A method for numerical solution of the advection equation

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ABSTRACT

The advection of substances in a fluid computed with a finite grid resolution is known to smooth out concentration gradients. A numerical method based on the determination of the zero, first and second order moments of the concentration in each cell is shown, through various 2-dimensional numerical experiments, to suppress the spatial truncation error substantially.

1. Introduction

B. R. Egan and J. R. Mahoney (1972) have developed a method of solving the problem of the transport of atmospheric pollutants. We have adapted their method as a basis for a further development which consists in a generalization to two dimensions, an approximative introduction of source and drain terms, and width correction which under certain conditions improves the calculational scheme.

We show some examples of the usefulness of the method by comparing with other methods and by a comparison between the analytic solution (which can be found for simple fields) and the numerical solution.

Generally speaking, eulerian difference schemes are applied to the solution of the advection equation. Sources and sinks of the pollutant in question are then easily attachted to the fixed, underlying coordinate system, as opposed to lagrangian schemes where the coordinate system moves with the mass of air in question. Eulerian difference schemes introduce, however, a numerical truncation error (pseudodiffusion) tending to smooth out any gradients of concentration of pollutants.

One of the most simple numerical methods to advect in an eulerian mesh is to move the mass in each cell in the direction of the velocity vector. The spatial average concentration in each cell is computed after every time step by accumulating the advected contributions from the neighbouring cells and taking into account the loss from itself by advection. This "Mass in Cell"-method (MIC) combines the lagrangian movement of the pollutant in the direction of the velocity vector with the fixed, underlying coordinate system. The MIC-method can be considered a special case of the "Particle in Cell Method" (Sklarew, 1971), which is a quasi-lagrangian method.

The spatial truncation error creates a pseudo-diffusion in the direction of the velocity vector. The normally used simple difference approximation methods (see e.g. Richtmyer, 1962), which move masses in the direction of the axes of the coordinate system, create a pseudodiffusion predominantly in the direction of these, however.

The method devised by Egan & Mahoney (1972) can be regarded as an extension of the MIC method, because not only is the mass in each cell accounted for, but also certain features of the mass distribution in each cell are taken into account. We can categorize the method as quasi-lagrangian, i.e. the masses are moved lagrangian in one time step, but a decomposition to the eulerian grid is performed immediately afterwards.

Apart from diffusion terms the differential equation governing the horizontal advection of atmospheric pollutants is given by

$$\frac{\partial c}{\partial t} = -\mathbf{v} \cdot \nabla c \qquad (1)$$

where c is the concentration of the pollutant and $\mathbf{v}$ is the horizontal component of the wind velocity.

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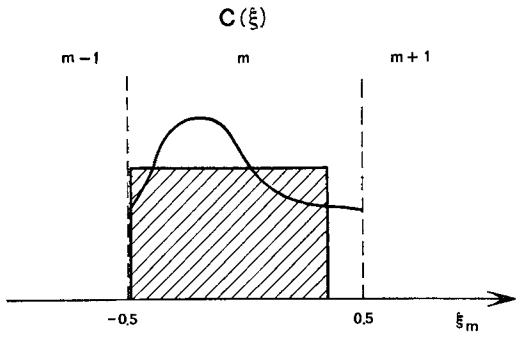

Fig. 1. An arbitrary distribution $C(\xi)$ in cell m is represented by the hatched rectangular distribution with the same area, centre of mass, and width.

In eq. (1) we have neglected source terms, deposition, and reaction terms. These terms, however, are easily incorporated in the numerical scheme, thus it is unnecessary to carry them along in the theoretical discussion of the scheme.

It is noted that eq. (1) is valid only in a non-divergent velocity field, which is the case for an incompressible fluid in three dimensions. If the horizontal velocity field is divergent, eq. (1) is still valid, providing suitable corrections are made. For instance, the mixing depth of the fluid could be determined from the vertical velocity component (Grønskei et al., 1973), or a vertical flux of mass could be found in a similar way.

2. General description of the advection procedure in one dimension

With the notation of Egan & Mahoney (1972) we replace the arbitrary distribution $C(\xi)$ in cell m, shown in Fig. 1, by a rectangular distribution of the same mass C_m, the same centre of mass F_m, and the same width R_m. It is advantageous to define the width R_m as the square root of the second moment of the distribution around the centre of mass (the first moment), multiplied by 12. We hereby achieve that a rectangular distribution across the interval $(-\frac{1}{2}, \frac{1}{2})$ has the width 1. Formally we can write as follows:

$$C_m = \int_{-0.5}^{0.5} C(\xi)\, d\xi \tag{2}$$

$$F_m = \int_{-0.5}^{0.5} C(\xi)\, \xi d\xi / C_m \tag{3}$$

$$R_m^2 = 12 \int_{-0.5}^{0.5} C(\xi)\, (\xi - F_m)^2\, d\xi / C_m \tag{4}$$

Following Egan & Mahoney, the advection is described by the so-called portioning parameter P_m, defined through the following equation (see Fig. 2).

$$P_m = \frac{2 \operatorname{sign}(\sigma_m)\,(F_m + \sigma_m) + R_m - 1}{2R_m} \tag{5}$$

P_m denotes how large a fraction of the material in cell m has been transferred to the neighbouring cell $m + 1$ sign (σ_m), sign $(\sigma_m) = 1$ for $\sigma_m \geqslant 0$, and sign $(\sigma_m) = -1$ for $\sigma_m < 0$. A closer investigation reveals that the above definition of P_m is true if $0 < P_m < 1$. If $P_m \leqslant 0$, no material is transferred to the neighbouring cell at all, while $P_m \geqslant 1$ implies that all the material is transferred. It is seen that a greater accuracy is achieved, if the velocity in the centre of mass, F_m, is used to determine σ_m. Usually the velocity in the centre of the cell has been applied.

3. Incorporation of source terms in the advection procedure

Let us assume that a source of source strength Q_m per unit of length is placed in cell m. We assume furthermore that Q_m is independent of position in the cell and independent of time. Under these conditions we get a mass distribution as shown in Fig. 3.

After some arithmetic we find the exact formulae for the masses, the centres of mass and the widths to be given by the following equations, where the sign ":=" should be read "contributions to":

Cell m

$$C := (1 - |\sigma_m|/2)\, Q_m \Delta t$$

$$F := \sigma_m/6\, \frac{3 - 2\sigma_m}{2 - \sigma_m}$$

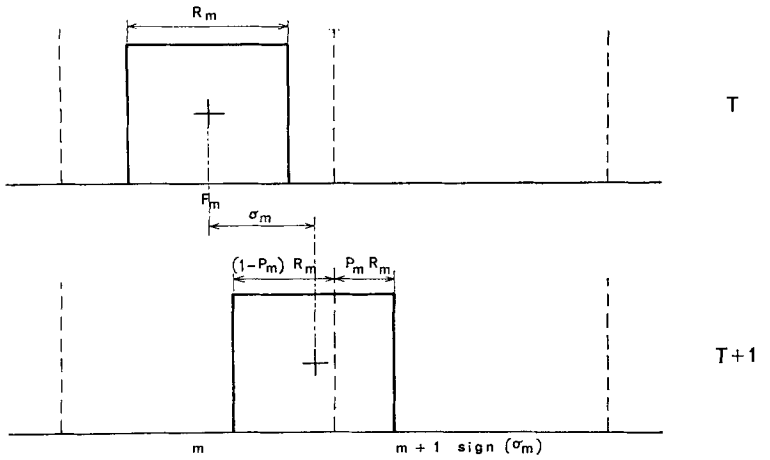

Fig. 2. Graphical explanation of the portioning parameter.

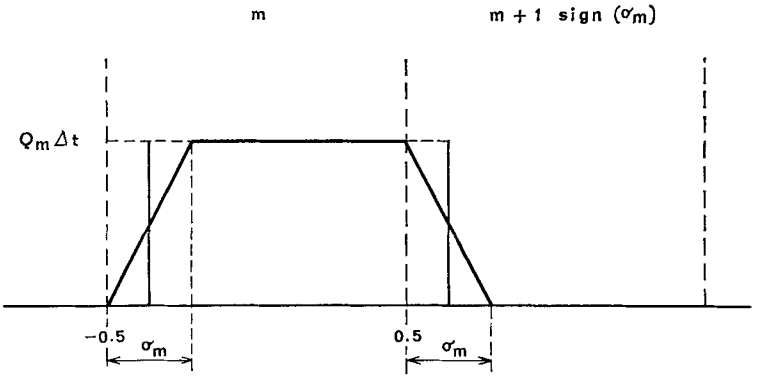

Fig. 3. Heavily drawn curve represents the true distribution of source contribution from cell m, after time Δt. Rectangular curve approximates the true distribution subject to mass conservation.

$$R^2 := \frac{\frac{\sigma_m^3}{27} + (1-\sigma_m)^3}{1-\sigma_m/2} + \frac{6\sigma_m\left(\frac{(\sigma_m-1)(\sigma_m-3)}{3(2-\sigma_m)}\right)^2 + 4(1-\sigma_m)\sigma_m^2\left(\frac{1+\sigma_m}{2-\sigma_m}\right)^2}{1-\sigma_m/2} \tag{6}$$

Cell $m+1$ sign (σ_m)

$$C := Q_m \Delta t\,|\sigma_m|/2$$

$$F := -\tfrac{1}{2}\,\text{sign}\,(\sigma_m) + \sigma_m/2 \tag{7}$$

$$R^2 := \sigma_m^2\ 6/81$$

A fair approximation to the exact picture, expressed in eqs. (6) and (7), is achieved by approximating the "triangles" with rectangles of the same area, i.e. the mass distribution is approximated under the condition of mass conservation. We then arrive at the following formulae which are easy to calculate:

Cell m

$$C := (1-|\sigma_m|/2)Q_m \Delta t$$
$$F := \tfrac{1}{2} - \tfrac{1}{2}(1-\sigma_m/2) = \sigma_m/4 \tag{8}$$
$$R := 1 - |\sigma_m|/2$$

Cell $m+1$ sign (σ_m)

$$C := \tfrac{1}{2}|\sigma_m| Q_m \Delta t$$
$$F := -\tfrac{1}{2}\,\text{sign}\,(\sigma_m) + \sigma_m/2 \tag{9}$$
$$R := |\sigma_m|/2$$

4. Sinks

Often an atomic or chemical chain of reactions is described by a set of coupled, linear differential equations. If we look at a chain with two species, A and B, where B's source Q_B is proportional to A's sink, D_A, i.e. $Q_B = k_{BA} D_A$, then we arrive at the following advection equations:

$$\frac{\partial C_A}{\partial t} = -\mathbf{v} \cdot \nabla C_A + Q_A - D_A \tag{10}$$

$$\frac{\partial C_B}{\partial t} = -\mathbf{v} \cdot \nabla C_B + k_{BA} D_A - D_B \tag{11}$$

The sulphur concentration has often been applied as an indicator of atmospheric pollution. A good approximation would be: the total amount of sulphur is equal to the sum of sulphur dioxide and sulphate ions. Eqs. (10) and (11) will then describe the state of sulphur in the atmosphere both spatially and temporally.

5. Incorporation of sink terms in the advection procedure

When treating the sink terms we shall distinguish the mass emitted in a previous step from the mass just emitted from the sources. We shall neglect sinks from the latter and consider only the former.

In the SO_2/SO_4^{--} system, SO_2 sinks are often described by an equation of the following form:

$$D_m = (\alpha_1 C_m + \alpha_2 C_m^2)\,\Delta t \tag{12}$$

where α_1 and α_2 are determined from measurements, and C_m is the mass of SO_2 in cell m. The form of eq. (12) can be interpreted as the first two terms of a power series. The two terms may also be interpreted one at a time. $\alpha_1 C_m$ represents the deposition of SO_2, and $\alpha_2 C_m^2$ the chemical transformation of SO_2 to SO_4. In the further treatment we shall adopt the former interpretation, assuming that all the SO_2 has been transformed into SO_4^{--}. In this way the SO_2 sink is simply considered a source for SO_4^{--}. We also assume that the total mass C_m is advected as the two contributions C_1 and C_2, C_1 assigned to cell m and C_2 to cell $m+1$ sign (σ_m). The corresponding centres of mass and widths are named F_1, R_1 and F_2, R_2 respectively. We find the sink terms D_1 and D_2 as follows:

$$D_1 = (\alpha_1 C_m + \alpha_2 C_m^2)\frac{C_1}{C_m}$$

$$D_2 = (\alpha_1 C_m + \alpha_2 C_m^2)\frac{C_2}{C_m} \tag{13}$$

Then we can find the corrected values of C_1 and C_2

$$C_1 := C_1 - D_1$$

$$C_2 := C_2 - D_2 \tag{14}$$

But the values of F_1, R_1 and F_2, R_2 will not be corrected, as we assume the sink comprises only a small part of the total mass in the cell. The terms (D_1, F_1, R_1) and (D_2, F_2, R_2) are attached to SO_4^{--} as source terms. In the same way we write for the SO_4^{--} sink:

$${}^{D}SO_4^{--} = (\beta_1 C_m + \beta_2 C_m^2)\,\Delta t \tag{15}$$

As in the SO_2 case, the term (15) only works on the mass emitted in previous time steps.

When connecting the formulae, representing the advection of mass released in previous time steps (corrected for sink terms) and those representing the advection of mass just released (source terms) we find:

$$C^{T+1} = \sum C_i \tag{16}$$

$$F^{T+1} = \frac{\sum C_i F_i}{C^{T+1}} \tag{17}$$

$$(R^{T+1})^2 = \frac{\sum C_i R_i^2}{C^{T+1}} = 12\left(\frac{\sum C_i F_i^2}{C^{T+1}} - \left(\frac{\sum C_i F_i}{C^{T+1}}\right)^2\right) \tag{18}$$

6. Width correction

When we defined the portioning parameter, P, it was implicitly assumed that the width of the mass distribution, R, had such a magnitude that there were no "ends" protruding into neighbouring cells as shown in Fig. 4.

Assume that the contributions in cell m appear as shown in Fig. 4 (---). This distribution is equivalent to the rectangular distribu-

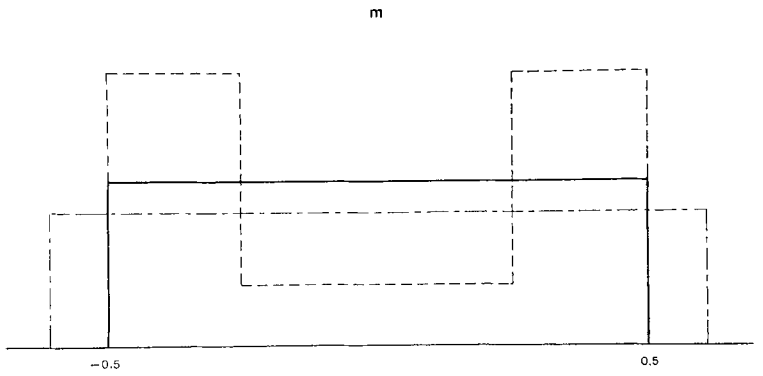

Fig. 4. Original mass distribution (---). Equivalent mass distribution (– – –). Width-corrected mass distribution (——).

tion (– – –). In order to move the mass sufficiently correctly at small velocities, using the portioning parameter notation, the rectangular distribution is contracted to: (——) subject to mass conservation and centre of mass conservation. Genererally, the correction above is made, when $R/2 > \min|F \pm \frac{1}{2}|$. Put $R_{\max}$ equal to $2 \min|F \pm \frac{1}{2}|$, then the correction can be written:

$$R = R_{\max} \tag{19}$$

Without width correction there might be advection in the limit $\sigma_m \to 0$, as P_m calculated from eq. (5) might become positive, was R greater than $R_{\max}$. Going back to the physical reason for introducing the portioning parameter, the above-mentioned advection is not wanted, because $\sigma_m \to 0$ corresponds to no advection at all. On the other hand, $R \geqslant R_{\max}$ reveals that the mass distribution is pushed towards the walls. In this case a relatively small velocity would cause a relatively large advection, and it would be inappropriate to make the width correction. In an actual case it might be difficult to decide whether to apply the width correction or not, as we shall see from the numerical experiments later.

7. General description of the advection procedure in two dimensions

As in the 1-dimensional case we use the two portioning parameters P_x and P_y, suppressing indices m and n:

$$P_x = \frac{2 \operatorname{sign}(\sigma_x)(F_x + \sigma_x) + R_x - 1}{2R_x} \tag{20}$$

$$P_y = \frac{2 \operatorname{sign}(\sigma_y)(F_y + \sigma_y) + R_y - 1}{2R_y} \tag{21}$$

In the most common case, where $0 < P_x < 1$ and $0 < P_y < 1$ the advection from cell m to its neighbouring cells is found from formulae analogous to those given by Egan & Mahoney (1972).

When P_x and/or P_y are greater than 1 and/or less than zero, we must apply different equations to calculate the advection. Formally, we can treat the above-mentioned cases by using the set of formulae referred to above. These formulae will also be correct in the cases P_x, $P_y \geqslant 1$ and $P_x, P_y \leqslant 0$, if we put P_x, P_y equal to one and zero respectively. The only exceptions are the equations for the centre of mass, which have to be modified. The formulae for the advection of source terms (area sources) also become quite analogous to the formulae for the line sources in 1 dimension, (8) and (9), as to the formulae for calculating the total contributions in each cell at the following time step, (16), (17), and (18). A detailed description of the computing procedure is given by Pedersen & Prahm (1973).

8. Numerical experiments

In order to illustrate the accuracy of the advection procedure we have calculated the advection in two cases with different initial

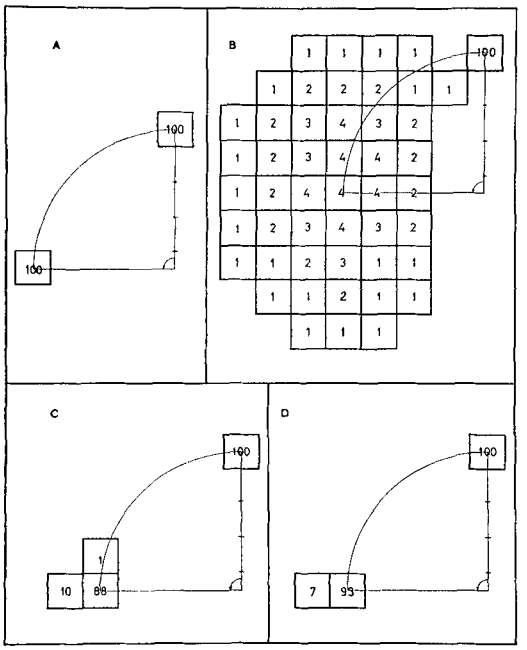

Fig. 5. Advection of a single particle of mass in a circular velocity field. $\Omega = 0.001$, $\Delta t = 30$, $T = 50$. (A) Analytical solution. (B) MIC method. (C) New advection procedure without width correction. (D) New advection procedure with width correction.

conditions, but in the same velocity field. Furthermore, we have studied a case with a continuous source. In all 3 examples the analytical solution is compared with 3 numerical methods:

(*a*) The chosen examples all have an analytical solution.

(*b*) The described advection procedure with decoupling of the first and second moment, i.e. without using the centre of mass, and the width in defining the portioning parameter. Instead, we define $P_x = |\sigma_x|$ and $P_y = |\sigma_y|$. The method is then reduced to the "Mass in Cell' method, as referred to earlier in the introduction. The pseudodiffusion achieves a magnitude dependent on the time step and the grid length.

(*c*) The described advection procedure without use of width correction.

(*d*) The described advection procedure, using width correction.

Example 1

Advection of a single particle of mass in a circular velocity field, which is given by:

$$\mathbf{v} = \Omega r \tag{22}$$

We have chosen $\Omega = 0.001$ sec^{-1} and to place the particle of mass = 100 in the cell $(m, n) = (0, 4)$. We use a time step $\Delta t = 30$ sec, whereby $\sigma_{\max} = 0.12$, ensuring the numerical stability. The stability criterion is

$$\sigma < 1 \tag{23}$$

The results from the methods (*a*), (*b*), (*c*), and (*d*) are seen in Fig. 5. The MIC method moves only 4% of the mass to the wanted cell, the rest is spread over an area of about $6 \times 9 = 54$ cells. A much better result is obtained in (*c*) using 1st and 2nd moments. Here, 88% of the mass is in the wanted cell. The incorporation of the width correction (*d*) improves the result even further. Now only 7% of the mass is situated outside the wanted cell.

Example 2

The initial conditions in this example have been taken from Molenkamp (1968), where a mass distribution is rotated through an angle. At time $T = 0$ we have:

$$A_0(x, y) = \begin{cases} 100(1 - 1/4r'') & r'' < 4 \\ 0 & r'' \geq 4 \end{cases} \tag{24}$$

where $r'' = ((x - x')^2 + (y - y')^2)^2)$, and (x', y') have been chosen so that the centre of the velocity field lies outside the mass distribution $A_0(x, y)$. In the actual case we use the following: $(x', y') = (0, 5)$, and like in example 1: $\Delta t = 30$, $\Omega = 0$, 001, $T = 40$. The analytical solution is naturally given by a new pyramidal mass distribution, turned approximately 72° compared with the original distribution.

Fig. 6A shows the rotation using the MIC method. The analytical solution is marked by the concentric circles. The inner circle corresponds to the value 80, the middle circle to 50 and the outer circle to 20. The centre cell of the pyramid has the value 100 in the analytical solution, while the MIC method has only retrieved about 45%. Fig. 6B and Fig. 6C show the results of the new advection procedure with and without the width correction. Without width correction a larger value is obtained in the centre cell than is the case with width correction. However, the mass is spread over a larger area without width correction than with width correction.

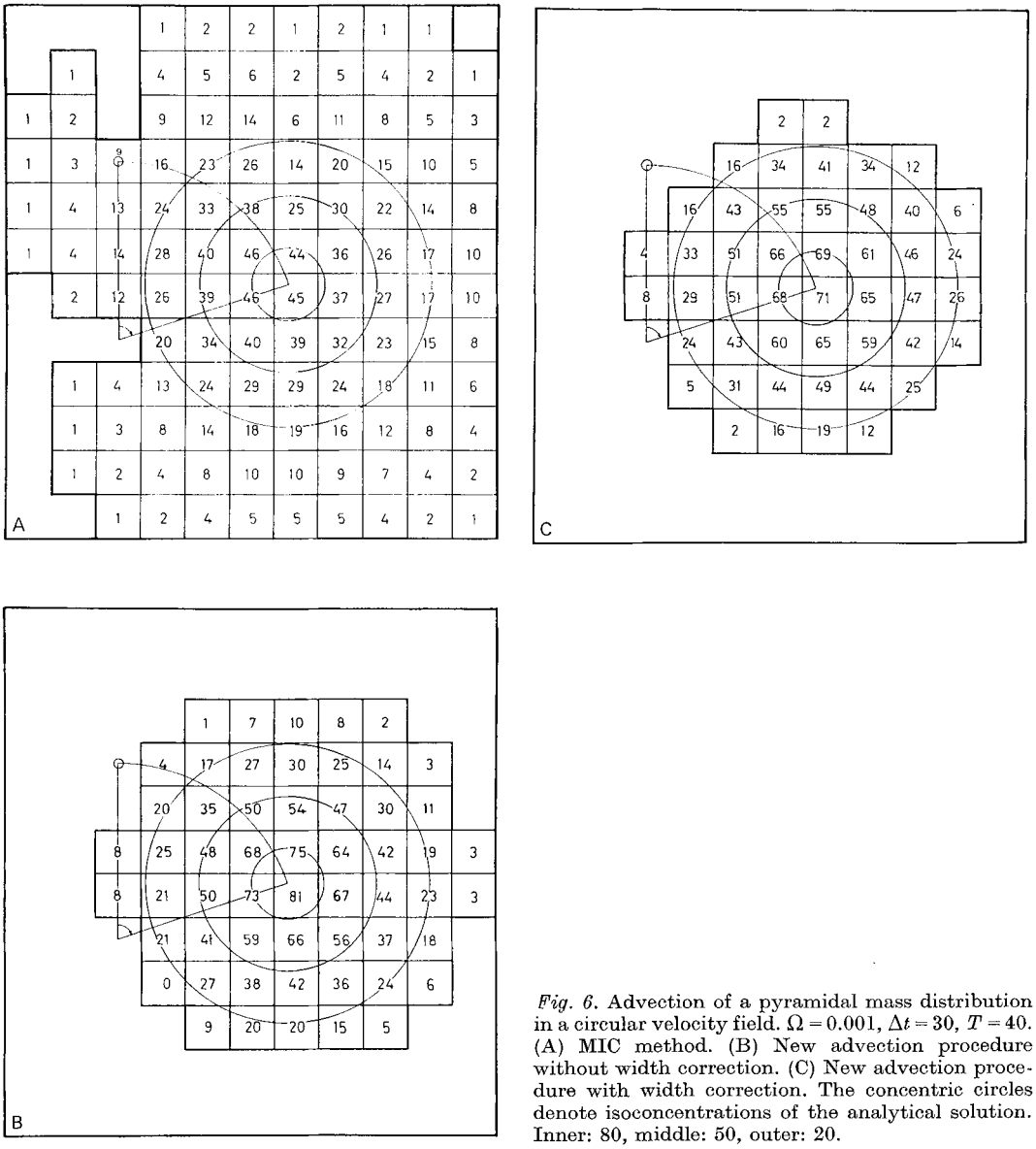

Fig. 6. Advection of a pyramidal mass distribution in a circular velocity field. $\Omega = 0.001$, $\Delta t = 30$, $T = 40$. (A) MIC method. (B) New advection procedure without width correction. (C) New advection procedure with width correction. The concentric circles denote isoconcentrations of the analytical solution. Inner: 80, middle: 50, outer: 20.

Example 3

In this example we place 6 sources of source strength $Q = 1$ as shown in Fig. 7. We use a velocity field $\mathbf{v} = (1,1)$, a time step $\Delta t = \frac{1}{2}$ and $T = 40$. Fig. 7A shows the analytical solution for $t \to \infty$. In Fig. 7B, 7C, and 7D we see the numerical solution using the MIC method, and the new method without and with width correction.

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This work was initiated in connection with the OECD NORDFORSK projects concerning transport of atmospheric pollutants.

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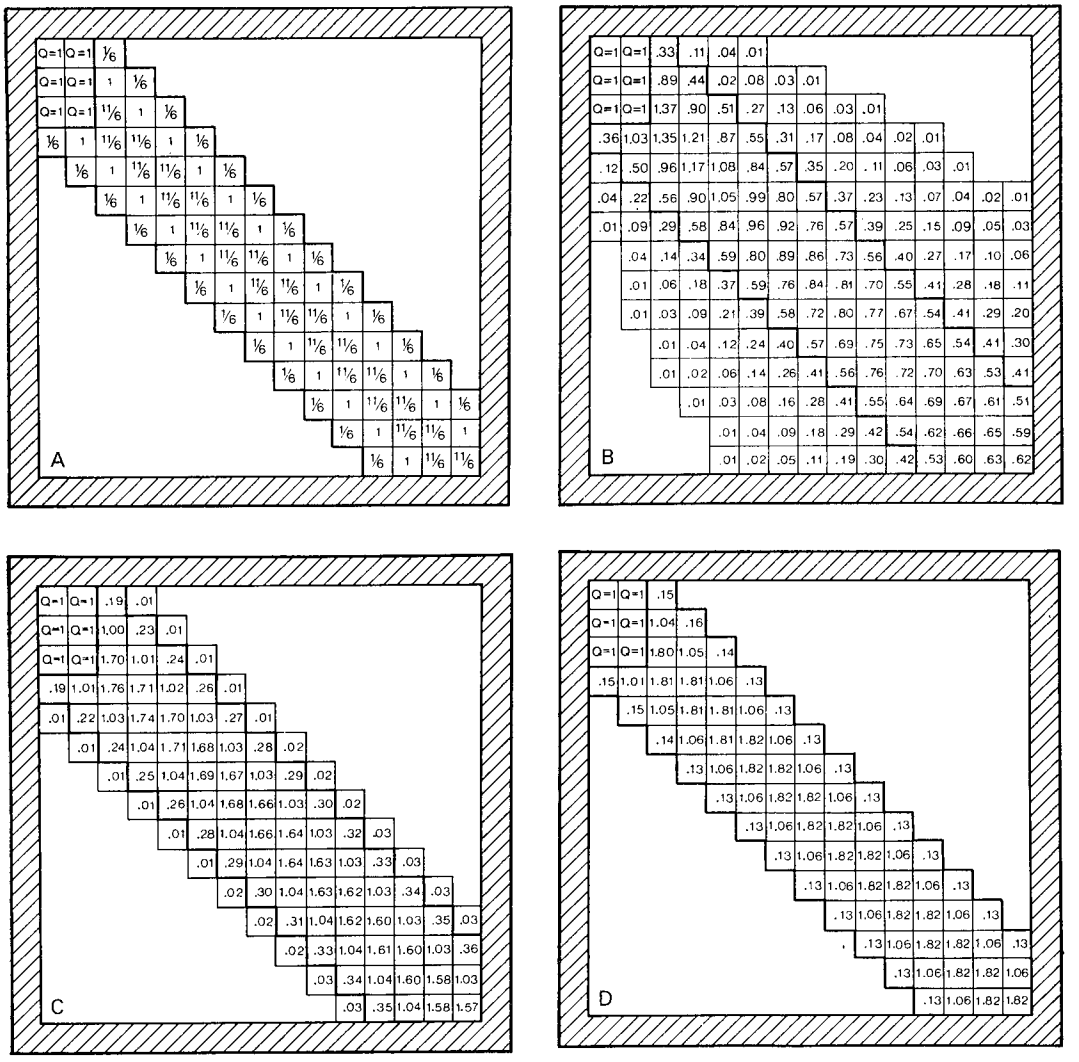

Fig. 7. Advection from a source field, $Q = 1$ situated in the top left-hand corner. The velocity field is homogeneous $(v_x, v_y) = (1,)$, $\Delta t = \frac{1}{2}$, $T = 40$. (A) Analytical solution for $t \to \infty$. (B) MIC method. (C) New advection procedure without width correction. (D) New advection procedure with width correction.

cussions and for drawing our attention to other publications in this field. Many thanks for helpful discussions must also be offerred to the modelling group in Oslo: J. Eliassen, R. O. Jensen, J. Nordø, and J. Saltbones.

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МЕТОД ЧИСЛЕННОГО РЕШЕНИЯ УРАВНЕНИЯ АДВЕКЦИИ

Известно, что вычисление адвекции субстанции в жидкости с постоянным разрешением сетки приводит к сглаживанию градиентов концентрации. С помощью различных двумерных численных экспериментов показано, что численный метод, основанный на определении моментов концентрации нулевого, первого и второго порядков в каждой ячейке, существенно подавляет ошибки пространственной аппроксимации.