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Choice of an Advection Scheme for Biogeochemical Models

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Abstract. Five advection schemes are compared and evaluated in the context of biogeochemical modeling. Using three schemes of comparable quality that have been used in recent biogeochemical models, we found that new production estimates vary by as much as 30%. Test experiments are presented that explain the large discrepancies in terms of the different types of numerical errors inherent to each scheme. One scheme is suggested for eddy-resolving models and another one for coarse resolution models.

1. Introduction

Net CO_2 uptake by phytoplankton can only occur when limiting nutrients, such as nitrate, are brought up into the well-lit upper ocean. The estimate of this uptake (or new production, NP) has motivated many numerical studies in the last ten years, using Ocean General Circulation Models (OGCMs) in conjunction with biogeochemical models. Nitrate is abundant at depth, and supplied to the euphotic layer by physical transport mechanisms such as convective mixing and vertical advection. Biogeochemical tracers are positive fields, often close to zero, and presenting sharp gradients in both the vertical and horizontal directions. Modeling their advection is a difficult task, as it requires schemes that preserve these gradients.

The earliest models of oceanic biogeochemical cycles have either used first order upstream differencing (UPS) [*Sarmiento et al.,* 1993] or second order centered differencing (CEN) [*Najar et al.,* 1992] for advecting biogeochemical tracers. Oschlies and Garçon [1999] and Oschlies [2000] have shown that neither of these scheme was satisfactory for this task. Indeed, CEN is non-diffusive but very dispersive and non-monotonic. Its use generates both negative tracer concentrations and unrealistic tracer accumulation. On the other hand, UPS is positive and monotonic but very diffusive. As a consequence the effective vertical nutrient transport within the euphotic layer is highly overestimated due to undesirable transport by numerical diffusion. In a similar problem involving age tracers, *Hecht et al.* [1998] drew the same conclusions, and also showed that flux correction is required to avoid unphysical results.

Recent developments of biogeochemical models reveal a sudden awareness of the importance of the numerical treatment of advection. More sophisticated transport algorithms have been incorporated and are now commonplace. Of these, the Multidimensional Positive Definite Advection Transport Algorithm (MPDATA) of *Smolarkiewicz* [1984], the Flux Corrected Transport (FCT) family of schemes [*Boris and Book,* 1976; *Zalesak*, 1979], and the Monotonic Upstream centered Scheme for Conservation Laws (MUSCL) [*Van Leer,* 1977; *Hourdin and Armengaud,* 1999] are among the most commonly used.

Our principal intention for this paper is to compare and evaluate MPDATA, FCT and MUSCL in the context of biogeochemical modeling. For complete comparison, results with CEN and UPS are also presented. The evaluation is based on three criteria : creation of unphysical values, diffusion and dispersion. The biogeochemical problem we examine is that of an oligotrophic region perturbed by the fertilizing effect of a growing baroclinic wave [see *Lévy et al.,* 2001 for more details]. This situation is encountered in subtropical gyres. It enables a focus on the NP enhancement due essentially to advection, without the complications of convection that would occur in basin-scale simulations.

2. Model and Advection schemes

The biogeochemical model consists of 6 tracers, expressed in terms of their nitrogen content, namely nitrate, ammonium, phytoplankton, zooplankton, detritus and dissolved organic matter [*Lévy et al.,* 2001]. Tracers are advected by the flow field, and are also subject to specific biogeochemical source/sink fluxes. Typical time scales of nitrate uptake vary from one day at the surface to ten days at 100m. The tracer equations are solved on-line with the OPA OGCM [*Madec et al.,* 1998; *Foujols et al.,* 2000]. The dynamical model provides the velocity field, and there is no feedback from the tracers on the flow.

Advection is formulated in terms of the divergence of the advective flux across the faces of the grid cells. This formulation yields conservative schemes. The schemes differ in their estimation of the flux. UPS approximates this flux as the product of the normal velocity at the cell face, the area of the cell face and the tracer concentration in the upstream cell; while in CEN, the tracer value at the cell face is approximated by the mean of the upstream and downstream cell values. The MPDATA scheme is based on UPS. By defining so called antidiffusive velocities, a scheme with three iterations is constructed that counteracts the diffusive effect of UPS. MPDATA is positive but not monotonic. The MUSCL scheme consists of a linear extrapolation of the tracer concentration to the cell face, which enables exact computation of the flux. The extrapolation is based on the upstream value, and the slope is estimated by finite differences. FCT is essentially a two-step method; CEN and UPS are combined with an antidiffusion operator to produce a positive intermediate order scheme. Flux limiters are applied in MUSCL and FCT in order to insure monotonicity. In MUSCL, this is done by limiting the slope, and in FCT by limiting the antidiffusion flux.

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Table 1. Averaged 0-150m NP during the entire duration of the experiments (mmoleN m^{-2} (d)$^{-1}$) and the local NP maximum value (mmoleN m^{-3} d^{-1}).

	Average	Maximum
CEN	0.35	0.34
UPS	0.72	0.15
MUSCL	0.41	0.12
FCT	0.32	0.14
MPDATA	0.48	0.13

3. Numerical experiments

An unstable zonal front in a periodic channel is allowed to evolve freely. The width of the channel is equal to one wavelength of the most unstable baroclinic wave (150 km), the meridional extent is 500 km, and the horizontal resolution is 6 km. There are 30 vertical layers covering 4000 m in depth, with 10 layers concentrated in the first 150 m (a typical resolution for current OGCMs). Simulations last 50 days with a time step of 6 minutes. The evolution of the front can be described as a succesion of three phases (Fig. 1). During the first 15 days, the front meanders, and the amplitude of the meanders increases with time. This phase corresponds to the linear growth of the baroclinic instability. Intense vertical velocities (up to 20 md^{-1}) are associated with this meandering, with upwelling in the northward branch and downwelling in the southward branch. Between days 15 and 30, non-linear terms become more important and an anticyclonic eddy forms in the northern part of the front. Vertical velocities are important both within the eddy and at the front (up to 10 md^{-1}). The w-pattern associated with the eddy has a quadripolar structure due to the curvature variation of the flow. During the last 20 days, the eddy detaches from the front and decays, with associated decaying vertical velocities.

Five biogeochemical experiments (BIO) are performed, which only differ in the advection scheme used for the transport of biogeochemical tracers. They are referred as the UPS, CEN, FCT, MUSCL and MPDATA experiments. Vertical mixing is parametrized in the form of a diffusion term, with a constant coefficient of $10^{-5} m^2 s^{-2}$, which corresponds to a stratified mixed-layer. The biogeochemical system is initially oligotrophic and at steady state. Nitrate is depleted in the first 100m.

An intermediate series of tracer experiments (TR), where biogeochemical source/sink terms are omitted, will serve as a basis to compare the performance of the various schemes. In these TR experiments, we consider a nitrate-like passive tracer whose initial concentration is 0 above 100m and 1 below.

4. Results of the TR experiments

Because there is no source or sink in the TR experiments, the physically acceptable tracer concentrations are between 0 and 1. This requirement is fulfilled with UPS, MUSCL and FCT which are monotonic schemes. The two schemes that can produce overshoots (CEN and MPDATA) do so. The overshoots are more frequent (8% versus 6% of the total grid cells, among 50 daily samples) and more pronounced (maximum cell concentration of +3.0 versus +1.5) with CEN than with MPDATA. Negative concentrations are found with CEN, which is the only non-positive scheme. They are found in as many as 30% of the grid cells in the top 100m.

Diffusion in the schemes is diagnosed from the time evolution of the tracer total variance (Fig. 2a). The highest loss of variance is obtained with UPS. Variance is on the contrary almost conserved using CEN, which is not diffusive. The loss of variance obtained with FCT, MUSCL or MPDATA falls between these two extremes, and are of similar magnitude. It appears nevertheless that among the three MUSCL is the most diffusive and FCT the least.

Analysis of the variance spectra of the tracer concentration enables a classification of the schemes in terms of their dispersion errors (Fig. 2b). These spectra exhibit a negative slope between 90 and 30 km wavelength, in agreement with the theory of the direct cascade. At wavelengths smaller than 30 km, the slope breaks and the variance is larger than that allowed by the cascade. This unusual form of the spectra reveals spurious accumulation of variance at small scales, associated with the dispersion errors of the transport scheme. On this basis, the dispersion errors of a scheme can be quantified by the amount of variance at small wavelengths. In between CEN, which is extremely dispersive, and UPS which is not, FCT is the most dispersive and MUSCL the least.

5. Results of the BIO experiments

The time evolution of NP is similar for all experiments (Fig. 2c). During the first phase (days 1 to 15), the jet instability triggers important vertical nitrate transport above 100 m, causing an increase in NP. During the second phase (days 15 to 30), NP reaches its maximum amplitude, both within the anticyclonic eddy and at the front, i.e. where vertical velocities are important. During the third phase (days

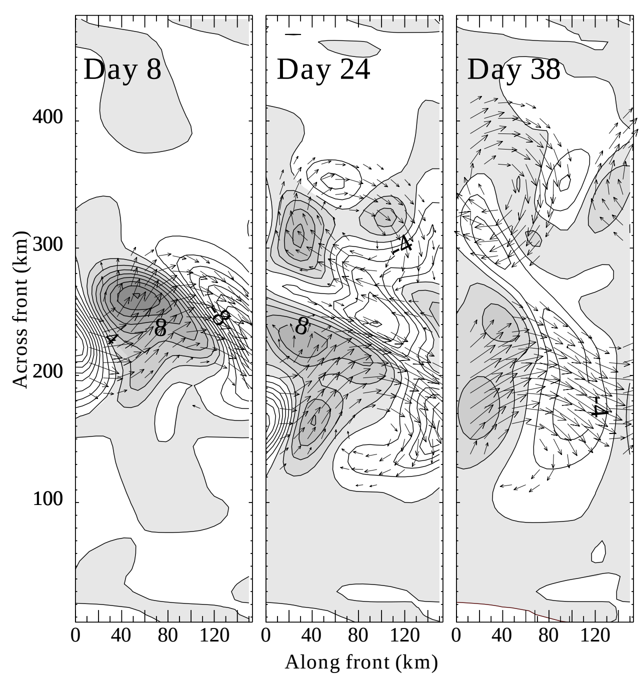

Figure 1. Time series of the horizontal (arrows) velocity at the surface and of the vertical velocity at 100 m (contours, with grey shading for upwelling). The contour interval for w is 2 m d^{-1} and the maximum horizontal velocity is 0.8 m s^{-1}.

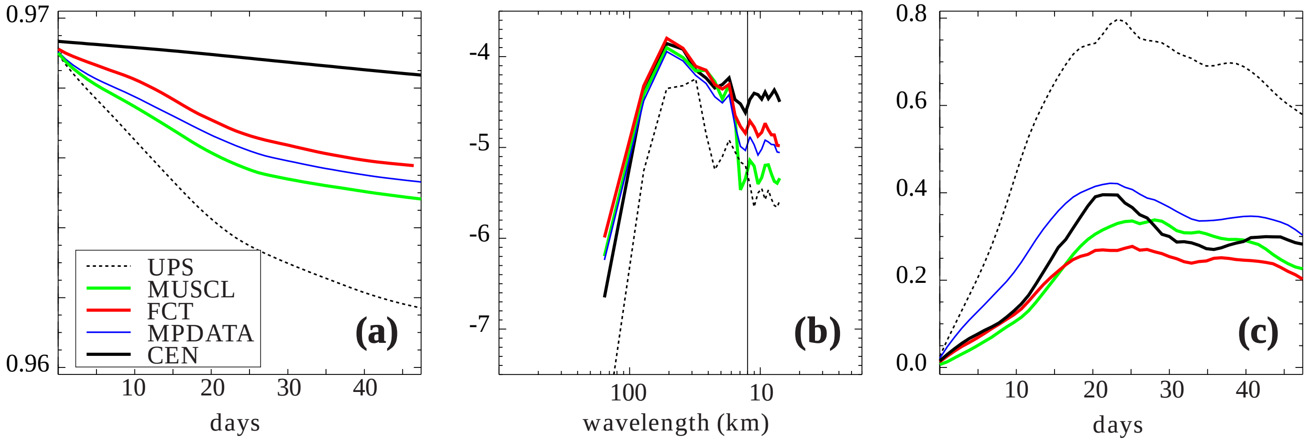

Figure 2. a/ Time evolution of the passive tracer total variance in the TR experiments. b/Variance spectra of the passive tracer field, integrated over the first 100m of the water column at day 50, in the TR experiments. c/ Time evolution of NP averaged over the entire domain and integrated over the first 150m, in the BIO experiments (in mmoleN m^{-2} $(d)^{-1}$).

30 to 45), NP slowly decreases, in response to the decreasing vertical velocities.

The experiments differ in the magnitude of simulated NP. The largest NP budget is obtained in UPS, followed by, in decreasing order, MPDATA, MUSCL, CEN and FCT (Fig. 2c and Table 1). Local NP maxima fall in a different order (Table 1): the smallest extremum values are obtained in MUSCL, followed by, in increasing order, MPDATA, FCT, UPS and CEN. Quantitatively, in UPS the NP budget is more than 100% higher than in the other experiments. This result is similar to that obtained by *Oschlies and Garçon* [1998], who compared model estimates of the annual North Atlantic production budget, using UPS and FCT. Excluding UPS, differences in NP budgets range between 10 and 30%. This range is robust over a variety of modifications to the basic model configuration: the addition of laplacian horizontal diffusion, enhancement of the vertical velocities (achieved following *Lévy et al.,* [2001], by an increasing the horizontal resolution), and increase/decrease of the phytoplankton maximum growth rate.

6. Discussion

The high sensitivity of NP estimates to the choice of advection scheme is clearly related to the difficulty of accurately computing the vertical nitrate transport. In most oceanic regions (as here), the vertical distribution of nitrate is characterized by a strong vertical gradient, located at the bottom of the euphotic layer. Upward advection of this gradient provides nitrate to the euphotic layer and enables NP to occur. When the numerical scheme used for the vertical advection of nitrate is diffusive, the amount of nitrate brought into the euphotic layer and thus the NP are overestimated. With a dispersive scheme, unrealistic nitrate accumulations at small scales yields an overestimation of NP in restricted small-scale areas, at the expense of larger scales. Closely related, when a non-monotonic scheme is used, undesirable under- and over-shoots are created. Consequently, NP is overestimated in regions of over-shoots, but underestimated in regions of under-shoots. This leads to the creation of unrealistic local NP extrema and consequently to an erroneous global NP budget.

The results of Table 1 can be rationalized in terms of these considerations. UPS and CEN represent two extremes, each one minimizing the effect of one kind of numerical error (i.e. diffusion versus dispersion and non-monotonicity) at the expense of the other. The large value of the global NP budget in UPS is due to diffusion, and is therefore an overestimation of the *true* solution. In CEN, the high local NP values are due to dispersion. In the other experiments (MPDATA, MUSCL and FCT), the solution is perturbed by a mixture of the different types of numerical errors. Among FCT and MUSCL, the higher local NP values in FCT and the higher global NP budget in MUSCL agree with the result established with the TR experiments, that the use of the FCT scheme generates more dispersion errors but less diffusion errors than the use of the MUSCL scheme. Between MPDATA and MUSCL, the non-monotonicity of MPDATA explains the larger local NP values. The global NP budget is also higher in MPDATA, suggesting that the cumulative effect of the large local values overshadows the effect of higher diffusion in MUSCL.

7. Conclusion

This work provides additional evidence that CEN and UPS are particularly poor options for biogeochemical modeling, and that the use of either FCT, MUSCL or MPDATA yields significant improvement. However, this study also reveals that numerical NP estimates using these three schemes vary by 10% to 30%. These large discrepancies come from different compromises made by each scheme over different types of numerical errors (diffusion, dispersion and non-monotonicity). The result is worth reporting as the magnitude of this sensitivity is comparable to other uncertainties in biogeochemical models, such as the estimation of biological parameters.

Regarding the question of which scheme should be used for biogeochemical modeling, we suggest a rejection of MPDATA, since it produces a non-negligible amount of unphysical values. While waiting for monotonic advection schemes that would minimize both diffusion and dispersion errors, the choice between FCT and MUSCL is more subtle. The MUSCL scheme is better in resolving the small scales, and is therefore a preferable choice for mesoscale and sub-mesoscale models. For coarse-resolution models, FCT appears to be a better option as it minimizes systematic NP overestimation through numerical diffusion.

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