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Implementing the trajectory-grid transport algorithm in an air quality model

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Abstract

Eulerian-based air quality models encounter a serious numerical problem in solving the advection equation. In addition, mass conservation is often violated when meteorological model output is used as input to air quality models. The trajectory-grid algorithm handles the advection and eddy-diffusion in the Lagrangian and Eulerian framework, respectively. It is very accurate and can be used to trivially solve the advection equation for molar mixing ratios to address (but not correct) the mass conservation issue. We incorporated the algorithm into the state-of-the-science comprehensive air quality model with extensions (CAMx). Applications of the model reveal the inaccuracy of the commonly used Bott advection scheme, and the subsequent compensating errors of the model. The results clearly call for a more reliable description of eddy diffusivity and emissions inventory in order to truly improve the reliability and predictive capability of air quality models.

Keywords: Air quality model; Trajectory-grid algorithm; Bott scheme; Advection equation; Mass conservation; Eddy diffusivity; Eulerian; Lagrangian; MM5; CAMx

1. Introduction

Eulerian-based air quality models (AQMs) suffer a serious numerical problem in solving the advection equation, accounting for a large fraction of numerical inaccuracies in the models. This is because grid-discretization leads to artificial dispersion and diffusion of the concentration profiles. Correction attempts can lead to distortion of the profiles and introduce spurious nonlinearity, leading to unpredictable outcome. Another problem AQMs face is that the input flow field may not conserve mass. When meteorological-model output is used as input to an AQM, mass-conservation violation can be due to (1) mass-conservation violation of the meteorological model itself, (2) difference in spatial and temporal resolution, in terms of grid size and time step, between the AQM and the meteorological model, and/or (3) use of time interpolation in the AQM to approximate the instantaneous meteorological model output read in at large time intervals. To address this problem, models may recalculate the wind field, typically by modifying the vertical velocity to satisfy the advection equation, or introduce artificial local and time-dependent emission sources and sinks to cancel the mass non-conservation. Neither approach is very satisfactory.

Chock et al. (1996) presented the trajectory-grid (TG) approach for solving the physical transport equation. The approach is Lagrangian for the advective transport

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and Eulerian for the diffusive transport. The basic idea of the approach for the advective transport is very simple. It rewrites the advection equation for, say, concentration, C, of a species in a velocity field $\mathbf{v}$, as one containing the full derivative of concentration with respect to time and a remaining term containing the velocity divergence.

$$\frac{\mathrm{d}C}{\mathrm{d}t} = \frac{\partial C}{\partial T} + \mathbf{v} \cdot \nabla C = -(\nabla \cdot \mathbf{v})C.$$

Thus, the equation is now describing the concentration profile of a species as this profile moves along the flow field. In other words, one can designate a set of points, or what we shall call pulses, on the concentration profile and trace the trajectories of these points along the wind field and modify their concentrations according to the velocity divergence along the trajectories. In the equation below, $C(t)$ is the concentration at the pulse location as the pulse moves along its trajectory prescribed by the wind field.

$$\begin{aligned} C(t) &= C(t_0)\ \exp\left(-\int_{t_0}^{t} (\nabla \cdot \mathbf{v})\, \mathrm{d}t\right) \\ &\approx C(t_0)\ \exp[-(\nabla \cdot \mathbf{v})(t - t_0)]. \end{aligned}$$

The method is intrinsically mass conserving, sign preserving and monotonic. It is also accurate because the species concentration is a solution to an ordinary differential equation and the trajectory can be made as accurate as necessary. Since the flow field is the same for all species at a given location and time, the movement of a concentration pulse constitutes the advective transport of concentrations of all species represented by the pulse so that the advective transport of concentrations of different species need not be treated separately. This is an important timesaving feature of TG. However, interpolative errors may occur when one needs to estimate the cell-center concentrations of a species in the modeling domain. But unlike the semi-Lagrangian methods, the errors do not propagate or grow because they are not fed back to the species concentrations at the pulse locations. Interpolation errors do occur in the diffusion step, but errors caused by the diffusion step are typically considerably smaller than those in Eulerian advection. Overall, the method yields a very accurate solution even for complex species concentration profiles. An application of the approach to the European chemical transport model was described by Chock et al. (1998). The approach has also been used to solve the condensation/evaporation equations in aerosol modeling accurately and with substantial time saving (Chock and Winkler, 2000; Gaydos et al., 2003). Here, we are describing our implementation of the TG approach in a state-of-the-science AQM called Comprehensive Air Quality Model with Extensions, or CAMx (Environ, 2004). The version we used is PMCAMx 3.01 (designated as CAMx hereafter), which contains an equilibrium aerosol module. In the course of this implementation, we also deal with the mass conservation issue.

2. The issue of mass conservation

Because we try to minimize the alterations of the meteorological model (MM5 in this case. See Grell et al., 1994.) output to be used in CAMx, we decided to retain the sigma coordinate instead of the physical coordinate used in CAMx. In addition, the vertical velocity, $\dot{\sigma}$, from MM5 can be used directly whenever both CAMx and MM5 refer to the same layer.

Many non-hydrostatic meteorological models, including MM5, do not conserve mass. In the case of MM5, there are two major reasons for failure to conserve mass. First, two terms corresponding to the heat fluxes from diabatic processes and subgrid-scale diffusion have been neglected in the pressure tendency equation (Dudhia, 1993). This will indirectly impact the accuracy of the estimated air density, though the terms are supposedly negligible compared to other terms in the equation. Second, and likely more important, the boundary condition, $\dot{\sigma} = 0$, at $\sigma = 1$ (bottom boundary) is generally not satisfied. This is because the σ levels are defined by reference (hydrostatic) pressures which are time independent, and for $\sigma = 1$, the reference pressure is prescribed according to the terrain height. But the actual surface pressure depends on location and time, which means that $\sigma = 1$ may be detached from (to be above or below) the surface, so that $\dot{\sigma}$ is no longer necessarily zero. This fact creates a lack of self-consistency in the model with mass conservation being one of the casualties.

As mentioned earlier, even if the meteorological model output is mass conserving, incorporating the output in an AQM need not guarantee mass conservation. An example of this was illustrated by Lee et al. (2004). To obviate such worries, CAMx determines the vertical velocity, w, by requiring that the continuity equation be satisfied, risking the possibility that the calculated vertical velocity may be unphysical. In addition, if the Bott scheme is used in the integration step to determine w, then the Bott scheme must also be used as the advection-equation solver to assure mass conservation. Therefore, the calculated vertical wind field is subject to the choice of the advection algorithm. Another interesting thing is that even though the grid structure is assumed to be terrain following, no correction involving the horizontal gradient of the terrain height for the vertical velocity is made. In other words, w need not be zero at the surface but is assumed so. As a result, the vertical velocity is effectively determined not for a terrain-following coordinate but