992</i>
southern England	n. a.	< 10	<i>Einsele, 1992</i>

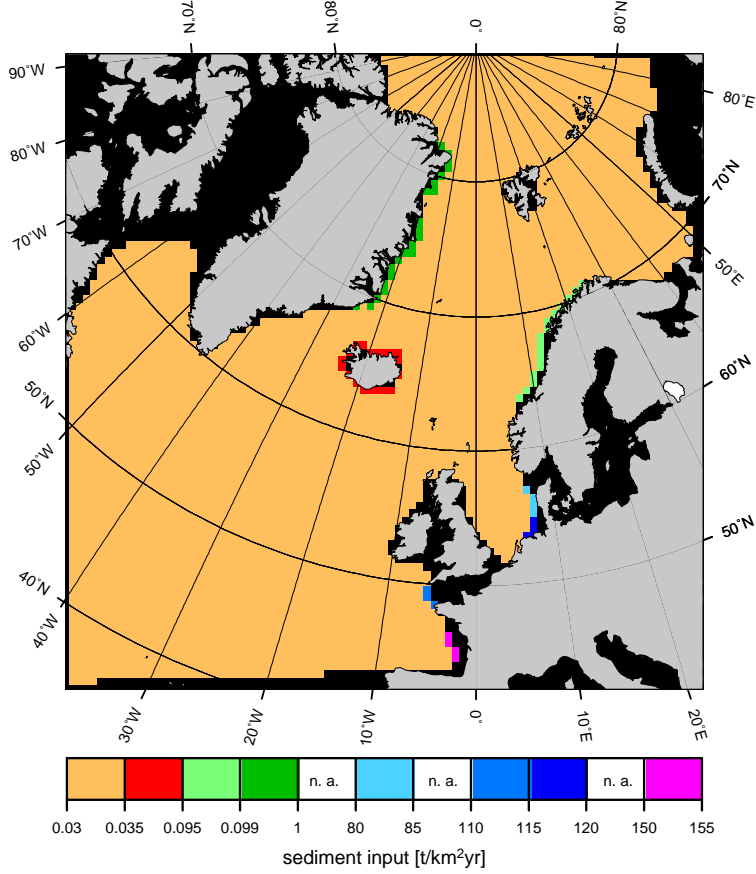


Figure 17: Sediment sources prescribed as initial conditions (see Table 1). In case of conversions the sediment density $\rho_s = 2.6 \text{ g/cm}^3$ and the porosity $\gamma = 0.75$ were used [Zanke, 1982].

All of our experiments were initialized with the same parameters (settling velocity of $0.05 \text{ cm s}^{-1} = 43.2 \text{ m d}^{-1}$ [Shanks and Trent, 1980], density of sediment, grain size, and sedimentological grain diameter, form factor of sediment particles, and sediment porosity). In both experiments using the sedimentation model SEDLOB, we employed reduced critical velocities to initiate bed load $v_{cm,b}$ and suspension load $v_{cm,s}$. These were set to 0.002 cm s^{-1} and 0.02 cm s^{-1} respectively. In control runs we figured out that a reduction is necessary to get realistic transports in the bottom layer in the deeper ocean basins. With these altered initial conditions the model was capable of eroding sediment when the critical velocities were weaker than the velocities predicted by the OGCM. Consequently, it produces more patchy sediment structures. Both simulations were run over 500 years. Unlike the OGCM, it is not possible to run SEDLOB into a steady state condition. The forward time integration lead to continuous changes of the bottom slope and therefore the critical velocities for initiating bed load and suspension load also changed. This is equivalent to the sediment

availability which influences the maximum possible sediment concentration and transport in the fluid depending on the bottom slope inclination.

Results and Discussion

In the first SEDLOB experiment (E1) only the eolian sediment input from the atmosphere was taken into account (Figure 18a), whereas the second experiment (E2) added lateral sediment input from rivers and icebergs (Figure 17). The sedimentation rate is given in centimeters/1000 years. The locations of the main sediment drifts south of Iceland and south of Greenland are well reproduced [Bohrmann *et al.*, 1990; McCave and Tucholke, 1986]. However, the sedimentation rate is affected by the chosen distribution of the sediment supply. Both experiments show similar sedimentation patterns. They are mostly formed along the margins of the current axes. Differences can be found especially in regions where strongly selective river sediment input was added to the eolian sediment portion (e.g., in the Bay of Biscay, or in the eastern German Bight). Higher sedimentation rates occur also in the coastal areas, where currents run approximately parallel to the shore line. Here the water takes up a „relatively low“ sediment input and accumulates it while moving along the coast. Whenever coastal currents depart from the coast to the open sea, the speed of the current slows down. Sediment transport capacity decreases and sediments are deposited. This phenomenon is found especially on continental slopes with a downward steepening bottom topography. An example of this is found off South–East Greenland where the East–Greenland Current flows through the Denmark Strait into the deep Irminger Basin. As well, this feature can be found to the south–southeast of Iceland and to the west of Lofoten, where the Norwegian Coastal Current turns to the east into the Norwegian Sea. Sediments are also deposited at higher rates on the Vøring Plateau. The higher sedimentation rates of these shelf–areas are in good agreement with the recorded sedimentation rates from sediment cores.

The high sedimentation rate area in the northeasternmost part of the model area has a different origin. In both experiments, E1 (Figure 18a) and E2 (Figure 18b), the high sedimentation rates are due to the closed northern boundary and are therefore an artifact. Figure 19 and Figure 20 show the artificial „return flow“ east of Franz Josef Land (northeastern Barents Sea). In Figure (15a, b), Figure 19, and Figure 20 the sediment

transport from North Scandinavia by the strong North Cape Current through the Barents Sea can be clearly seen. The southern model boundaries are responsible for artificially low sedimentation rate areas south of 50°N. In the OGCM the inflow of the North Atlantic Current is maintained using a southern sponge layer where the numerical solution is restored to modern climatology in a narrow latitudinal belt near this latitude [Seidov *et al.*, 1996]. Because of the lack of information concerning the sediment transport in the water column across these walls, we cannot arrive at reasonable sediment dynamics in this location.

The high sediment input to the English and French shelf-areas from southern England and the French rivers Seine and Loire is responsible for the observed high sedimentation rates [Einsele, 1992]. Contrarily, the runoff from the German rivers Elbe and Weser is not limited to the river mouths. Although most of the sediment is deposited in the eastern German Bight, some is still transported to and deposited in the Norwegian Channel and on the southern Vøring Plateau (63°N, 5° – 7°W).

A comparison of the experiments E1 and E2 shows that small local changes in the sediment supply can affect the sediment distribution in remote areas. These changes are clearly seen in the transport through gateways and along vertical cross-sections. Figure 21a (Experiment E1) and Figure 21b (Experiment E2) show the transport in the water column and at the bottom in tons/km²yr. Both experiments indicate that most of the sediment transport occurs in the bottom layer. The transport through the cross-section increases with the increase of additional lateral sediment supply everywhere except for two locations. Whether the decrease found between Svalbard and Franz Josef Land is a real feature or an artifact created by the closed northern boundary cannot be answered with this model. In Experiment E2 (Figure 21b), the bottom transport over the Iceland–Faeroe–Ridge changes from a southward sediment transport (Figure 21a) to a northward transport. In this region, the currents are generally parallel to the Iceland–Faeroe–Ridge (Figure 15b; 20). In a set of several supplementary experiments we discovered that a small shift of this cross-section to the north, or to the south resulted in a change of the transport direction.

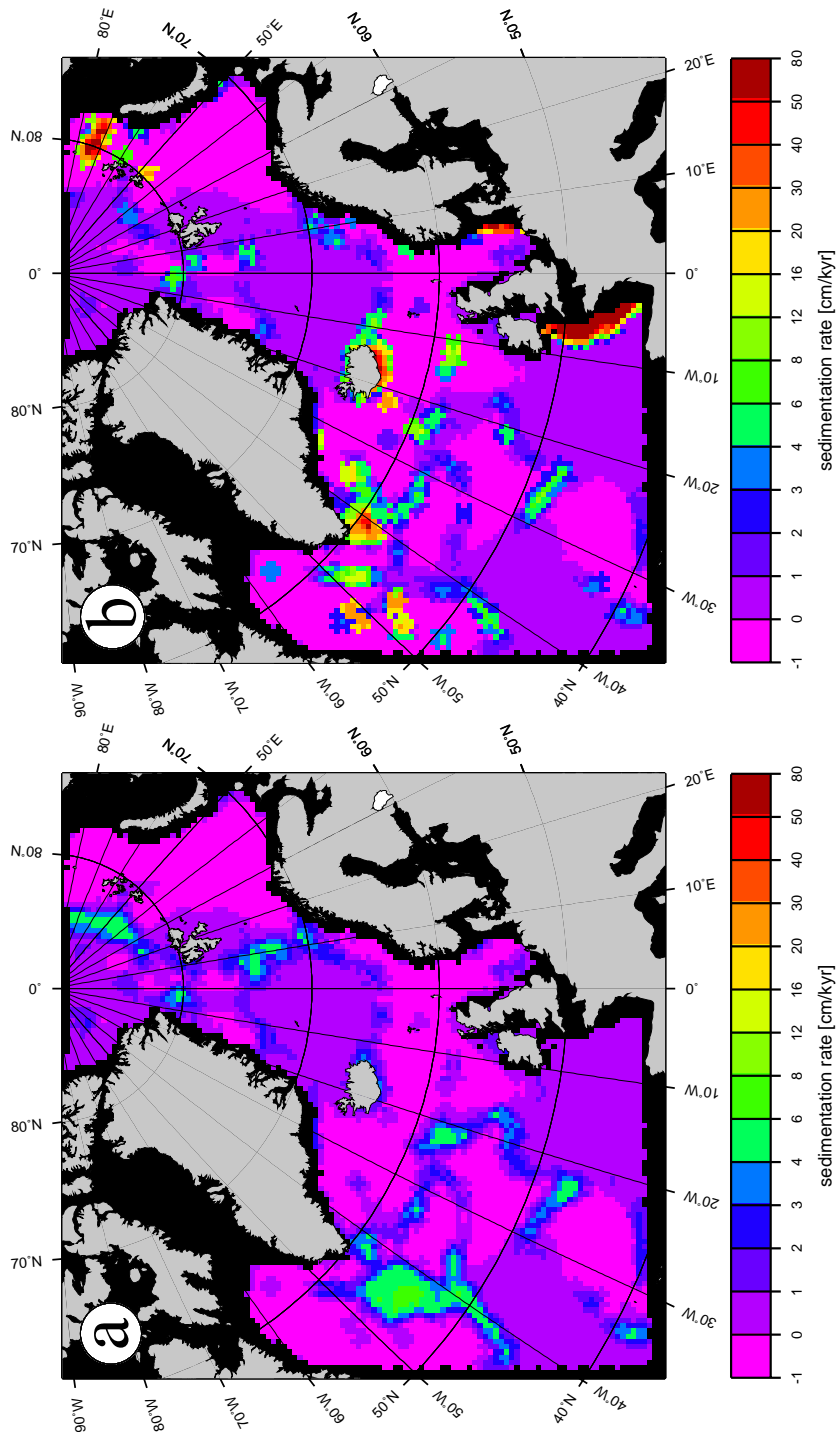


Figure 18: Present-day sedimentation rate (centimeters/1000 years). (a) Experiment E1: Only the eolian sediment input from the atmosphere ($1 \times 10^{-13} \text{ g/cm}^2 \text{ s} \approx 0.0864 \text{ mg/cm}^2 \text{ d}$) is considered [Honjo, 1990; Miller et al., 1977]. The critical velocities for starting of bed load $v_{cm,b}$ and for beginning of suspension load $v_{cm,s}$ are set to 0.002 cm s^{-1} respectively 0.02 cm s^{-1} . (b) Experiment E2: Additional sediment sources are applied; see Table 1 and Figure 17.

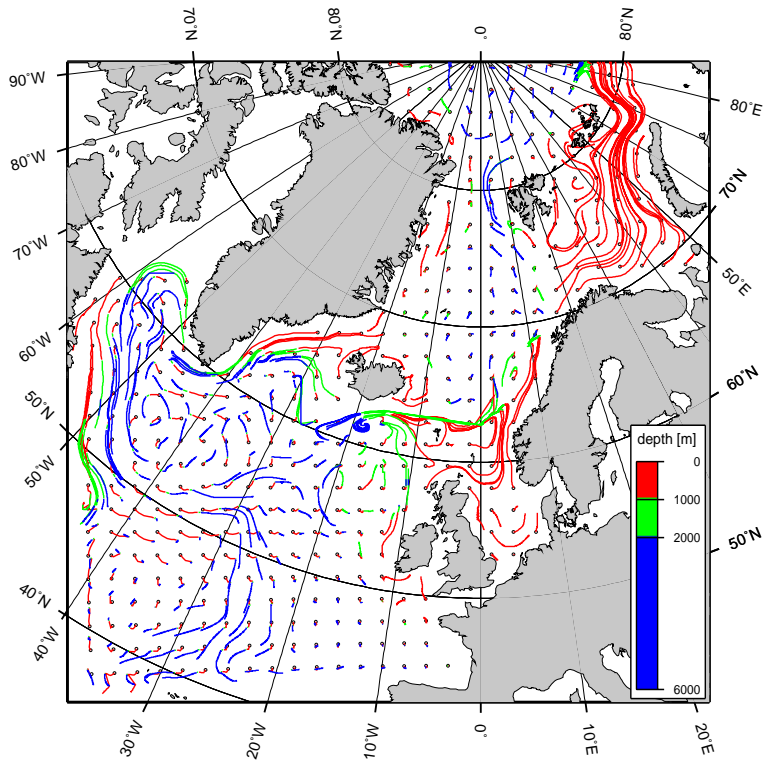


Figure 19: Trajectories of 495 Lagrangian particles for the 3-D water motion tracing during two years. The small circles show the location where the particles were launched. The settling velocity is 0.05 cm/s. The depth is indicated by colors from the color palette.

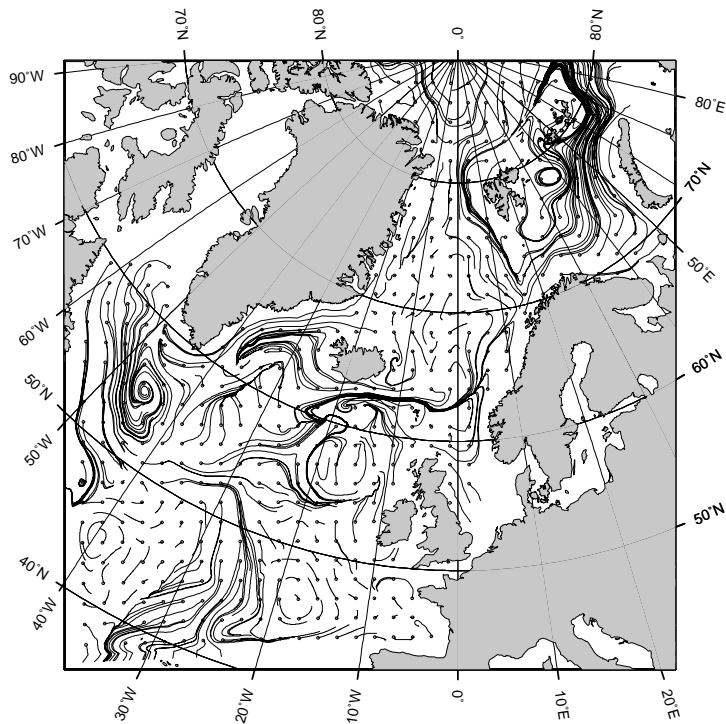
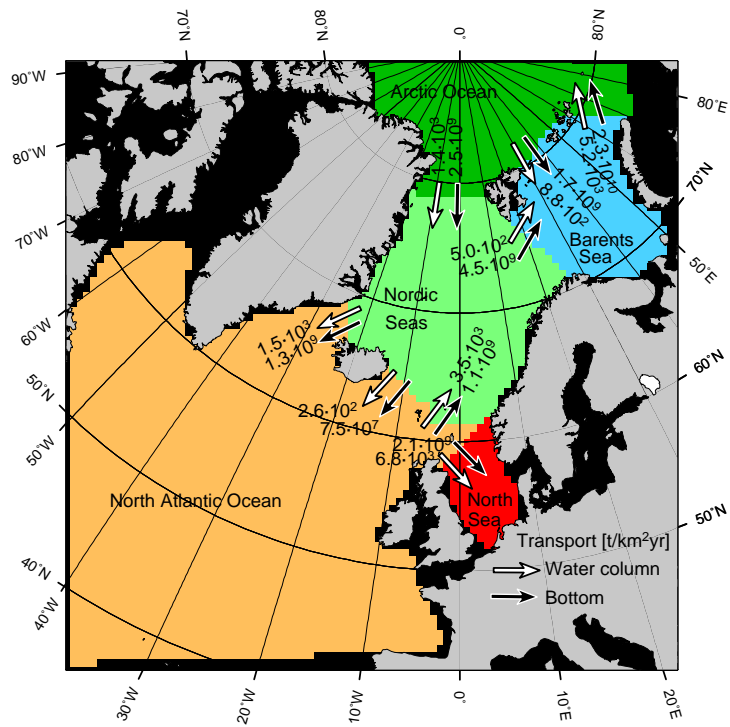


Figure 20: Trajectories of 495 Lagrangian particles started in the bottom layer. The small circles show the location where the particles were launched. This experiment was run over 10 years.

a)



b)

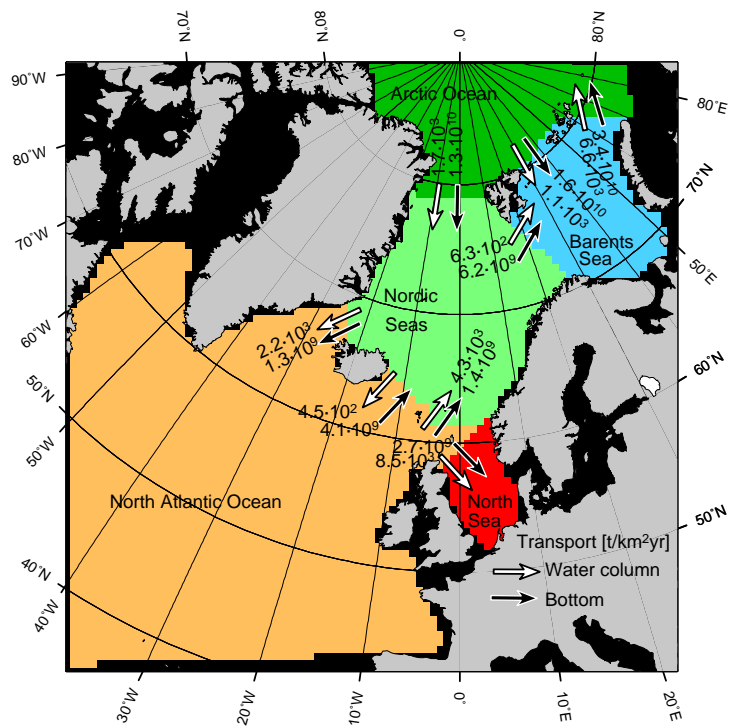


Figure 21: Calculated transport rates for the three-dimensional water column and for the bottom layer: experiment E1 (a) and experiment E2 (b).

Conclusions

Integrated numerical models of oceanic circulation, sedimentation, and tracing water volumes lead to a better understanding of the complexity of interactions in the climatically forced ocean–sediment system. Two 3–D numerical models, SEDLOB and PATLOB, were developed to reconstruct the sedimentary history of the North Atlantic. Both models consist of a 3–D submodel for the water column and a 2–D bottom layer to model the specific features of near–bottom process motion. The models were tested using different horizontal and vertical resolutions in the North and northeastern Atlantic. High resolution experiments aimed at the simulation of detailed features of sediment flux through gateways and cross–sections were discussed. The models are initialized using the output of an OGCM and different sediment sources. We supplied material by vertical eolian input from the atmosphere and from lateral sediment input by rivers and ice. In all experiments, the critical velocities for movement of bed load and suspension load were reduced to arrive at more realistic transports at the bottom in ocean basins. The employed polynomial equations for the sediment transport and the critical velocities were modified by an empirical function to introduce the dependence on bottom slope.

The simulated sediment distribution fits well the observed location of the main sediment drifts south of Iceland and Greenland. Additional lateral sediment input did not change the regional distribution of the high sedimentation areas. However, these changes in the input did affect the sedimentation rates and the transport through the cross–sections. The increased sediment transport was predicted by the models both in the main body of water, and within the bottom layer. In comparison to the distribution within the water column the transport in the bottom layer showed a weaker response to the addition of lateral sediment sources. The calculation of cross–section transport is a valuable tool in mass balancing through oceanic gateways.

In both experiments with SEDLOB we found that coastal downward currents lead to reduced bottom current velocities and therefore to a reduced sediment transport capacity. This effect is especially pronounced in the areas of steep bottom gradients.

Finally, we want to emphasize that both models may be coupled to any OGCM which provides the adequate input data fields of temperature, salinity, velocity and convection depth.

Acknowledgments

This research was supported by the Deutsche Forschungsgemeinschaft (DFG) and SFB313 of Kiel University. We appreciate Avan Antia's und Derek Dreger's help on correcting our English. We thank Johannes Wendebourg for his very useful comments and suggestions which led to improvement of the manuscript.

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Appendix

Symbols and definitions		
c_x, c_y, c_z	= Courant–numbers	—
C	= sediment concentration in the fluid	g/cm ³
C_n	= sediment concentration at time step n	g/cm ³
d	= grain size	cm
$dx_{i,j}, dy_{i,j}, dz_k$	= grid spacing	cm
D^*	= sedimentological grain diameter $\left(\frac{\rho'g}{v^2}\right)^{\frac{1}{3}} d$	—
FF	= form factor	—
g	= gravitational acceleration	g cm/s ²
h_{sed}	= change of bottom topography due to erosion, transport, and deposition	cm
H	= water depth	cm
i, j, k	= zonal, meridional, and vertical grid indices	—
n	= time step, $n=1, 2, 3, \dots$	—
p, p_{surf}	= pressure, surface pressure	g/cm s
q	= total sediment transport	cm ³ /cm s
q_B, q_S	= bed load and suspension load transport	cm ³ /cm s
Q	= sediment source term	cm ³ /cm s ²
$r_{x,n}, r_{y,n}, r_{z,n}$	= zonal, meridional, and vertical location inside of the numerical grid at time step n	cm
\vec{r}	= location of a particle	cm
t, t_n, t_0	= time, time at time step n , starting time	s
T	= temperature	°C
S	= salinity	‰
u, v, w	= zonal, meridional, and vertical velocity components	cm/s
u_{bot}, v_{bot}	= reduced zonal and meridional bottom velocity components	cm/s
\vec{v}, \vec{v}_{bot}	= three–dimensional and two–dimensional velocity vector	cm/s
w_s, w_g	= settling velocity, total vertical velocity	cm/
x, y, z	= zonal, meridional, and vertical component of the grid	cm

Δt	= time step	s
$\Delta x, \Delta y, \Delta z$	= zonal, meridional, and vertical grid spacing	cm
γ	= sediment porosity	—
∇, ∇_H	= three- and two-dimensional Laplacian operator	cm^{-1}
μ	= dynamic viscosity of sea water	g/cm s
ν	= kinematic viscosity of sea water	cm^2/s
ϕ	= bottom slope	°
ρ_F, ρ_S	= density of sea water and sediment	g/cm^3
ρ'	relative density $\frac{\rho_S - \rho_F}{\rho_F}$	—