CREATION AND TESTING OF FLUX-TYPE ADVECTION SCHEMES FOR AIR POLLUTION MODELING APPLICATION

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INTRODUCTION

Many advection schemes are described in the literature (*WMO*, 1979) but none of them possesses all properties of the exact solution of the advective equation. One of the most widely used schemes is developed by *Bott* (1989). In the Bott scheme, the change of concentration for one time step is calculated as difference between advective fluxes at the cell edges and fluxes determined by integration of proper polynomial fitting the concentrations in the neighboring grid points. Upper and lower limitation and **normalization** are applied. The produced scheme is conservative and positively definite with small numerical diffusion. These properties make the Bott scheme very attractive for further improvements and optimizations. The TRAP scheme (*Syrakov*, 1995, *Syrakov and Galperin*, 1997) is such a daughter scheme. It is built supposing that the shape of the so called "flux area" is trapezoidal and its value is calculated as a product of the Courant number and the concentration in the middle of the trapezium. Some variants of TRAP scheme are elaborated and tested, decreasing the order of the fitting polynomial *(Syrakov*, 2003). In this paper, four new variants of the TRAP scheme are presented. They are obtained by special determination of fitting polynomials and the normalization procedure is omitted. The new created schemes are tested and compared with mother ones using the two-dimensional rotational test of *Smolarkiewicz* (1982).

DESCRIPTION OF THE BESSEL VARIANT OF THE TRAP-SCHEME (*TrB*)

The one-dimensional case will be considered here. The one-dimensional advection equation in non-divergent and discrete form is

$$\partial C/\partial t - \partial uC/\partial x = 0; \qquad C_i^{n+1} = C_i^n - (Fr_i - Fl_i)^n \qquad (1)$$

where $C(x,t)$ is the concentration of the tracer, $u(x,t)$ – the transport velocity, x, t – space and time, Fr_i and Fl_i – the rightmost and leftmost fluxes at the edges of the i^{th} cell. The problem made dimensionless by introducing the Courant number $U_i^n = u_i^n \Delta t/\Delta x$ and setting $\Delta x = \Delta t = 1$.

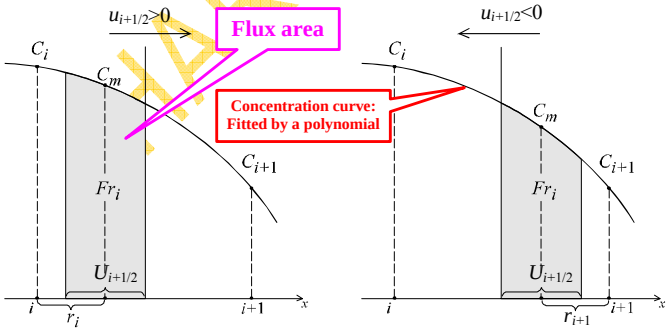

Fig.1; Flux trough the right edge of cell i at positive and negative transport velocity

According to the TRAP concept, the flux area is approximated by rectangular trapezium laying on its height (*Fig.1*) and its value Ar_i can be calculated as a product of this height (i.e. the Courant number) and the half-sum of both bases. Estimates for these concentrations can be obtained using the proper approximating polynomial. In TRAP, a single estimate for the point in the middle of the passed distance (the trapezium height) is obtained exploiting the same polynomial, instead. According to *Fig.1*, this distance is $r = (1 - U_{i+1/2})/2$ and is the same in both cases of

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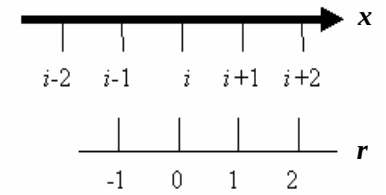
positive and negative transport velocity. It is obvious that this approach substantially reduces the amount of calculations.

Bott (1989) recommends a 4th order Lagrangean polynomial as best fit of concentration profile. In the ***TrB***-variant of the TRAP scheme (*Syrakov and Galperin*, 1997) a Bessel type polynomial of 3rd order is applied, instead:

$$C^b(r) = b_0 + b_1 r + b_2 r^2 + b_3 r^3, \quad (2)$$

In order to determine the coefficients b_k a local coordinate system (4-point pattern) is introduced with origin in point i as shown in Scheme 1. Known the grid values of the concentration, a system of four ordinary algebraic equations results:



Scheme 1

$$\begin{aligned} &at \quad r=-1: \quad C_{i-1} = b_0 - b_1 + b_2 - b_3 \\ &at \quad r=\ 0: \quad C_i = b_0 \\ &at \quad r=\ 1: \quad C_{i+1} = b_0 + b_1 + b_2 + b_3 \\ &at \quad r=\ 2: \quad C_{i+2} = b_0 + 2b_1 + 4b_2 + 9b_3 \end{aligned} \quad (3)$$

Its solution gives the polynomial coefficients:

$$\begin{aligned} b_0 &= C_i \\ b_1 &= \left(-2C_{i-1} - 3C_i + 6C_{i+1} - C_{i+2}\right)/6 \\ b_2 &= \left(C_{i-1} - 2C_i + C_{i+1}\right)/2 \\ b_3 &= \left(-C_{i-1} + 3C_i - 3C_{i+1} + C_{i+2}\right)/6 \end{aligned} \quad (4)$$

This local approach of polynomial fitting (separate coefficients for each cell) leads to a small numerical diffusion, but in case of strong gradients in the concentration field some values of the polynomial can become negative or unrealistically high. That is why the next step is to introduce lower and upper limits for the flux area (*Bott*, 1989).

$$\begin{aligned} &0 \le Ar_i < C_i, \quad at \quad U_{i+1/2} > 0 \\ &0 \le Ar_i < C_{i+1}, \quad at \quad U_{i+1/2} < 0 \end{aligned} \quad (5)$$

Bott introduces an additional procedure, called here **normalization**, aiming to account for the fact that the polynomial is built over grid values at grid points. Flux area is multiplied by

$$C_i/A_i \text{ when } U_{i+1/2} > 0 \text{ and } C_{i+1}/A_{i+1} \text{ when } U_{i+1/2} < 0, \quad (6)$$

where $C_i \Delta x = C_i$ is the entire mass in the cell and here A_i is estimate via equations (2) and (4):

$$A_i = \int_{-1/2}^{1/2} C_i^b(x)dx, \text{ i.e. } \begin{aligned} A_i &= \left(C_{i-1} + 22C_i + C_{i+1}\right)/24, \quad at \quad U_i > 0 \\ A_{i+1} &= \left(C_i + 22C_{i+1} + C_{i+2}\right)/24, \quad at \quad U_i < 0 \end{aligned} \quad (7)$$

Finally, the change of concentration in the cell is determined after equation (1) having $Fl_i = Fr_{i-1}$. At each time step, the procedure recurs for each consecutive cell.

The introduction of Bessel polynomial leads to some important results. Firstly, the lower order leads to a smaller number of coefficients, so the computation is faster. Secondly, the number of the boundary points decreases. Finally, the highest order of accuracy of the Bessel polynomial is in the region $0.25 \le r \le 0.75$, i.e. around the cell edge, where the flux is located. The results from the experiments made with the Bott's scheme and some variants of TRAP scheme are presented in *Syrakov* (2003) and show that the schemes possess practically equal simulation abilities, but TRAP schemes are much faster. As a final conclusion the Bessel variant of TRAP scheme (***TrB***) was recommended for practical use.

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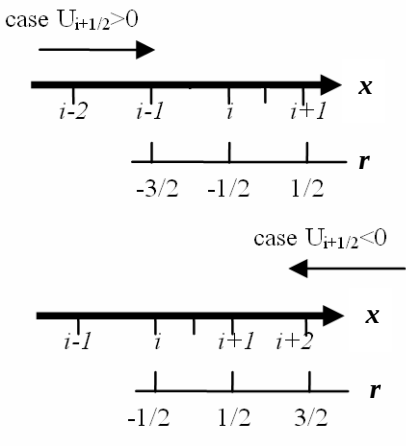
SECOND ORDER TRAP-SCHEME (*Tr2)*

It was shown in *Syrakov* (2003) that the decrease of the order of approximation from 4 to 3 leads to acceleration of computations without considerable change for the worse. Further decrease of this order is worth to be checked: The interpolation polynomial has the form:

$$C^2(x)=d_0+d_1x+d_2x^2 \qquad (8)$$



Scheme 2

The 3-point grid pattern has its origin in point $i+1/2$ (shifted pattern), its position depending on the transport direction as shown in **Scheme 2**. Following the approach of the equation (3), the polynomial coefficients are:

$$\begin{array}{ll} U_{i+1/2}>0 & \begin{aligned} d_0 &= (-C_{i-1}+6C_i+3C_{i+1})/8 \\ d_1 &= -C_i+C_{i+1} \\ d_2 &= (C_{i-1}-2C_i+C_{i+1})/2 \end{aligned} \\ U_{i+1/2}<0 & \begin{aligned} d_0 &= (3C_i+6C_{i+1}-C_{i+2})/8 \\ d_1 &= -C_i+C_{i+1} \\ d_2 &= (C_i-2C_{i+1}+C_{i+2})/2 \end{aligned} \end{array} \qquad (9)$$

Because of the shifted pattern, the flux area is calculated by multiplying the Courant number with the value of the argument in equation (8) $r_i=-U_{1+1/2}/2$. Bott's limiters and **normalization** procedure, equations (5) and (6), are applied, mass-in-cell determined as

$$A_i=d_0-d_1/2+d_2/3 \ \text{ at } U_{i+1/2}>0 \ \text{ and } A_{i+1}=d_0+d_1/2+d_2/3 \ \text{ at } U_{i+1/2}<0 \qquad (10)$$

SELF-NORMALIZING TRAP SCHEMES (*Tr3_n1, Tr3_n2, Tr2_n1, Tr2_n2*)

Further optimization of the TRAP scheme can be achieved applying the so called self-normalizing proposed by *Galperin* (1998). Keeping in mind that C_i, $C_{i\pm1}$ etc. are the average concentrations in the respective cells, the coefficients of polynomials are determined in such way that the integral of the polynomial, taken between cell edges, is equal to the mass in it. As a result, the necessity of normalization step fells out.

Two self-normalizing schemes can be built as variants of the schemes described above, exploiting normal and shifted patterns. Here, the first 3rd order scheme, ***Tr3_n1***, will be described in details. The parameters of the other three schemes will be given in a table.

The same 4-point pattern as shown in **Scheme 1** is used. According to Galperin's approach, the system of linear equations (11) is derived. Its solution gives the unknown coefficients of the polynomial (2):

$$\begin{aligned} &at \ \ r=-1: \ \ C_{i-1}=\int_{-3/2}^{-1/2}C^3(x)dx=p_0-p_1+\frac{13}{12}p_2-\frac{5}{4}p_3 \\ &at \ \ r=\ 0: \ \ C_i=\int_{-1/2}^{1/2}C^3(x)dx=p_0+\frac{1}{12}p_2 \\ &at \ \ r=\ 1: \ \ C_{i+1}=\int_{1/2}^{3/2}C^3(x)dx=p_0+p_1+\frac{13}{12}p_2+\frac{5}{4}p_3 \\ &at \ \ r=\ 2: \ \ C_{i+2}=\int_{-3/2}^{-1/2}C^3(x)dx=p_0+2p_1+\frac{49}{12}p_2+\frac{17}{2}p_3 \end{aligned} \qquad (11)$$

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$$
\begin{aligned}
p_0 &= \left(-C_{i+1} + 26C_i - C_{i-1}\right)/24 \\
p_1 &= \left(-5C_{i+2} + 27C_{i+1} - 15C_i - 7C_{i-1}\right)/24 \\
p_2 &= \left(C_{i+1} - 2C_i + C_{i-1}\right)/2 \\
p_3 &= \left(C_{i+2} - 3C_{i+1} + 3C_i - C_{i-1}\right)/6
\end{aligned}
\qquad (12)
$$

The rightmost flux is calculated exploiting r_i = (1 - $U_{i+1/2}$)/2; the Bott limiters (equation (5)) are applied, **normalization omitted**. Finally, the new time level concentration is calculated after equation (1).

Table 4. Polynomial coefficients and arguments for the other three schemes

Scheme	pattern	Polynomial coefficients		r_i – argument
Tr3_n2	**4-points, shifted, origin in point *i*+1/2**	$p_0 = \left(-C_{i+2} + 7C_{i+1} + 7C_i - C_{i-1}\right)/12$ $p_1 = \left(-C_{i+2} + 15C_{i+1} - 15C_i + C_{i-1}\right)/12$ $p_2 = \left(C_{i+2} - C_{i+1} - C_i + C_{i-1}\right)/4$ $p_3 = \left(C_{i+2} - 3C_{i+1} + 3C_i - C_{i-1}\right)/6$		r_i = -$U_{i+1/2}$/2
Tr2_n1	**3-point, origin in point *i***	$U_{i+1/2}>0$	$d_0 = \left(-C_{i-1} + 26C_i - C_{i+1}\right)/24$ $d_1 = \left(-C_{i-1} + C_{i+1}\right)/2$ $d_2 = \left(C_{i-1} - 2C_i + C_{i+1}\right)/2$	r_i = (1- $U_{i+1/2}$)/2
		$U_{i+1/2}<0$	$d_0 = \left(23C_i + 2C_{i+1} - C_{i+2}\right)/24$ $d_1 = \left(-3C_i + 4C_{i+1} - C_{i+2}\right)/2$ $d_2 = \left(C_i - 2C_{i+1} + C_{i+2}\right)/2$	
Tr2_n2	**3-points, shifted, origin in point *i*+1/2**	$U_{i+1/2}>0$	$d_0 = \left(-C_{i-1} + 5C_i + 2C_{i+1}\right)/6$ $d_1 = -C_i + C_{i+1}$ $d_2 = \left(C_{i-1} - 2C_i + C_{i+1}\right)/2$	r_i = -$U_{i+1/2}$/2
		$U_{i+1/2}<0$	$d_0 = \left(2C_i + 5C_{i+1} - C_{i+2}\right)/6$ $d_1 = -C_i + C_{i+1}$ $d_2 = \left(C_i - 2C_{i+1} + C_{i+2}\right)/2$	

NUMERICAL EXPERIMENTS

The described variants of TRAP scheme have passed the two-dimensional rotational test (*Smolarkiewicz*, 1982). Instantaneous releases with cone-shaped initial profile are rotated over a grid field of 101×101 points with Δx=Δy=1. The wind rotates with a constant angular velocity $\omega \approx 0.1$ (~600 time steps per rotation) centered at point (51, 51). Keeping in mind that the initial concentration field C^0_{ij} is the exact solution of the advection equation after one or several full rotations, the following criteria for estimation of the simulation quality are established:

Table 2. Estimates for simulation quality of numerical advection schemes (rotational test)

Estimate	Meaning
Cmax = max(C_{ij})/max(C^o_{ij})	**Cmax**<1 – presence of numerical diffusion
Cmin = min(C_{ij})/max(C^o_{ij})	**Cmin**<0 absence of positive definiteness
CM = $(\sum_{ij} C^o_{ij} - \sum_{ij} C_{ij}) / \sum_{ij} C^o_{ij}$	**CM** - normalized difference of masses. **CM**≠0 denotes absence of conservativeness
DXc = $\sum_{ij} iC_{ij} / \sum_{ij} C_{ij} - \sum_{ij} iC^o_{ij} / \sum_{ij} C^o_{ij}$ **DYc** = $\sum_{ij} jC_{ij} / \sum_{ij} C_{ij} - \sum_{ij} jC^o_{ij} / \sum_{ij} C^o_{ij}$	**DXc** and **DYc** estimate the displacement of the mass centre due to numerical effects. **DXc** = **DYc** = 0 after a full rotations indicate ideal transport ability
T = $\Delta T_{calculation}/\Delta T^{ref}$,	Relative speed of performance, ΔT^{ref}=ΔT^{TrB}

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Table 3. Values of the simulation quality estimates after six rotations.

Persents (%)		*TrB*	*Tr3_n1*	*Tr3_n2*	*Tr2*	*Tr2_n1*	*Tr2_n2*
Cone shape (6 rotations)	**Cmax**	85.9	89.1	89.1	81.3	80.8	80.8
	Cmin	0.0	0.0	0.0	0.0	0.0	0.0
	CM	-0.8	-0.2	-0.2	-1.2	-0.8	-0.8
	DXc	-0.16	-0.16	-0.16	-0.15	-0.15	-0.15
	DYc	0.52	0.52	0.52	0.52	0.52	0.52
	T	100	43.4	41.5	48.2	35.1	34.6

In *Table 3*, the cone-source values of these static estimates are presented. Experiments with other initial shapes – Gaussian, point, cylinder, cube etc. are made as well. None of these schemes rotates the point source (absolute discontinuity) well. All schemes give their best results on the gauss shape (absolute smoothness) and more or less good ones on the cone shape (intermediate case). One can see that the two 3rd degree self-normalizing schemes (***Tr3_n1*** and ***Tr3_n2***) perform the rotations best, considering all criteria. They are rather fast and their conservation of mass characteristics are very satisfying, but they are not very good in rotating sharp gradients. The self-normalizing schemes of 2nd degree are very fast and describe well the rotation of shapes with discontinuity.

All these schemes have successfully passed the deformational test of *Smolarkiewicz* (1982), as well. They are modified to be able to work on non-homogeneous grid (*Syrakov*, 2003).

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