Mass conservation

A very important issue for any air quality model is the mass conservation. It means that off-line fields of wind and surface pressure supplied by the meteorological pre-processor should satisfy the continuity equation:

$$\frac{\partial p^*}{\partial t} + \nabla_H \cdot (p^* V_H) + \frac{\partial}{\partial \sigma}(p^* \dot{\sigma}) = 0 \qquad (1)$$

In terms of an air quality model it implies that the model maintains a uniform mass mixing ratio field of an inert tracer in an arbitrary wind field [*Odman and Russel*, 2000]. It can be exactly realized only if the air quality model and a meteorological driver supplying input data are on-line coupled or have the same *discretization*, i.e. grid structure, time step, and finite-difference formulation. However, many off-line transport models (including considered one) have the discretization different from that used in the meteorological driver. Besides, time resolution of the off-line meteorological data (6 hours for the model involved) is often considerably lower than the model time resolution (~10 minutes) defined by the numerical stability of the explicit scheme. It requires temporal interpolation of the meteorological data. All mentioned above can lead to a considerable mass inconsistency and the uniform tracer field cannot be maintained. A possible approach to adjust the input meteorological fields to the model discretization is derivation of vertical wind velocity $\dot{\sigma}$ from the continuity equation (1) at each time step [*Odman and Russel*, 2000].

For the exact mass conservation it is important to apply to solution of equation (1) the same numerical scheme used for species advection description. The solution is performed in two steps:

Step 1. Solution of the horizontal constituent of the air continuity equation for p^* using Bott advection scheme:

$$\frac{\partial p^*}{\partial t} = -\nabla_H \cdot (p^* V_H) \qquad (2)$$

For the initial condition the surface pressure at the beginning of the time step $(p^*)_t$ is used. As a result a tree-dimensional distribution of the intermediate pressure $(p_k^*)_{t+\Delta t/2} = f(x, y, \sigma)$ is obtained.

Step 2. Solution of the vertical constituent of the air continuity equation for the vertical velocity $\dot{\sigma}$:

$$\frac{\partial p^*}{\partial t} = -\frac{\partial}{\partial \sigma}(p^* \dot{\sigma}) \qquad (3)$$

The intermediate pressure $(p_k^*)_{t+\Delta t/2}$ from the Step 1 is used as the initial condition; and the surface pressure at the end of the time step $(p^*)_{t+\Delta t} = f(x,y)$ interpolated from the input data is considered as a final condition. Keeping notations from [*Bott*, 1989a] the surface pressure at the end of the time step can be express as follows for each layer k of the model domain:

$$(p^*)_{t+\Delta t} = (p_k^*)_{t+\Delta t/2} - I_k^{up} - I_k^{down} + \frac{\Delta\sigma_{k-1}}{\Delta\sigma_k} I_{k-1}^{up} + \frac{\Delta\sigma_{k+1}}{\Delta\sigma_k} I_{k+1}^{down}, \qquad k = 1, K_{max}, \quad (4)$$

where the integrals of mass coming up and down though the upper and lower borders of the gridcell, respectively, are given by:

$$I_k^{up} = \int_{-1/2}^{-1/2+\alpha_k^{up}} p^*(\xi) d\xi, \quad I_k^{down} = \int_{1/2-\alpha_k^{down}}^{1/2} p^*(\xi) d\xi, \qquad (5)$$

pressure distribution in a gridcell is approximated by the 2nd order polynomial:

$$p^*(\xi) = \sum_{n=0}^{2} a_{k,n} \xi^n, \quad \varepsilon = \frac{\sigma - \sigma_k}{\Delta\sigma_k}, \qquad (6)$$

where $a_{k,n}$ are coefficient of the polynomial.

The local Courant numbers are calculated as follows:

$$\alpha_k^{up} = \frac{|\dot\sigma_k^{up}|\Delta t}{\Delta\sigma_k}, \qquad \alpha_k^{down} = \frac{|\dot\sigma_k^{down}|\Delta t}{\Delta\sigma_k} \qquad (7)$$

The integrals of mass coming though the gridcell borders are derived from Eq. (4):

$$\begin{cases} I_k^{up} = (p_k^*)_{t+\frac{\Delta t}{2}} - (p^*)_{t+\Delta t} - I_k^{down} + \dfrac{\Delta\sigma_{k-1}}{\Delta\sigma_k} I_{k-1}^{up}, & I_k^{up} > 0 \\ I_{k+1}^{down} = \dfrac{\Delta\sigma_k}{\Delta\sigma_{k+1}} \left((p^*)_{t+\Delta t} - (p_k^*)_{t+\frac{\Delta t}{2}} + I_k^{down} - \dfrac{\Delta\sigma_{k-1}}{\Delta\sigma_k} I_{k-1}^{up} \right), & I_k^{up} \le 0 \end{cases} \quad k = 1, K_{max} (8)$$

The calculation is started from the lowest layer where the mass flux through the ground surface is absent: $I_0^{up} = 0$ and $I_1^{down} = 0$. Substituting the polynomial approximation (6) to the Eqs. (5) and equating the obtained expressions to the values of the mass integrals calculated in Eq. (8) one can derive linear algebraic equations for the local Courant numbers α_k^{up} or α_k^{down} at borders of each gridcell $(k = 1, K_{max})$

$$\sum_{n=0}^{2} \frac{a_{k,n}}{(n+1)2^{n+1}} (-1)^n \left[1 - \left(1 - 2\alpha_k^{up}\right)^{n+1}\right] = I_k^{up} \qquad (9)$$

$$\sum_{n=0}^{2} \frac{a_{k+1,n}}{(n+1)2^{n+1}} \left[1 - \left(1 - 2\alpha_{k+1}^{down}\right)^{n+1}\right] = I_{k+1}^{down} \tag{10}$$

Only one of Eqs. (9) and (10) is taken for each gridcell border. For example, for the upper border of gridcell k Eq. (9) is chosen if $I_k^{up} > 0$ and Eq. (10) in the opposite case. The Eqs. (9) or (10) are solved for a_k^{up} or a_k^{down}, respectively, using the Newton's method. Vertical velocities are derived from the appropriate Courant numbers using expressions (7).

Bott A. [1989a] A positive definite advection scheme obtained by nonlinear renormalization of the advective fluxes. *Mon. Wea. Rev.* **117**, 1006-1015.

Odman M. T. and Russell A. G. [2000] Mass conservative coupling of non-hydrostatic meteorological models with air quality models. In: Gryning S.-E. and Batchvarova E. (Eds.) Air pollution modelling and its application XIII. Kluwer Academic/Plenum Publishers, New York, 651-660.