Advection and diffusion

The species continuity equation describing the atmospheric transport and dispersion of a pollutant on the stereographic projection with the vertical (σ–p) coordinate has the following form:

$$\frac{\partial}{\partial t}(qp^*) = -\nabla_H \cdot (qp^*\mathbf{V}_H) - \frac{\partial}{\partial \sigma}(qp^*\dot{\sigma}) + \frac{\partial}{\partial \sigma}\left[K_z\left(\frac{g\rho}{p^*}\right)^2 \frac{\partial}{\partial \sigma}(qp^*)\right] + \sum_i S_i \tag{1}$$

where $q = c/\rho$ is a species mass mixing ratio;

c and ρ are the volume concentration and the local air density;

$p^* = p_s - p_t$ is the difference between the local surface pressure p_s and the model top pressure p_t;

$\sigma = (p - p_t)/p^*$ is the vertical σ-coordinate, where p is a local air pressure;

$\dot{\sigma} = d\sigma/dt$ is the vertical scalar velocity in the (σ–p) coordinate;

∇_H and $\mathbf{V}_H$ denote horizontal divergence operator and wind velocity respectively;

K_z is the vertical eddy diffusion coefficient; and g is the gravitational acceleration.

In the continuity equation we omitted horizontal eddy diffusion because of the coarse horizontal grid resolution. The local air density ρ at fixed σ-layer is coupled with air temperature T_a and the pressure difference p^* through the equation of state:

$$\rho = \frac{\sigma p^* + p_t}{R_a T_a}$$

where R_a is the gas constant for moist air.

The first two terms on the right hand side of the continuity equation describe horizontal and vertical advection of a pollutant in the atmosphere. The third term represents vertical eddy diffusion, the last term describes variety of sources and sinks (emissions, chemical transformations, depositions etc.). The equation is solved by means of the operator-splitting procedure [e.g. *Yanenko*, 1971; *Marchuk*, 1975; *McRae et al.*, 1982]. Following this method, the original equation is approximated by several operator-split equations describing different physical and chemical processes, which are solved sequentially during each time step.

Advection

The sub-equation of the continuity equation (1) describing horizontal advection has the following form:

$$\frac{\partial}{\partial t}(qp^*) = -\frac{1}{R_E \cos\varphi}\left[\frac{\partial}{\partial\lambda}(qp^*V_\lambda) + \frac{\partial}{\partial\varphi}\left(qp^*V_\varphi \cos\varphi\right)\right], \tag{2}$$

where λ and φ are the geographical longitude and latitude; R_E is the Earth radius; V_λ and V_φ are zonal and meridional components of the wind velocity respectively.

Equation (2) is solved numerically using Bott flux-form advection scheme [*Bott*, 1989a; 1989b, 1992]. This scheme is mass conservative, positive-definite, monotone, and is characterized by comparatively low artificial diffusion [see e.g. *Dabdub and Seinfeld*, 1994]. In order to reduce the time-splitting error in strong deformational flows the scheme has been modified according to [*Easter*, 1993]. The original Bott scheme has been derived in the Cartesian coordinates. To apply the scheme to the transport in spherical coordinates it has been modified taking into account peculiarities of the spherical geometry. Detailed description of the Bott advection scheme in the spherical coordinates is presented in [*Travnikov*, 2001].

The vertical advection part of equation (1) is written as follows:

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

This one-dimensional advection equation is solved using the Bott scheme with second-order area-preserving polynomials generalized for a grid with variable step $\Delta\sigma$.

Eddy diffusion

The non-linear equation for vertical eddy diffusion:

$$\frac{\partial}{\partial t}(qp^*) = \frac{\partial}{\partial\sigma}\left[K_z\left(\frac{g\rho}{p^*}\right)^2 \frac{\partial}{\partial\sigma}(qp^*)\right] \tag{4}$$

has been approximated by the second-order implicit numerical scheme in order to avoid restrictions of the time step caused by possible sharp gradients of the species mixing ratio. The obtained finite-difference equation is solved by means of the decomposition - backsubstitution method.

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

Bott A. [1989b] Reply to comment on "A positive definite advection scheme obtained by nonlinear renormalization of the advective fluxes" *Mon. Wea. Rev.* **117**, 2633-2636.

Bott A. [1992] Monotone flux limitation in the area-preserving flux-form advection algorithm. *Mon. Wea. Rev.* **120**, 2592-2602.

Dabdub D., Seinfeld J. H. [1994] Numerical advective schemes used in air quality models – sequential and parallel implementation. *Atmos. Environ*. **28**, 3369-3385.

Easter R. C. [1993] Two modified versions of Bott's positive-definite numerical advection scheme. *Mon. Wea. Rev.* **121**, 297-304.

Marchuk G. I. [1975] *Methods of numerical mathematics*. Springer-Verlag, New York. 316 p.

McRae G. J., Goodin W. R., Seifeld J. H. [1982] Numerical solution of the atmospheric diffusion equation for chemically reacting flows. *J. Comp. Phys.* **45**, 1-42.

Travnikov O. [2001] Hemispheric model of airborne pollutant transport. EMEP/MSC-E Technical Note 8/2001, Meteorological Synthesizing Centre - East, Moscow, Russia

Yanenko N. N. [1971] The method of fractional steps. The solution of problems of mathematical physics in several variables. *Springer-Verlag*, New York. 160 p.