The sensitivity of a 3D biogeochemical-like tracer model to advection schemes

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\begin{abstract}
Multidimensional Positive Definite Advection Transport Algorithm (MPDATA) and Monotonic Upstream Schemes for Conservation Laws (MUSCL) are compared and evaluated in a biogeochemical-like tracer model. Based on the MUSCL scheme, an adapted scheme for \( \sigma \)-coordinate models (MUSCL\_VD) is presented. These schemes are first implemented in idealized experiments configured for a closed channel with and without a seamount, and conservation is confirmed. MUSCL\_VD and MUSCL generate the same results in the flat bottom case, while MUSCL\_VD is the only scheme that avoids unphysical values in the seamount experiments. When implemented in a three-dimensional model of the Gulf of Maine (GoM) with realistic topography and real-time forcing, the modeled distributions of an inert tracer concentration are sensitive to the advection schemes. The experiment with MUSCL shows persistent overshoots. MPDATA and MUSCL\_VD produce similar spatial distributions and seasonal cycles with MUSCL\_VD being slightly more diffusive in the horizontal and less so in the vertical. These two schemes are about equally efficient in computation.
\end{abstract}

1. Introduction

Advection plays an important role in determining distributions of biogeochemical elements in marine ecosystem models. Even though the pure advection equation seems simple in its mathematical form, it highlights many aspects of difficulties in the numerical treatment. Designing or choosing a scheme (such as the center difference, forward or backward scheme), one needs to look at accuracy (both the amplitude and the phase), stability, diffusion, dispersion, computational complexity, and conservation properties. Because of its simplicity and computational efficiency, the center difference scheme is the most popular scheme for solving partial differential equations (PDEs). Although it is free of numerical diffusion, the center difference scheme does not guarantee non-negative values for the transported constituents. This is problematic in marine ecosystem models as all biogeochemical state variables are scalars and have to be positive semi-definite at all times. On the other hand, the upstream scheme is the simplest first-order advection scheme that guarantees positive values, but it is often too diffusive. Finite difference discretizations of second or higher order accuracy for solving PDEs might produce oscillations and negative values of a scalar due to dispersive ripples (Smolarkiewicz, 1984). Over and undershoots caused by the advection scheme can be reduced by adding additional mixing but excessive mixing tends to reduce gradients in property and element distributions.

Experience in the modeling community strongly indicates that biogeochemical simulations require advection schemes with better numerical qualities. To overcome the implicit dispersion in the center difference scheme and the diffusion in the upstream scheme, Smolarkiewicz (1984) constructed a positive definite scheme, which has evolved to become the Multidimensionally Positive Definite Advection Transport Algorithm (MPDATA). MPDATA employs an iterative method to reduce excessive diffusion by calculating an anti-diffusive velocity that can be derived analytically from the truncation error of the upstream advection scheme. MPDATA is known to be conservative, fully multidimensional, and computationally efficient. According to Smolarkiewicz and Grabowski (1990) and Smolarkiewicz and Szmelter (2005), MPDATA is more computationally efficient than other positive definite schemes; yet it maintains the properties of upward differencing such as the strict preservation of the sign of the transported field and it has a relatively small phase-error. Monotonic Upstream Scheme for Conservation Laws (MUSCL) (van Leer, 1977, 1979) is another popular positive definite advection scheme for scalar simulations because the scheme does not generate spurious oscillations; hence the positive-definite property is automatically maintained. Lévy et al. (2001) suggested the MUSCL is the best choice among center difference, upstream, MUSCL, and MPDATA for mesoscale and sub-mesoscale biogeochemical models while MPDATA is rejected because of the occurrence of non-physical values.
Studies aimed at examining advection schemes often focus on test cases in idealized ocean basins. In Lévy et al. (2001), the idealized rectangular channel had a constant depth of 4000 m, and the runs lasted only 50 days. In this study three schemes are compared:

1. a generalized form of MUSCL derived by Lin et al. (1994),
2. a modified MUSCL for variable depth, and
3. the second-order MPDATA with different time resolutions.

These are compared not only in idealized experiments but also in a biogeochemical-like tracer model for the Gulf of Maine (GoM) to better understand how the advection schemes impact an inert tracer in the presence of realistic, complex topography and apparent seasonal and inter-annual forcing. MPDATA and MUSCL are chosen because of their relative simplicity and their known ability to work with mode-split treatments that are commonly adopted in free-surface ocean models such as the Princeton Ocean Model (POM) and the Regional Ocean Modeling System (ROMS).

The GoM is a semi-enclosed sea located between Cape Cod and southwestern Nova Scotia. The main connection between the GoM and the North Atlantic is the Northeast Channel, a deep submerged valley separating the elevated Georges and Browns Banks (Fig. 1). Nutrient-rich water from the Atlantic moves into the GoM via the Northeast Channel, and eventually settles in the three deep basins (namely, Jordan, Wilkinson, and Georges Basin) of the Gulf (Townsend, 1998). Physical processes such as advection, mixing and stratification are among the driving mechanisms for large variations of the GoM ecosystem dynamics at seasonal to interannual time scales (Schlitz and Cohen, 1984; Fournier et al., 1984; Townsend, 1998; Petrie and Yeats, 2000; Thomas et al., 2003). This suggests that the GoM, characterized by highly convoluted coastlines and highly variable bathymetry, is well suited for a case study to examine advection schemes in realistic applications.

In this study, an inert tracer is added to a three-dimensional physical–biogeochemical model of the GoM to examine how the modeled concentration varies in experiments with different advection schemes. Our main objective is to compare and evaluate MPDATA and MUSCL in the context of the GoM model. The evaluation is based on three criteria: conservation, dispersion and the creation of non-physical values, and diffusion. The organization of this paper is as follows. The physical–biogeochemical model of the GoM is introduced in Section 2. Reviews of MPDATA and MUSCL are presented in Section 3. Model results from both idealized experiments and the GoM simulations that employ different advection schemes are then evaluated in Section 4. These are followed by a summary and concluding remarks in the final section.

2. The physical–biogeochemical model

The physical model is the Gulf of Maine Ocean Observing System (GoMoOS) nowcast/forecast system (Xue et al., 2005), which has been used to issue 48-h forecasts of physical conditions since January 2002. This study focuses on the period between 2002 and 2006, during which we have consistent open boundary forcing. The biogeochemical model is adapted from the Carbon, Si(OH)4, Nitrogen Ecosystem (CoSINE) model developed by Chai et al. (2002) and Dugdale et al. (2002). The CoSINE model has been used in studies of decadal variability in primary production, nutrient and pCO2 distributions in the Pacific (Chai et al., 2003; Jiang and Chai, 2005), and responses of diatom productivity and biogenic silica export to iron enrichment in the equatorial Pacific (Chai et al., 2007). In this paper, only an inert tracer is analyzed to examine the similarities and differences associated with different advection schemes. This tracer is influenced purely by physical forcing without undergoing any biogeochemical cycle, but it shares the same numerical algorithm as the other biogeochemical state variables.

Considering the time rate of change of a biogeochemical element concentration, the governing equation is given by the following.

$\frac{\partial C}{\partial t} + \text{advection} = \text{diffusion} + \text{SMSc}$

(1)

Here, $\text{SMSc}$ represents the net of source-minus-sink, which is nil for an inert tracer. The analytical formulations of advection and diffusion terms are the same as those for the temperature and salinity in the physical model. Numerically, the advection term for temperature and salinity is approximated by the second-order center difference, while the advection term for biogeochemical elements is approximated by several different schemes discussed in Section 3 below. Diffusion includes both the horizontal diffusion calculated based on the Smagorinsky scheme (1963) and the vertical diffusion calculated based on the second-order turbulence closure of Mellor and Yamada (1982).

Initial concentration of the inert tracer, $C_0$, is prescribed by a piecewise linear profile:

$C_0 = \begin{cases} 0.01Z + 1.0 & \text{for } 0 < Z < 350 \text{ m} \\ 4.5 & \text{for } Z \geq 350 \text{ m} \end{cases}$

(2)

i.e., the concentration increases from the lowest value of 1.0 mmol m$^{-3}$ at the surface to the highest value of 4.5 mmol m$^{-3}$ at 350 m and is set at 4.5 mmol m$^{-3}$ below 350 m. Upstream advection is prescribed at the open boundary for the inert tracer, such that for inflows the exterior concentration that has the values as prescribed.
by the initial profile (Eq. (2)) is transported to the boundary, whereas for outflows the modeled concentration at the neighboring interior grid is transported to the boundary. In addition, a sponge layer of 10-grid cells is imposed along the open boundaries to restore the inert tracer concentration to the initial distribution (Eq. (2)), and the values at levels below 350 m depth are fixed at 4.5 mmol m\(^{-3}\). The sponge layer is implemented for the benefit of biogeochemically active nutrients, but it is also applied to the inert tracer for a consistent numerical treatment. Zero flux is prescribed at land boundaries except at the head of the rivers, where zero concentration is specified for the discharged river water.

### 3. Advection schemes

The GoMOOS nowcast/forecast system of Xue et al. (2005) is based on the POM. POM belongs to the class of \(\sigma\)-coordinate ocean models, in which the vertical coordinate is scaled to the height of the water column. In the original POM code, the advection term is approximated using the center difference scheme with second-order accuracy in both space and time (Mellor, 1998). In this study, advection terms in the physical model still use the center difference scheme, whereas advection schemes based on MPDATA and MUSCL are utilized for the biogeochemical elements including the inert tracer.

MPDATA is positive definite, and the accuracy can be increased via an iterative procedure: the first pass in MPDATA is a simple upstream differencing, which is positive definite with first-order accuracy; the second pass increases the accuracy of the calculation by estimating and compensating the truncation error of the first pass; additional passes may be used to estimate the residual error of the previous passes and this results in successively more accurate solutions (Smolarkiewicz, 1984; Smolarkiewicz and Margolin, 1998). In the first pass, the physical velocity is used for advecting the tracer. In the second and subsequent passes, the velocity is calculated from the field that is being advected and has no physical significance. These velocities are known as anti-diffusive velocities. Two iterations result in the most basic MPDATA scheme with a second-order accuracy in both time and space. Additional iterations can reduce the error, but the scheme remains to be second-order. In practice, the benefit of more than four iterations is negligibly small and more than two iterations in multidimensional problems could result in deformation of the solution or even instability (Smolarkiewicz, 1984). Using a third-order Taylor series expansion can lead to the positive definite advection algorithm with third-order accuracy for the constant coefficient case (Smolarkiewicz and Margolin, 1998).

In this study, MPDATA is limited to two iterations to achieve second-order accuracy by utilizing the anti-diffusive velocities to counteract the diffusive effect of the upstream scheme (Smolarkiewicz and Grabowski, 1990; Smolarkiewicz and Szmelter, 2005). In contrast to the pseudo velocities of the original MPDATA, the recursive velocities do not necessarily satisfy the Courant–Friedrichs–Lewy (CFL) conditions and must be appropriately bounded to ensure stability (Margolin and Smolarkiewicz, 1998). Therefore, we have tested the second-order MPDATA with different time resolutions. MPDATA\(_{t5}\) and MPDATA\(_{t1}\) represent the second-order MPDATA with a time step of \(5 \Delta t\) and \(\Delta t\), respectively.

### Table 1

<table>
<thead>
<tr>
<th>Experiments</th>
<th>Time step</th>
<th>CPU time s/day</th>
<th>Max</th>
<th>Min</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPDATA(_{t5})</td>
<td>(5 \Delta t)</td>
<td>241.26</td>
<td>30.00</td>
<td>0.0</td>
</tr>
<tr>
<td>MPDATA(_{t1})</td>
<td>(\Delta t)</td>
<td>292.29</td>
<td>11.09</td>
<td>0.0</td>
</tr>
<tr>
<td>MUSCL</td>
<td>(\Delta t)</td>
<td>332.45</td>
<td>29.34</td>
<td>0.0</td>
</tr>
<tr>
<td>MUSCL(_{VD})</td>
<td>(\Delta t)</td>
<td>292.39</td>
<td>6.73</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Here, \(\Delta t = 216\) s, is the internal time step set in the physical model. The main motivation for applying larger time steps to biogeochemical elements is to minimize the computational time. MPDATA\(_{t5}\) saves about 18\% of the time (Table 1). Note this is with a single biogeochemical state variable. Saving in computational time is substantial when the full CoSiNE model with 10 biogeochemical state variables is invoked. One might argue that this practice violates the CFL condition. Surprisingly, problems occur only on Nantucket Shoals, an area that is shallow. This shall be discussed further in Section 4.

Another type of advection scheme tested with the biogeochemical model is based on Lin et al. (1994), which is a second-order variant of the MUSCL scheme initially proposed by van Leer (1977, 1979). The MUSCL scheme linearly extrapolates the tracer concentration to the cell face, which is then used to calculate the flux. Extrapolation is based on the upstream value, and the slope of extrapolation is limited to ensure monotonicity. Several different expressions of limiters were proposed by van Leer (1977, 1979). Lin et al. (1994) derived a generalized form of the second-order van Leer scheme, and applied it to a three-dimensional atmospheric general circulation model to simulate moisture transport. They found that the distinct advantage of the scheme is its ability to transport sharp gradients without producing spurious oscillations and non-physical negative mixing ratios. These findings were confirmed by Lévy et al. (2001) and Christian (2007). When the scheme of Lin et al. (1994) is implemented in the GoM model, it appears to produce surface distributions with small-scale variability closely resembling the bottom topography (see Fig. 7c below). This is likely associated with the particular form of the advection term in the POM,

\[
\frac{\partial (uDC)}{\partial x} + \frac{\partial (vDC)}{\partial y} + \frac{\partial (oC)}{\partial z}.
\]

### Fig. 2

Time series of the domain averaged concentration in an idealized channel with a flat bottom (a) and with a seamount (b). All experiments are forced with the surface wind given by Eq. (8) in the text.
Here, $D$ is the depth of the water column. To compute the fluxes at cell faces, the contributed code posted at the POM website extrapolates the product, $DC$, with the slope being approximated by

$$\Delta D_{i+1/2} = \text{sign}([\Delta D_{i+1/2}]_{avg}) \min \left\{ [\Delta D_{i+1/2}]_{avg}, \right.$$

$$\times 2\text{DIM}(D_{i+1/2}, D_{i+1/2}), 2\text{DIM}(D_{i+1/2}, D_{i+1/2}) \right\}$$

(3)

Here, $\text{sign}()$ is the SIGNUM function, and $\text{DIM}()$ computes the positive difference between two numbers. $i$ is the grid index, and $i + 1/2$ represents half grid to the right. Monotonicity can be guaranteed if the lower and upper limits are set to the following.

$$D_{i+1/2}^{\min} = \min \{D_{i+1/2}, D_{i+1/2}, D_{i+1/2}\}$$

$$D_{i+1/2}^{\max} = \max \{D_{i+1/2}, D_{i+1/2}, D_{i+1/2}\}.$$  

(4a)

(4b)

Note that the constraint in (3) forces the product, $DC$, to be bounded by $D_{i+1/2}^{\min}$ and $D_{i+1/2}^{\max}$. What is actually desired is that the distribution of concentration is bounded by $C_{i+1/2}^{\min}$ and $C_{i+1/2}^{\max}$. In coastal seas...

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**Fig. 3.** Time series of the bottom concentration along the center of the channel at $y = L_y/2$ in the experiments with a flat bottom (a) and with a seamount (b).
where variations in water depth between neighboring grids are much more dramatic than the variations in concentration, Eqs. (4a) and (4b) can result in erroneous distributions in concentration.

To make sure that the bounds are in fact imposed on the concentration, we have modified the contributed code by associating $D_i$ with the velocity components $u$ and $v$ and the limiter is now applied to the variable $C_i$ as in Lin et al. (1994):

$$D_i = \text{DIM}(C_i+1/2; C_i-1/2; C_i+1/2).$$

This modified MUSCL for variable depth is called MUSCL_VD thereafter. All experiments discussed in this paper were timed on a machine with two dual-core Opteron 2.4 GHz CPUs. MPDATA_t1 and MUSCL_VD are comparable in terms of computational efficiency. MUSCL, on the other hand, uses $\sim 14\%$ more time (see Table 1).

4. Numerical results

4.1. Idealized seamount experiments and conservation of the schemes

Before being applied in the GoM simulations, the schemes are tested in an idealized channel with and without a seamount. The channel is 512 km in length ($L_x$) and 320 km in width ($L_y$). A uniform resolution of 8 km is used in the horizontal and there are 21 sigma levels in the vertical. The maximum depth of the domain is 1000 m and a seamount is specified in the middle of the domain with the peak rising to 100 m below the surface as given by the following.

$$h = 1000 \times \left[1 - 0.9 \times e^{-\frac{-16 \times y^2 - y^2}{2 \times 100^2}}\right].$$

Temperature and salinity are set to constant values of 20 °C and 35 PSU while the initial concentration of the inert tracer is prescribed by Eq. (2). In all experiments an oscillatory wind is imposed in the along channel direction, which has an amplitude of 0.1 N m$^{-2}$ and period of 10 days.

$$\tau_l = \tau_0 \sin(\pi y/\eta) \sin(2\pi t/T_0).$$

A cyclic boundary condition is applied at two ends of the channel, which tapes the ends together to form a circular zonal belt. All

![Fig. 4. Time series of the domain-wide maximum concentration of the inert tracer throughout the 5-year integration from 2002 to 2006. (a) MPDATA_t5, (b) MPDATA_t1, (c) MUSCL, and (d) MUSCL_VD.](image-url)
experiments are integrated for 100 days. The domain-averaged concentration is shown in Fig. 2, which tends to vary only on the order of $10^{-6}$ (the truncation accuracy) in all experiments. This suggests that MPDATA, MUSCL, and MUSCL_VD as implemented are conservative to the same order of accuracy as the center difference scheme used in the POM. The time series of the bottom concentration in the flat bottom channel (Fig. 3a) suggests that MUSCL_VD is essentially identical to MUSCL in the case of a flat sea floor. The bottom concentration is lower in the experiments with MUSCL and MUSCL_VD than in the experiments with center difference and MPDATA because (1) the vertical exchange appears to be more vigorous in the experiments with MUSCL and MUSCL_VD (though not shown, these two experiments have higher surface concentration) and (2) the experiments with center difference and MPDATA appear to generate overshoots that are obvious in the first few oscillation periods with $C > 4.5$ mmol m$^{-3}$. In the presence of the seamount (Fig. 3b), the experiment with MUSCL produces erroneous responses right over the seamount, where the concentration is clearly out of bound. The other three schemes produce similar bottom concentration with the center difference scheme being the least diffusive followed by MPDATA and MUSCL_VD.

4.2. The GoM experiments

In the GoM case, we compare the modeled inert tracer concentrations resulted from the variants of advection schemes based on MPDATA and MUSCL (Table 1). Most of the comparisons use daily averaged concentrations except in Fig. 5 instantaneous values are used. Discussions on the predicted circulation can be found in Xue et al. (2005), in which predictions for 2002 and 2003 were compared with in situ observations. Model skills in predicting physical variables are rather consistent throughout the years from 2002 to 2006.

4.2.1. Dispersion and creation of non-physical values

Because there is neither a sink nor a source for the inert tracer and zero concentration is imposed at the head of the rivers, physically acceptable tracer concentration values should be between 0 and 4.5 mmol m$^{-3}$. However, over and undershoots due to numerical dispersions of the schemes can result in modeled concentrations outside of the bounds. The lowest concentration in the model is still zero as both the MPDATA and MUSCL schemes are positive definite. However, a maximum concentration of

Fig. 5. Bottom concentration of inert tracer (a) and salinity (b) at 9:00 UST on 21 December 2004 in the experiment with MUSCL_VD. Areas in white represent concentration >7 mmol m$^{-3}$. (c and e) The time series of bottom concentration and cross shore velocity, respectively, along the transect $i=142$ that passes the center of the abnormal values. (d and f) The time series of bottom concentration and along shore velocity, respectively, along the transect $j=11$ that passes the center of the abnormal values.
30 mmol m\(^{-3}\) is set to cap the overshoots in the model. To detect possible over and undershoots in the model associated with each of the schemes, we first conduct a global search for the maximal and minimal values. As expected the minimum is always zero. The resultant time series of the maximum is shown in Fig. 4.

When larger time steps are used with the MPDATA scheme, the concentration appears to be under control for the first 4–5 months, but the maximum value in the domain increases quickly to well exceeding 4.5 mmol m\(^{-3}\) (Fig. 4a) with the highest value reaching 30 mmol m\(^{-3}\) (Table 1). When the time step is reduced to $\Delta t$, MPDATA\(_{t1}\) behaves much better such that the maximum concentration oscillates around 4.75 mmol m\(^{-3}\) most of the time except on a few occasions when the concentration spikes to as high as 11 mmol m\(^{-3}\) (Fig. 4b). In contrast, overshoots in the experiment with MUSCL appear from the beginning of the integration. The maximum concentration appears to have a quasi-annual cycle with low in winters and high in summers (Fig. 4c). The experiment with MUSCL\(_{VD}\) has the best capability to cap the domain-wide maximum concentration at ~4.5 mmol m\(^{-3}\) except for a few spikes (Fig. 4d). Although MUSCL\(_{VD}\) is considered monotonic, the

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**Fig. 6.** Concentration of the inert tracer at the first sigma level at the end of 5-year integration (31 December 2006). Contours shown are 1.0 and 4.5 mmol m\(^{-3}\), respectively. (a) Experiment with MPDATA\(_{t5}\); (b) MPDATA\(_{t1}\); (c) MUSCL; and (d) MUSCL\(_{VD}\).

**Fig. 7.** Similar to Fig. 6 but for the concentration at the lowest sigma level.
simulated concentration does not have to be monotonic because of the diffusion terms in Eq. (1). It is expected that spurious, localized spikes dissipate gradually over time. Unlike the persistent overshoots on Nantucket Shoals in MPDATA_t5 (see below), the spikes in MPDATA_t1 and MUSCL_VD occur mostly in November through March. They result from

Fig. 8. Time series of the surface concentration at the Nantucket Shoals station (see Fig. 1 for the location). (a) MPDATA_t5; (b) MPDATA_t1; (c) MUSCL; and (d) MUSCL_VD.

Fig. 9. Similar to Fig. 8 for the station in Minas Basin in the upper Bay of Fundy.
exceptionally strong vertical motions at isolated locations. For example, the spike in the experiment with MUSCL_VD (Fig. 4d) in December 2004 is generated near the bottom on the slope (Fig. 5a). Similar abnormal values can also be seen in salinity (Fig. 5b) and temperature. They are generated due to numerical noise in the physical model as shown by the time series in Fig. 5c–f. A sudden divergence, very localized, occurs in the velocity field, which leads to the anomalously high values of concentration that are damped gradually over time in response to diffusions present in the model. The numerical noise can be suppressed by increasing the horizontal mixing coefficient in the model. Here, we have decided to keep the horizontal mixing coefficient small in the nowcast/forecast system as long as the numerical integration can be carried forward. Another location where spikes appear is the Minas Basin in the upper Bay of Fundy (see Fig. 9 below), where the velocity becomes very large when occasionally the water depth becomes extremely shallow. All spikes are damped gradually over time, but the base value in MPDATA_t1 is noticeably higher than 4.5 mmol m$^{-3}$, which is non-physical since all values in the initial and boundary conditions are $<4.5$ mmol m$^{-3}$ at all times and there is no net source inside the model. This echoes the conclusion of Lévy et al. (2001) and the findings from the idealized experiments shown in Fig. 3a.

To examine where overshoots occur, Figs. 6 and 7 show, respectively, horizontal distributions of the inert tracer at the top and bottom sigma levels at the end of the 5-year integration. Initial concentration at the top sigma level is nearly homogeneous from 1 near shore to 1.14 mmol m$^{-3}$ on the slope. Concentration at the surface (see Fig. 6) has increased after 5 years, mostly greater than 1.5 mmol m$^{-3}$ in the inner Gulf. Relatively lower concentration (<1.5 mmol m$^{-3}$) can be seen in the vicinity of several estuaries in MUSCL_VD (Fig. 6d). Although not shown, plume water with concentration less than 1 mmol m$^{-3}$ can be found near the coast during high discharge periods. Mixing is particularly prominent over the side of Georges Bank. Overshoots, on the other hand, with values considerably greater than 4.5 mmol m$^{-3}$ occur on Nantucket Shoals in MPDATA_t5 (Fig. 6a) and along the shelf break in MUSCL (Fig. 6c). Values less than 0.5 mmol m$^{-3}$ appear in the upper Bay of Fundy in both experiments with MPDATA (Fig. 6a and b).

At the bottom sigma level, the initial concentrations are within the range from 1 to 4.5 mmol m$^{-3}$, mirroring the irregular bottom topography to 350 m. Overshoots are again found in MPDATA_t5 (Fig. 7a) on Nantucket Shoals and in MUSCL at the shelf break (Fig. 7c). Similarly, values below 0.5 mmol m$^{-3}$ are found in Minas Basin in the experiments with MPDATA. There is no obvious overshoot in MUSCL_VD (Fig. 7d) with the maximum value enclosed by the contour of 4.5 mmol m$^{-3}$ on the slope less than 4.51 mmol m$^{-3}$. However, the maximum value enclosed by the contour of 4.5 mmol m$^{-3}$ in MPDATA_t1 is $\sim 4.75$ mmol m$^{-3}$.

Comparisons of the inert tracer concentration at different times of the year (not shown) suggest similar differences between schemes such that MPDATA_t5 generates overshoots on Nantucket Shoals, that MUSCL results in overshoots in the slope region south of Georges Bank, and that MPDATA_t1 has low concentration values trapped in Minas Basin. Overall, distributions of the inert tracer are similar in MPDATA_t1 and MUSCL_VD (Figs. 6 and 7b and d) with the extreme values better constrained in MUSCL_VD.

4.2.2. Time evolution of the concentration
To investigate the causes for over and undershoots, Figs. 8 and 9 show, respectively, time variations of the inert tracer concentration.

![Fig. 10. Similar to Fig. 8 but for the station on Georges Bank. Dashed lines in (b) and (d) indicate the times (end of March, June, September and December in 2006) when the cross sections are taken and shown in Fig. 12.](image-url)
in Nantucket Shoals and Minas Basin. Since both Nantucket Shoals and Minas Basin are well mixed, only the surface time series are shown. The Nantucket Shoals station is located in the sheltered area between Cape Cod and Martha’s Vineyard-Nantucket (see Fig. 1). The values are again significantly higher in MPDATA_t5 (Fig. 8a) as this location is near the center of the overshoot in this experiment, which is why the time series mimics the variation of the domain-wide maximum shown in Fig. 4a. Clearly, using 5Δt triggers numerical instability in the model although its extent is effectively capped by the upper limit of 30 mmol m⁻³. An additional experiment using a time step of 2Δt for biogeochemical variables was also conducted. Results are otherwise similar to those in MPDATA_t5 except that the overshoots are somewhat smaller in magnitude.

On the contrary, concentration is the lowest (between 0.5 and 1 mmol m⁻³) in MPDATA_t1 (Fig. 8b) despite that the values are relatively high in the part of Nantucket Shoals that is more open (Fig. 6b). In MPDATA_t1 the concentration tends to decrease from the initial value of 1 to about 0.5 mmol m⁻³ in the first 2–3 months, well before any significant amount of river water reaches the site. This also appears to be a common feature of MPDATA_t1 in relatively sheltered areas with strong currents as the trend is similar for the station in Minas Basin (Fig. 9b). In the experiment with MUSCL, the concentration at the Nantucket Shoals station increases from 1 to 2.5 mmol m⁻³ in the first year (Fig. 8c), reflecting the increase of surface concentration in the entire domain during the same period. Annual cycles are clear in the following years with lows in January/February and highs in May. The concentration in MUSCL_VD (Fig. 8d) has similar trends of MUSCL but with lower values and smaller annual cycles.

At the station in Minas Basin, the concentration is below 1 mmol m⁻³ most of the time in both MPDATA_t5 and MPDATA_t1 (Fig. 9a and b). The reason appears to be numerical as described above. However, the concentration is high in MUSCL (Fig. 9c),

![Figure 11](figure11.png)

**Fig. 11.** Time evolution of the inert tracer profiles at the Jordan Basin station. (a) MPDATA_t5, (b) MPDATA_t1, (c) MUSCL, and (d) MUSCL_VD. The white lines in (b) and (d) indicate the times (end of March, June, September, and December in 2006) when the cross sections are taken and shown in Fig. 13.
which is unique to this scheme. There are sharp jumps of concentration in both MPDATA_t1 and MUSCL_VD, which are due to the numerical noise that diminishes the water depth. It is important, however, that these jumps relax back to the values that they should be.

Although there is no non-physical value, time series' at two other stations (on Georges Bank and in Jordan Basin) are shown to illustrate differences among the schemes. The Georges Bank station is located near the center of the Bank where water depth is less than 40 m. Initially, the concentration increases from 1 mmol m$^{-3}$ at the surface to ~1.4 mmol m$^{-3}$ at the bottom, but the water column mixes quickly in all experiments to reach a vertically uniform distribution in only a few tidal cycles. This station appears to be vertically well mixed throughout the 5 years of integration despite the presence of strong annual and inter-annual variations. Hence, Fig. 10 shows time evolution of the surface concentration only. MPDATA_t1 (Fig. 10b) and MUSCL_VD (Fig. 10d) produce similar results at the Georges Bank station with the latter being ~0.5 mmol m$^{-3}$ higher except in the first year (i.e., 2002). The concentration increases steadily in MUSCL_VD while it is almost unchanged in MPDATA_t1. More importantly, these two experiments appear to have similar annual cycles with the minimum in early winter, followed by a quick increase to the maximum in late winter, and then a slow decrease from spring to fall. On the other hand, the concentration can reach considerably higher values in MPDATA_t5 (Fig. 10a) and MUSCL (Fig. 10c), and the seasonal cycle in these two experiments are out of phase with the ones in MPDATA_t1 and MUSCL_VD.

Fig. 12. Distributions of the salinity and inert tracer at the Georges Bank cross-section (see Fig. 1 for the location) on 31 March 2006 (a), 30 June 2006 (b), 30 September 2006 (c), and 31 December 2006 (d). The top panels in (a–d) show the salinity, the middle panels the inert tracer in MUSCL_VD, and lower panels the inert tracer in MPDATA_t1.
The Jordan Basin station is in much deeper water (~220 m) so that the vertical profiles are used to illustrate the time evolution of the entire water column in these four experiments (Fig. 11). The concentration at this station ranges from 1 to 3.15 mmol m\(^{-3}\) initially and reduces to less than 3.0 mmol m\(^{-3}\) in all experiments. The initial gradient is greatly reduced during the first two months in all cases, which can be attributed to the strong winter mixing in the GoM. Temporal variations are quite similar in all four experiments with a fairly regular annual cycle in the last three years such that the surface concentration is lower in May, June and July but higher in late fall and early winter. MUSCL produces a period of inverse gradient in the summer and fall of 2003 and 2004 when the concentration in the upper water column is higher than the concentration in the lower water column. Otherwise the resulted time series are similar between MUSCL and MUSCL_VD. When compared with the time series in the experiments with MPDATA, phase delays in the vertical from February to June are consistent, while the gradient is larger in MUSCL_VD in fall and winter.

4.2.3. Diffusion

Diffusion associated with the advection schemes is another concern, which is often best illustrated near frontal zones. Two sections, one across Georges Bank from south to north and another across Jordan Basin and the Eastern Maine Coastal Current (see Fig. 1 for locations), are used to compare the diffusion in MPDATA_t1 and MUSCL_VD as MPDATA_t5 and MUSCL are deemed unsatisfactory.

The idealized experiments suggest that MUSCL_VD is more diffusive than MPDATA_t1 (Fig. 3b). In the GoM simulations,
distributions of the bottom concentration appear to suggest the same because the bottom front along the southern flank of Georges Bank is slightly sharper in MPDATA_t1 (Fig. 7b). Similarly, high concentration (>3.5 mmol m$^{-3}$) from the slope water comes into the GoM through the Northeast Channel in the fall (though not shown, the 3.5 mmol m$^{-3}$ isoline is near the entrance of the Northeast Channel on 30 September 2006 in both experiments), which tends to spread wider in MUSCL_VD (Fig. 7d). As a result, the concentration on Georges Bank is higher in MUSCL_VD than in MPDATA_t1 as seen in Fig. 10b and d.

Fig. 12 shows north–south sectional distributions of the inert tracer across Georges Bank in these two experiments with comparison with the sectional distribution of salinity since the salinity is also a conservative tracer in the water column but it is calculated using the center difference scheme that has the smallest numerical diffusion among all schemes as shown in Fig. 3. The front on the northern flank appears to be a subsurface feature both for the salinity and the inert tracer in MUSCL_VD with a bulge moving onto the Bank near the bottom. In MPDATA_t1, the upslope movement of higher concentration tends to be closer to the bottom slope. The upslope intrusion of high concentration water from depth onto the Bank is even more pronounced on the southern flank in MPDATA_t1, likely due to the sharper topographic gradient there.

Along the Jordan Basin/EMCC cross-section, concentration increases from near the coast at the surface to the southern end at the bottom because the coastal water is influenced by river waters with zero concentration and the southern end is influenced by the slope water intrusion with high concentration (Fig. 13). Tracer distributions are qualitatively similar in these two experiments although the slopes of the isopleths are more similar for the salinity and the tracer in MUSCL_VD, which tend to be steeper in MPDATA_t1. The upslope intrusion extends more vertically but less horizontally in the experiment with MPDATA_t1, e.g., near 43 and 44.5°N. This appears to affect the property distribution in Jordan Basin. For example, in MPDATA_t1 the dome associated with the slope water disappears in September (Fig. 13c).

5. Conclusions

Based on two types of advection schemes, MPDATA and MUSCL, this work compares and evaluates the similarities and discrepancies between the schemes in a biogeochemical-like tracer model. The MUSCL based on Lin et al. (1994) is modified to allow explicit treatment of variable depth (MUSCL_VD). Conservation associated with the schemes is verified in a circular channel with and without a seamount. The modified MUSCL_VD and MUSCL produce almost identical results in the flat bottom case, while the original MUSCL produces overshoots over the seamount.

These advection schemes are then applied to a conservative tracer in a 3D model for the GoM with realistic topography and forcings. The second-order MPDATA is also implemented with different time resolutions: $\Delta t$ (MPDATA_t1) and 5$\Delta t$ (MPDATA_t5). Modeled results are sensitive to the advection schemes:

1. The experiments with MPDATA_t5 and MUSCL exhibit persistent overshoots. Decreasing the time step in MPDATA can reduce the occurrence and the magnitude of the overshoots. The original MUSCL that places the limiters on the product DC produces small-scale variability mimicking topographic features in some places.
2. By comparing the inert tracer concentration at different times of the year, MPDATA_t1 and MUSCL_VD produce similar spatial distributions and similar seasonal cycles. MUSCL_VD appears to be slightly more diffusive in the horizontal, but less so in the vertical.

3. In MUSCL_VD the concentration is capped at the physically allowable limit of 4.5 mmol m$^{-3}$ except for a few short lived spikes due to numerical noise in the physical model. On the other hand, the maximum concentration has a positive bias in MPDATA with values greater than the allowable upper limit of 4.5 mmol m$^{-3}$ at all times. Furthermore, MPDATA_t1 tends to generate low concentrations trapped in Minas Basin and Nantucket Shoals.

4. Overall, MUSCL_VD emerges as a viable choice in terms of avoiding non-physical values, conservation, and diffusion, and it is computationally as efficient as MPDATA_t1.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.ocemod.2009.05.001.

References


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