Annex B

CALCULATION OF THE VERTICAL VELOCITY

A possible approach to adjust the input meteorological fields to the model discritization is derivation of vertical wind velocity σ from the continuity equation for air at each time step [*Odman and Russel*, 2000]. For the exact mass conservation it is important to apply the same numerical scheme used for description of species advection to solution of the continuity equation. 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:

$$\frac{\partial p^*}{\partial t} = -m^2 \nabla_H \cdot \left(p^* \frac{V_H}{m} \right) \qquad \text{(B.1)}$$

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 $(p^*)_{t+\Delta t/2} = f(x,y,\sigma)$ is obtained.

Step 2. Solution of the vertical constituent of the air continuity equation for the vertical velocity σ :

$$\frac{\partial p^*}{\partial t} = -\frac{\partial}{\partial \sigma}\left(p^* \sigma \right) \qquad \text{(B.2)}$$

The intermediate pressure $(p^*)_{t+\Delta t/2}$ 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

$$\left(p^*\right)_{t+\Delta t} = \left(p_k^*\right)_{t+\Delta t/2} - I_k^{up} - I_k^{down} + \frac{\Delta\sigma_{k-1}}{\Delta\sigma_k} I_{k-1}^{up} + \frac{\Delta\sigma_{k+1}}{\Delta\sigma_k} I_{k+1}^{down}, \qquad k = 1, K_{max}, \qquad \text{(B.3)}$$

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

$$I_k^{up} = \int_{-1/2}^{-1/2+\alpha_k^{up}} p^*(\xi)d\xi, \qquad I_k^{down} = \int_{1/2-\alpha_k^{down}}^{1/2} p^*(\xi)d\xi, \qquad \text{(B.4)}$$

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

$$p^*(\xi) = \sum_{n=0}^{2} a_{k,n}\xi^n, \qquad \xi = \frac{\sigma - \sigma_k}{\Delta\sigma_k} \qquad \text{(B.5)}$$

and the local Courant numbers are calculated as follows:

$$\alpha_k^{up} = \frac{\left|\sigma_k^{up}\right|\Delta t}{\Delta\sigma_k}, \qquad \alpha_k^{down} = \frac{\left|\sigma_k^{down}\right|\Delta t}{\Delta\sigma_k} \qquad \text{(B.6)}$$

The integrals of mass coming through the gridcell borders are derived from Eq. (B.3):

$$\begin{cases} I_k^{up} = \left(p_k^*\right)_{t+\Delta t/2} - \left(p*\right)_{t+\Delta t} - I_k^{down} + \dfrac{\Delta\sigma_{k-1}}{\Delta\sigma_k} I_{k-1}^{up}, & I_k^{up} > 0 \\ I_{k+1}^{down} = \dfrac{\Delta\sigma_k}{\Delta\sigma_{k+1}}\left(\left(p*\right)_{t+\Delta t} - \left(p_k^*\right)_{t+\Delta t/2} + I_k^{down} - \dfrac{\Delta\sigma_{k-1}}{\Delta\sigma_k} I_{k-1}^{up}\right), & I_k^{up} \le 0 \end{cases}, \qquad k = 1, K_{max}\,. \tag{B.7}$$

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 (B.5) to the Eqs. (B.4) and equating the obtained expressions to the values of the mass integrals calculated in Eq. (B.7) 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}):

$$\sum_{n=0}^{2} \frac{a_{k,n}}{(n+1)2^{n+1}} (-1)^n \left[1 - \left(1 - 2\alpha_k^{up}\right)^{n+1}\right] = I_k^{up} \tag{B.8}$$

$$\sum_{n=0}^{2} \frac{a_{k+1,n}}{(n+1)2^{n+1}} \left[1 - \left(1 - 2\alpha_{k+1}^{down}\right)^{n+1}\right] = I_{k+1}^{down} \tag{B.9}$$

Only one of Eqs. (B.8) and (B.9) is taken for each gridcell border. For example, for the upper border of gridcell *k* Eq. (B.8) is chosen if $I_k^{up} > 0$ and Eq. (B.9) in the opposite case. The Eqs. (B.8) or (B.9) are solved for α_k^{up} or α_k^{down}, respectively, using the Newton's method. Vertical velocities are derived from the appropriate Courant numbers using expressions (B.6).