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Bartnicki, J.

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PREFACE

Under a collaborative agreement with the Institute for Meteorology and Water Management, Warsaw (Poland), Jerzy Bartnicki works with IIASA's Acid Rain Project on modeling atmospheric transport and deposition of pollutants. This paper reports on a new method for solution of the advection equation of an air pollution transport model. This new method turned out to be a useful tool in the uncertainty analysis of the RAINS (Regional Acidification INformation and Simulation) model carried out in the project.

Leen Hordijk
Leader, Acid Rain Project

ACKNOWLEDGEMENTS

I would like to thank Krzysztof Abert from the Institute of Meteorology and Water Management in Warsaw for many valuable discussions about the method and especially about the filtering procedure. I am also very grateful for all comments and remarks of my colleagues from IIASA, and in particular, I wish to acknowledge the contribution of Maximilian Posch who provided me with the three-dimensional graphics used in this paper. I would also like to express my gratitude to Dr. Jerzy Pruchnicki from the Institute for Meteorology and Water Management in Warsaw who supported part of the work done in Warsaw. Finally I would like to thank Dr. Leen Hordijk who agreed to review the entire manuscript of this paper.

ABSTRACT

A numerical Positive Definite Pseudo-Spectral (PDPS) method for the solution of the advection equation is presented. The method consists of two parts. For each time step first a solution using a pseudospectral method is computed. Then the solution is corrected by a filtering procedure which eliminates negative values. The numerical test with the rotational velocity field and different initial conditions shows that the present method has the accuracy of the pseudospectral one without producing negative values. An additional advantage of the PDPS method is the elimination of spurious artificial shortwaves typical for the pseudospectral solution.

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AN EFFICIENT POSITIVE DEFINITE METHOD FOR THE NUMERICAL SOLUTION OF THE ADVECTION EQUATION

Jerzy Bartnicki

1. INTRODUCTION

The partial differential advection-diffusion equation is most frequently used for the mathematical description of the long range transport of air pollutants. This equation is also a basic one for the atmospheric part of the IIASA RAINS (Regional Acidification INformation and Simulation) model described by Alcamo et. al. (1985) and Hordijk (1985). The atmospheric module of RAINS consists of the source-receptor matrices computed by MSC-W (Meteorological Synthesizing Centre-West) in Oslo, using the Long Range Transport (LRT) model developed by Eliassen and Saltbones (1983). This LRT trajectory model is used by the Co-operative Programme for Monitoring and Evaluation of the Long Range Transmission of Air Pollutants in Europe (EMEP) for routine calculations. In order to use this or any other LRT model within RAINS, it is important to evaluate the uncertainty and

credibility of the results. Among different types of sources of uncertainty in LRT models the error introduced by the numerical method used to solve the advection-diffusion equation can be an important one, especially for models with nonlinear chemical reactions.

The main goal of this paper is to present a numerical method which can be used for the solution of the advection-diffusion equation without producing negative values. Therefore the method could be applied to nonlinear problems as well with high accuracy typical for the pseudospectral approach and without losing stability (which occurs when negative values appear). When solving the advection-diffusion equation, the diffusive part is relatively less important than the advective part concerning numerical problems. Also from the physical point of view, in the synoptic scale of motions, the diffusion term is small compared to the advective one and is even neglected in some models (e.g. in the MSC-W model). Therefore only an application of the method to the advection equation is presented in this paper, however, it can be used for the advection-diffusion equation as well.

2. NUMERICAL METHOD

Among many different methods used for the numerical solution of the advection equation, the spectral (Orszag, 1971a) and pseudospectral (Gottlieb and Orszag, 1977) approach are relatively efficient and accurate. The accuracy of these methods is better compared with finite difference methods (Orszag, 1971b), and also to other methods (Long and Pepper, 1981; Chock, 1985). Another advantage of the spectral methods is the simple mathematical formulation which makes them convenient for practical applications, especially when using numerical Fast Fourier Transform (FFT) (Coo-

ley and Tukey, 1965). Spectral and pseudospectral methods have been successfully applied to the air pollution transport models by Christensen and Prahm (1976) and Wangle et al. (1978). Unfortunately, the accurate pseudospectral and spectral methods can produce negative values during the numerical solution of the advection equation. For many practical problems, like air pollutant transport involving nonlinear chemistry, this phenomenon makes the pseudospectral method unstable. There are other methods, like the flux-corrected transport (FCT) method (Boris and Book, 1976; Zalesiak, 1979) and a positive definite algorithm developed by Smolarkiewicz (1984) that can be applied in this case. However, these methods either require a long computational time or are significantly less accurate than the pseudospectral solution. This paper presents a combined numerical method: The Positive Definite Pseudo-Spectral (PDPS) method, which eliminates completely negative values on one hand, and is of the same order of accuracy as a pseudospectral approach, on the other hand.

2.1. Problem Formulation

The multidimensional advection equation to be solved has the following form:

$$\frac{\partial c}{\partial t} + \sum_{j=1}^{N} u_j \frac{\partial c}{\partial x_j} = 0 \qquad (1)$$

where $c = c(\boldsymbol{x},t)$ is the concentration (could be arbitrarily scalar),

assumed to be non-negative.

$u_j = u_j(\boldsymbol{x},t)$ is the j-th velocity component

$(\boldsymbol{x},t) = (x_1,\ldots,x_N,t)$ are the space and time coordinates

The numerical method presented in this paper involves two basic steps at each time step when solving equation (1):

(1) The pseudospectral method is applied to equation (1) at time t and a solution which contains also negative values of the concentration is achieved.

(2) The filtering procedure, which removes all negative values of the concentration, is used to get the solution at time $t+\Delta t$.

Let $c^m = c(\boldsymbol{x}, m\,\Delta t)$ be the concentration field with periodic boundary conditions at time $m\,\Delta t$. We are looking for the concentration $c^{m+1} = c(\boldsymbol{x}, (m+1)\Delta t)$ at time $(m+1)\Delta t$ in the uniform mesh of size $M_1 \times M_2, \ldots, \times M_N$ where the location of the mesh points is given by:

$$x_j = m_j\,\Delta x_j; \quad m_j = 0,1,2,\ldots, M_j - 1 \tag{2}$$

where

$$\Delta x_j = \frac{2\pi}{M_j} \tag{3}$$

for any $j = 1,2,\ldots,N$.

The pseudospectral method can be represented by an operator $\hat{P}$ which, applied to the discrete concentration field c^m at time $m\,\Delta t$, produces the concentration $\tilde{c}^{m+1}$ at time $(m+1)\Delta t$:

$$\tilde{c}^{m+1} = \hat{P}(c^m) \tag{4}$$

The concentration $\tilde{c}^{m+1}$ can still include negative values. The filtering procedure can be represented by the operator $\hat{F}$ which transforms $\tilde{c}^{m+1}$ to c^{m+1} containing non-negative values only:

$$c^{m+1} = \hat{F}(\tilde{c}^{m+1}) \tag{5}$$

Thus, the positively defined pseudospectral method can be defined as:

$$c^{m+1} = \hat{F} \cdot \hat{P}(c^m) \tag{6}$$

In principle the operator $\hat{P}$ can represent also other methods, not only the pseudospectral method. However, because of its simplicity and accuracy, the pseudospectral approximation is a rather efficient one for the numerical solution of equation (1).

2.2. Pseudospectral Solution

The pseudospectral approach developed by Gazdag (1973) has been chosen as the operator $\hat{P}$. The principle of Gazdag's method is to approximate the time derivatives by a truncated Taylor series, and then replace the time derivatives by the space derivative terms, which are computed using the spectral method. Mathematically the method can be described as follows. Assuming that we know the concentration c^m at time $m\,\Delta t$, the concentration c^{m+1} at the next time step $(m+1)\Delta t$ can be approximated by the truncated Taylor series

$$c^{m+1} = c^m + \frac{\partial c^m}{\partial t} \cdot \Delta t + \frac{\partial^2 c^m}{\partial t^2} \cdot \frac{\Delta t^2}{2!} + \tag{7}$$
$$+ \frac{\partial^3 c^m}{\partial t^3} \cdot \frac{\Delta t^3}{3!} + \cdots + \frac{\partial^p c^m}{\partial t^p} \cdot \frac{\Delta t^p}{p!}$$

Following Gazdag (1973), the time derivatives of c can be expressed in terms of the space derivatives of c and u_j by making use of equation (1):

$$\frac{\partial c}{\partial t} = -\sum_{j=1}^{N} u_j \frac{\partial c}{\partial x_j} \tag{8}$$

$$\frac{\partial^2 c}{\partial t^2} = -\sum_{j=1}^{N} \left\{ \frac{\partial u_j}{\partial t} \cdot \frac{\partial c}{\partial x_j} + u_j \frac{\partial}{\partial x_j} \cdot \frac{\partial c}{\partial t} \right\} \tag{9}$$

. .

. .

$$\frac{\partial^{l+1} c}{\partial t^{l+1}} = -\sum_{j=1}^{N} \sum_{r=0}^{l} \binom{l}{r} \frac{\partial^r u_j}{\partial t^r} \cdot \frac{\partial}{\partial x_j} \left[\frac{\partial^{l-r} c}{\partial t^{l-r}} \right] \tag{10}$$

The superscript m has been omitted in the above equations for convenience. Equations (8-10) show how to compute any order time derivative of c from the lower order time derivatives of u_j and c. The first order time derivative of c can be computed directly from the basic advection equation. It remains only to compute space derivatives of c which is done with the spectral method. Denoting the set of all grid points (Equations 2-3) by R, the finite Fourier transform C of c can be written as

$$C(\boldsymbol{k},t) = \frac{1}{M_1 \cdot M_2 \cdot \cdots \cdot M_N} \cdot \sum_{\boldsymbol{x} \in R} c(\boldsymbol{x},t) \exp(-i\, \boldsymbol{k} \cdot \boldsymbol{x}) \tag{11}$$

where $i = \sqrt{-1}$ and $\boldsymbol{k}$ is the wave vector

$$\boldsymbol{k} = (k_1,\ldots,k_j,\ldots,k_N) \tag{12}$$

whose components assume integer values within the limits

$$-K_j < k_j \leq K_j; \quad K_j = \frac{M_j}{2} \tag{13}$$

From $C(\boldsymbol{k},t)$ the partial derivatives of $c(\boldsymbol{x},t)$ can be computed as

$$\frac{\partial c(\boldsymbol{x},t)}{\partial x_j} = \sum_{|k_j| < K_j} i \cdot k_j\, C(\boldsymbol{k},t) \exp(i\boldsymbol{k} \cdot \boldsymbol{x}) \tag{14}$$

The numerical computation of the space derivatives described by Equations (11-14) can be carried out sufficiently fast by the use of the numerical Fast Fourier Transform (FFT, Cooley and Tukey, 1965). According to Gazdag (1973) it gives very accurate results and therefore he called it Accurate Space Derivative (ASD) method.

2.3. Filtering Procedure

The pseudospectral method described in the previous paragraph provide the concentration in the grid system at time $(m+1)\Delta t$, assuming that the concentration at time $m\Delta t$ is known (also the velocity and its time derivatives). Unfortunately, the new concentration field may contain negative values. The presence of negative concentrations is a common phenomenon for different numerical methods used for the solution of the advection equation. According to Adam (1985), this is mainly due to the wrong numerical propagation speed of the shortest waves in the spectrum. He suggests, that the situation can be improved by applying digital filters. However, the most common linear filters do not completely remove the negative values. The main features of a perfect filtering procedure are: (1) To remove negative values. (2) To conserve total mass. (3) To preserve the shape of the function. (4) To preserve the maxima. (5) To be free of shortwave noise. Unfortunately, none of the existing numerical filters satisfy all above requirements.

2.3.1. Method

The multidimensional nonlinear filtering procedure developed in this paper fulfills at least some of the conditions mentioned above. It completely removes negative values and conserves the total mass with an accuracy of 0.001%. Filtered maxima and the shape of the function are relatively close to the original ones. The procedure can be explained as follows. Let c_j be the concentration in the j-th point of the one-dimensional grid system consisting of N points ($j = 1,...,N$). If all c_j values are non-negative the filter does not change them. Let us assume now that the concentration field has N_1

positive values ($c_j > 0$), N_2 zero values ($c_j = 0$) and N_3 negative values ($c_j < 0$). Obviously

$$N_1 + N_2 + N_3 = N \tag{15}$$

As assumed under Equation (1) we have:

$$M_1 > M_3 \tag{16}$$

where

$$M_1 = \sum_{\substack{j=1 \\ c_j>0}}^{N} c_j \tag{17a}$$

is the "positive" mass and

$$M_3 = -\sum_{\substack{j=1 \\ c_j<0}}^{N} c_j \tag{17b}$$

is the "negative" mass. With the above assumptions the filtering procedure is defined by the following algorithm:

1. Compute the negative mass M_3 and check if it is greater than zero. If not, stop.
2. Compute the number of positive concentrations N_1.
3. Check the sign of the concentration c_j for $j = 1,\ldots,N$
   (a) If $c_j > 0$, subtract the negative mass divided by the number of positive concentrations: $c_j := c_j - \frac{M_3}{N_1}$
   (b) If it is zero, do nothing.
   (c) If it is negative, set it to zero: $c_j := 0$.
4. Go to 1.

2.3.2. A One-Dimensional Example

The filtering procedure lined out in the previous paragraph is illustrated by a simple one-dimensional example with a grid system consisting of 11 points. The initial distribution shown in Figure 1a is typical for the intermediate solution of the advection equation with "delta" function (concentrations at all points except one are equal to zero) as initial condition. Two negative values of the concentration are present in the distribution: -4 at point number 4 and -5 at point number 8. After the first iteration (Figure 1b) only one negative value remains: -0.8 at point number 11. The second and final iteration (Figure 1c) gives a distribution without negative values. The maximum is slightly lower: 13 instead of 15 but the shape of the final distribution is quite close to the initial one (Figure 1d). From Figure 1d it can be also seen that the short waves present in the initial distribution have been removed from the final one.

The basic feature of the algorithm presented above is the conservation of mass, which can be expressed as

$$M_1 - M_3 = const. \tag{18}$$

The algorithm is convergent and stable (this will be proved in the next section), and also simple in its numerical realization. Numerical experiments with different initial distributions indicate that the typical number of iterations necessary to achieve a non-negative distribution is not greater than two. Also the additional computer-time spent for filtering is small ($\leq$ 10%) compared to the computer-time required by the pseudospectral method.

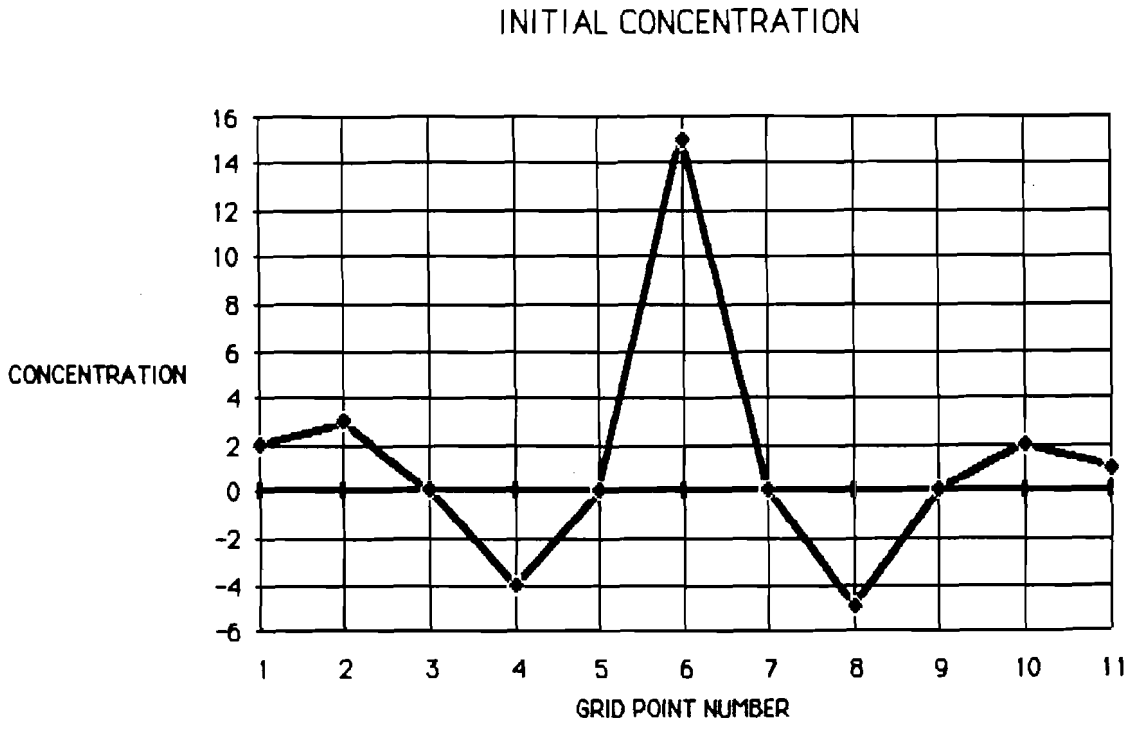

Figure 1a. One dimensional test for the filtering procedure: Initial distribution of the concentration.

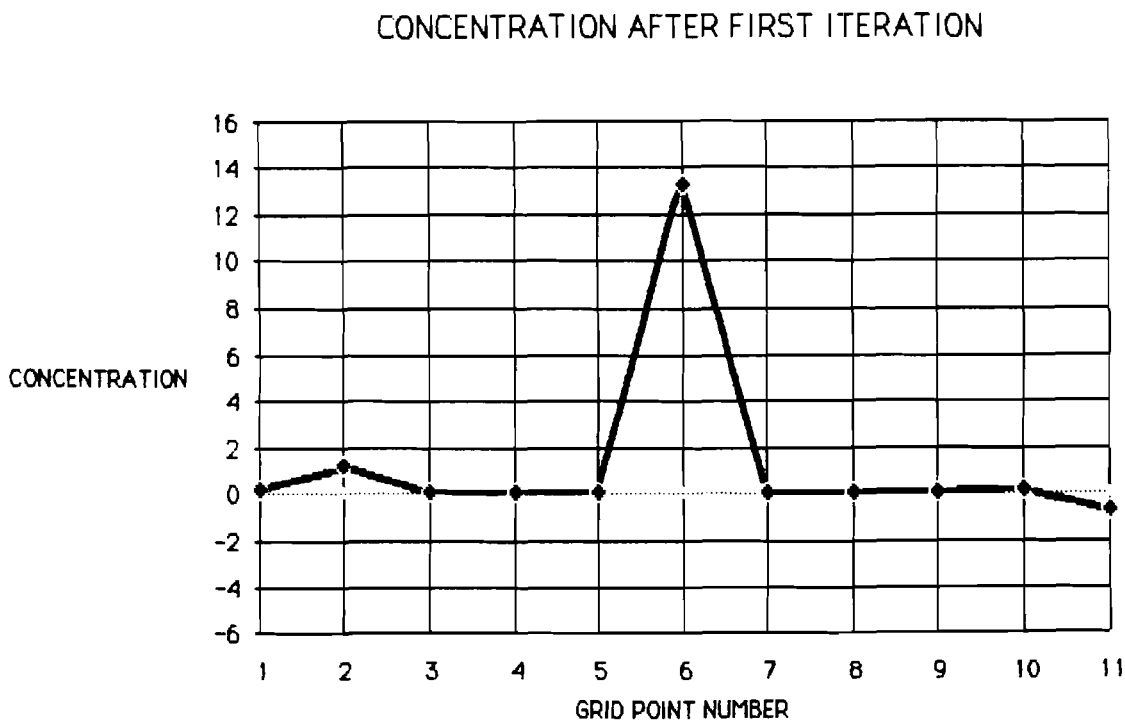

Figure 1b. One dimensional test for the filtering procedure: Distribution after first iteration.

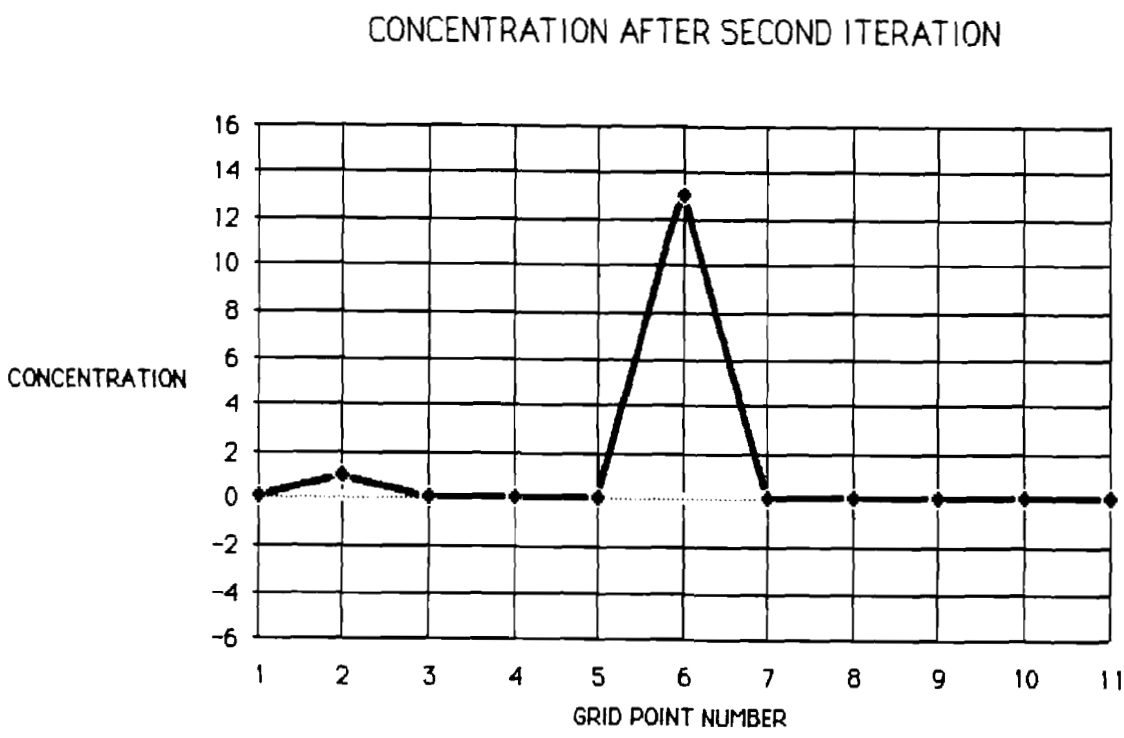

Figure 1c. One dimensional test for the filtering procedure: Distribution after second and final iteration.

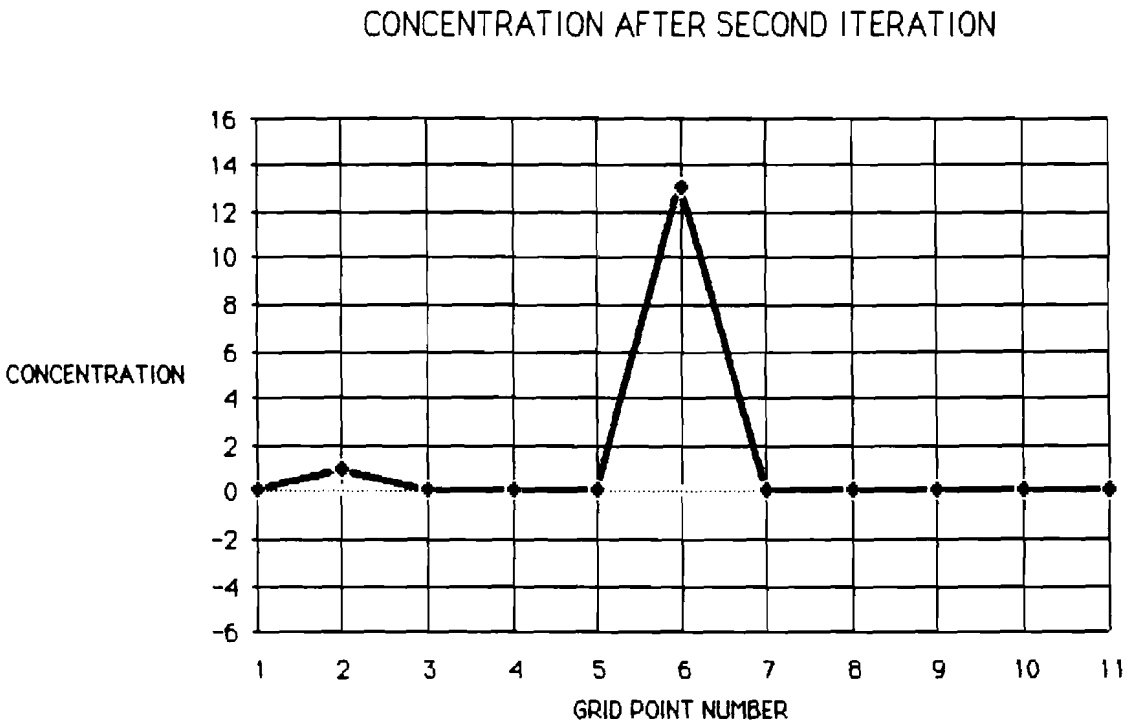

Figure 1c. One dimensional test for the filtering procedure: Distribution after second and final iteration.

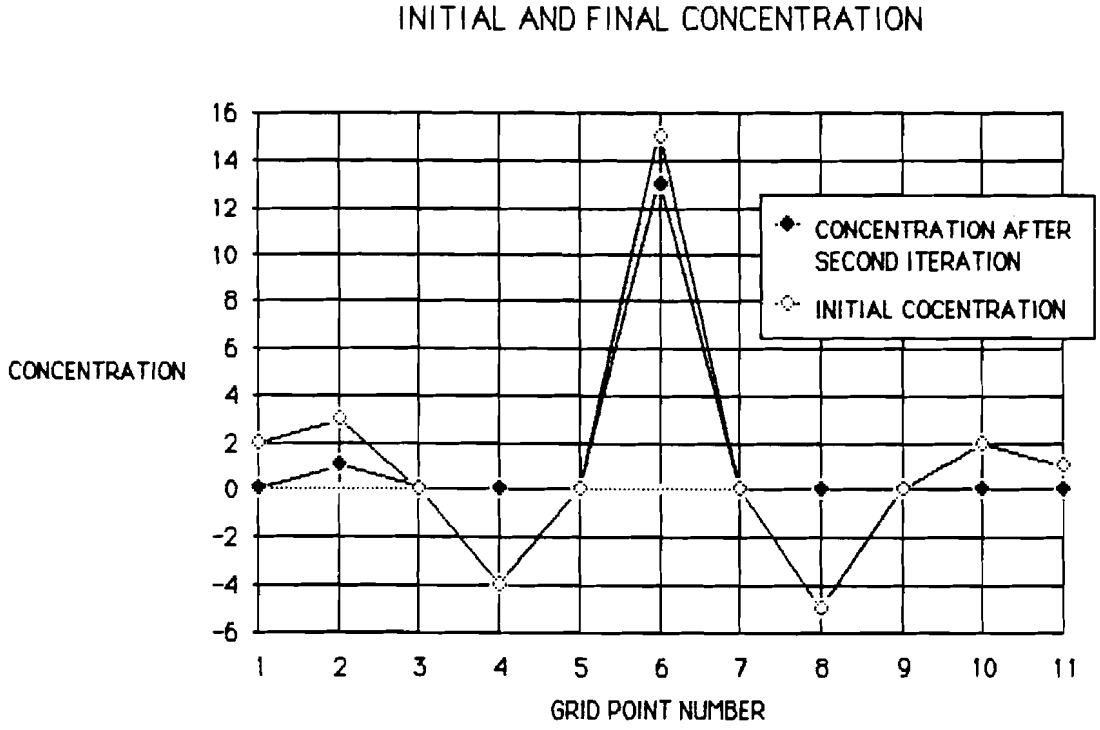

Figure 1d. One dimensional test for the filtering procedure: Comparison of initial and final distribution of the concentration.

2.4. Stability and Convergence

The PDPS method described by equation (6) is a superposition of the operator $\hat{P}$ -- the pseudospectral method -- and $\hat{F}$ -- the filtering procedure. The stability of the pseudospectral method is discussed in detail by Gazdag (1973). He proved that the stability condition is satisfied for truncated Taylor series of order 3,4,7 and 8.

For the filtering procedure there are three possibilities: (1) The initial value of the concentration is negative ($\tilde{c}_j < 0$) and becomes zero after filtering ($c_j = 0$). (2) The initial concentration is equal to zero ($\tilde{c}_j = 0$) and remains zero ($c_j = 0$). (3) The initial concentration is positive ($\tilde{c}_j > 0$) and finally remains non-negative, because the part of the negative mass subtracted from it cannot be larger than the original value ($0 \leq c_j < \tilde{c}_j$). Therefore, the following condition is fulfilled by the filtering procedure:

$$0 \leq c_j \leq |\tilde{c}_j| \quad j = 1,\ldots,N \tag{19}$$

where

$\tilde{c}_j$ - concentration at point j before filtering

c_j - concentration at point j after filtering

A simple implication of relation (19) is that the amplification factors are less than one. This means that the filtering procedure is stable and also that the PDPS method, as a superposition of two stable operators, satisfies the stability condition.

The filtering procedure is also convergent. This is obvious when only non-negative values are present in the initial distribution. Let us assume now an initial distribution with N_1 positive values, N_2 zero values and N_3 negative values of the concentration in the initial distribution. Due to

Equation (16) the negative mass M_3 is smaller than positive mass M_1. According to the filtering procedure all negative values become equal to zero and zero values are not changed. From each positive value of the concentration the negative mass averaged over the number of positive values is subtracted. If each positive value is greater than the average negative mass, the filtering procedure is completed after the first iteration. If not, there are positive values lower than the average negative mass, and they become equal to zero during the second iteration. It means that after each iteration the number of zeros increases at least by the number of negative values. Assuming that the filtering procedure is not convergent, there will be zeros only after less than $N - N_3$ iterations, which is impossible because of the conservation of mass (Eq. 18). Thus the filtering procedure is convergent.

3. ADVECTIVE TEST

In order to check the accuracy of the method described in the previous paragraph, a numerical advective test has been performed. A standard artificial velocity field has been used with the "frozen" initial shape moving around the axis of rotation. Three different initial conditions have been chosen: cone, rectangular block and smooth shape. The test was performed both for the Positive Definite Pseudo-Spectral (PDPS) method, and Pseudo-Spectral (PS) approach (Gazdag, 1973).

3.1. Basic Equation

The equation describing the rotation of the "frozen" initial condition has been frequently used for testing numerical methods (Orszag, 1971a; Gazdag, 1973; Long and Pepper, 1981; Christensen and Prahm, 1976). It has the

following form:

$$\frac{\partial c}{\partial t} - \omega y \frac{\partial c}{\partial x} + \omega x \frac{\partial c}{\partial y} = 0 \tag{20}$$

where ω is angular velocity

$$\omega = \frac{2\pi}{T} \tag{21}$$

and T is the period of rotation. Equation (1) was solved numerically on a grid consisting of 32 × 32 points. The time step was equal $\frac{T}{400}$ which means that one full revolution required 400 time steps. The analytical and numerical solutions were compared after 10 rotations. In addition, several parameters were computed during each run. Namely:

(1) Mass conservation (in %) - M

$$M = \frac{\sum_{i=1}^{32}\sum_{j=1}^{32} c(i,j)}{\sum_{i=1}^{32}\sum_{j=1}^{32} c_0(i,j)} \times 100 \tag{22}$$

where $c_0(i,j)$ is the initial concentration

(2) Conservation of the square of the mass (in %) - SM

$$SM = \frac{\sum_{i=1}^{32}\sum_{j=1}^{32} c^2(i,j)}{\sum_{i=1}^{32}\sum_{j=1}^{32} c_0^2(i,j)} \times 100 \tag{23}$$

(3) Minimum of $c(i,j)$ - MIN

(4) Maximum of $c(i,j)$ - *MAX*

(5) Maximum absolute error - *MER*

$$MER = \max_{i,j}(|c(i,j) - c_0(i,j)|) \tag{24}$$

(6) Average absolute error - *AER*

$$AER = \frac{1}{32 \times 32} \sum_{i=1}^{32} \sum_{j=1}^{32} |c(i,j) - c_0(i,j)| \tag{25}$$

All above parameters are functions of time and are different for each initial condition. The maximum of each tested initial condition was kept constant and equal 100.

3.2. Cone Shape Initial Condition

The "cone" shape initial condition (Figure 2a) is a standard one and was applied as a test case to almost all numerical methods used for solving an advection equation. In the grid system the "cone" shape is defined as:

$$c(i,j) = \begin{cases} 100 \cdot (1 - r/4) & \text{if } r \le 4 \\ 0 & \text{if } r > 4 \end{cases}$$

$$r = \sqrt{(i-8)^2 + (j-16)^2}; \quad i,j = 1,\ldots,32 \tag{26}$$

In Figures (2b) and (2c) the numerical solutions after ten rotations are shown for the PDPS and PS methods, respectively. The difference in shapes is small and both numerical solutions are quite close to the analytical one. However, negative values appear in the PS solution.

The mass conservation M, defined by Equation (22), is equal to 100% during the entire run for both PDPS and PS with accuracy better than 0.001%. The square mass conservation SM, defined by Equation (23), is

shown in Figure 3. The square mass is well conserved by the PS method (99.7% after 10 rotations) and slightly worse by the PDPS method (92.6% after 10 rotations). In the latter case the square mass decreases rapidly during the first rotation and then stays almost at the same level.

The minimum values *MIN* are shown in Figure 4 for both methods. In case of PDPS negative values are not created and the numerical minimum is equal to the analytical one, which is zero. In case of PS negative values are created, reaching -1.81 after ten rotations.

The analytical maximum *MAX* is equal to 100 and is slightly above the numerical ones (Figure 5). After ten rotations the maximum for the PDPS method is equal to 91.75 whereas it is 94.02 for the PS method. For both methods the maximum decreases mainly during the first rotation and then stays at the same level.

For both PDPS and PS the maximum absolute error *MER*, defined by Equation (24), occurs at the top of the cone. It is slightly higher for PDPS than for PS (Figure 6), and is less than 10 after ten rotations.

For the PS method the average absolute error *AER*, defined by Equation (25), increases rapidly during the first rotation and then, with some fluctuations, remains at the same level of 0.14 (Figure 7). In case of the PDPS method, *AER* increases slowly, reaching 0.172 after ten rotations.

3.3. Rectangular Block Initial Condition

The "Rectangular Block" initial condition is shown in Figure 8a. It is defined on the grid as:

$$c(i,j) = \begin{cases} 100 & \text{if } 5 \le i \le 11 \text{ and } 13 \le j \le 19 \\ 0 & \text{otherwise} \end{cases} \qquad i,j = 1,\ldots,32 \qquad (27)$$

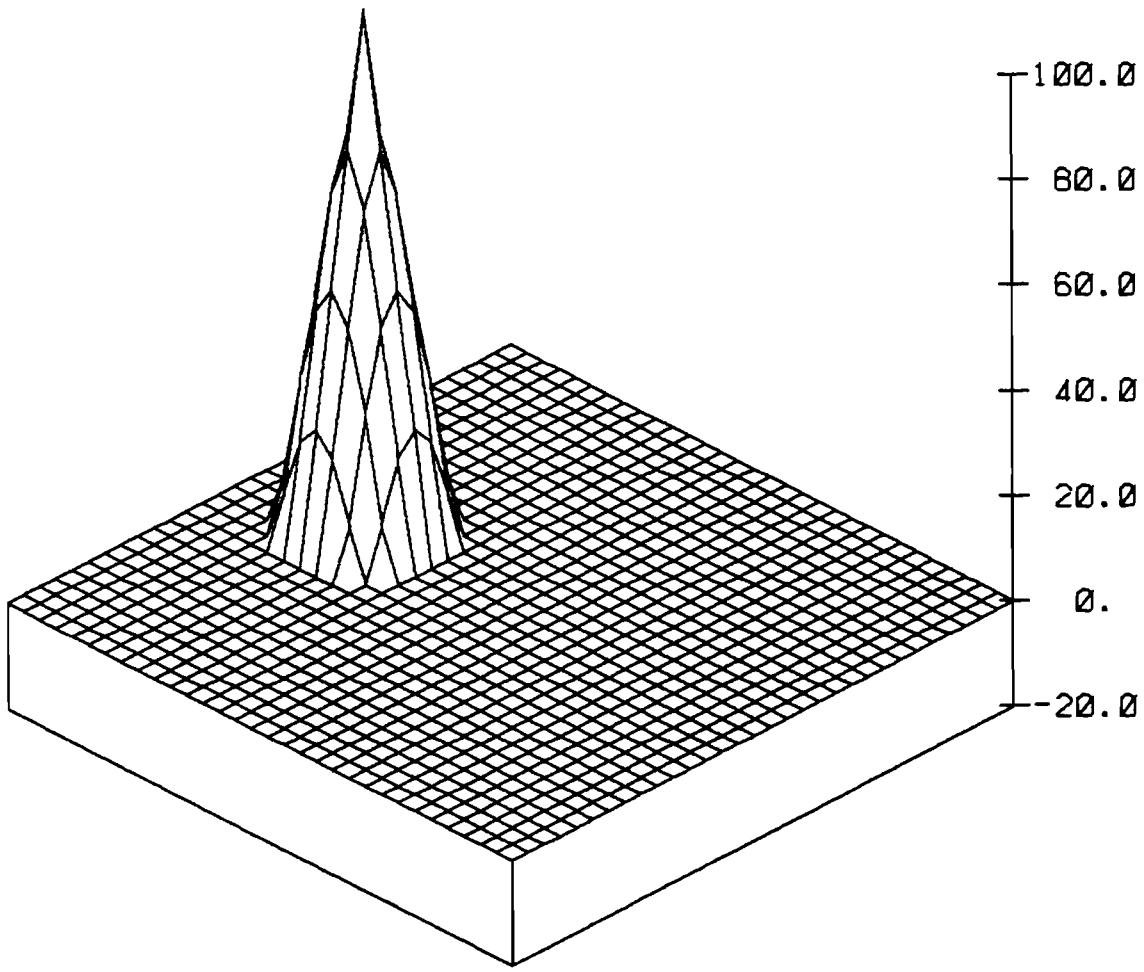

Figure 2a. Shape of the cone after 10 rotations: analytical solution.

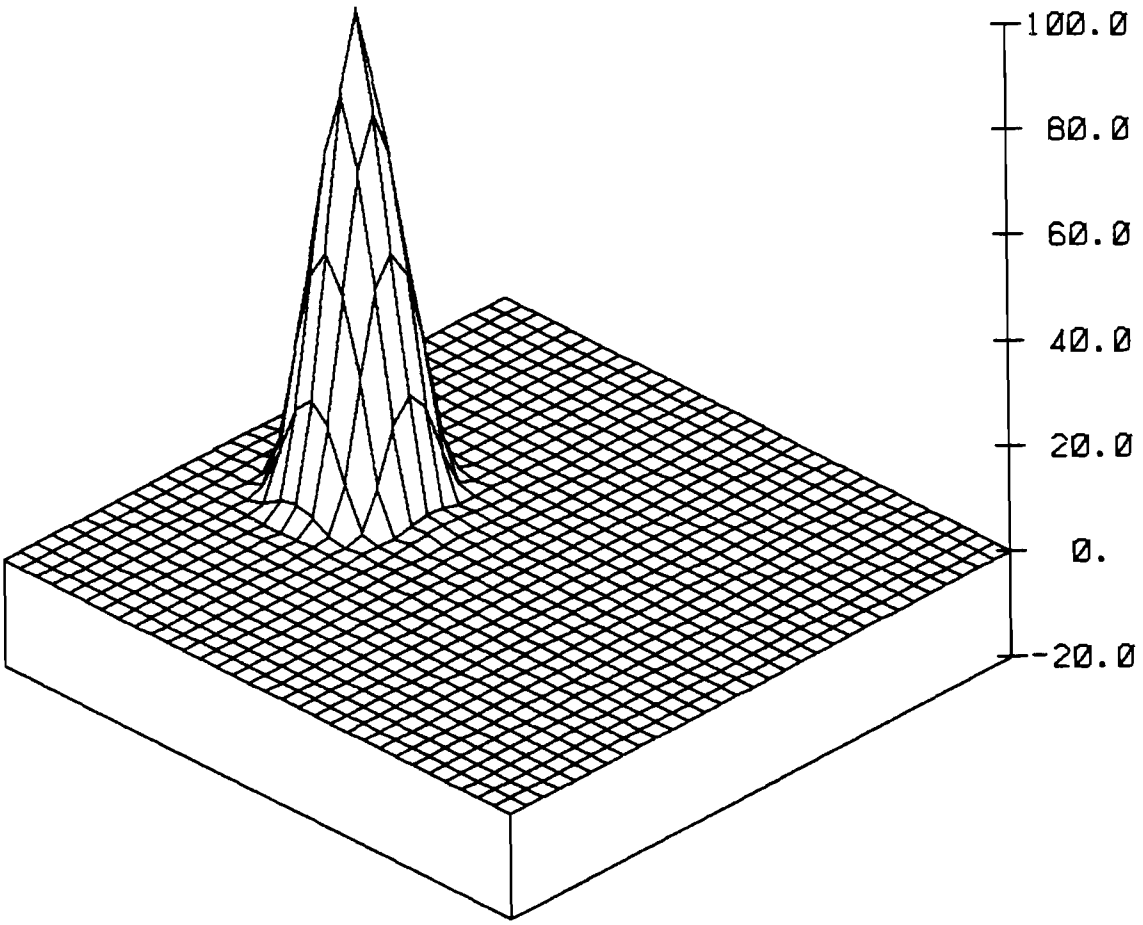

Figure 2b. Shape of the cone after 10 rotations: PDPS method.

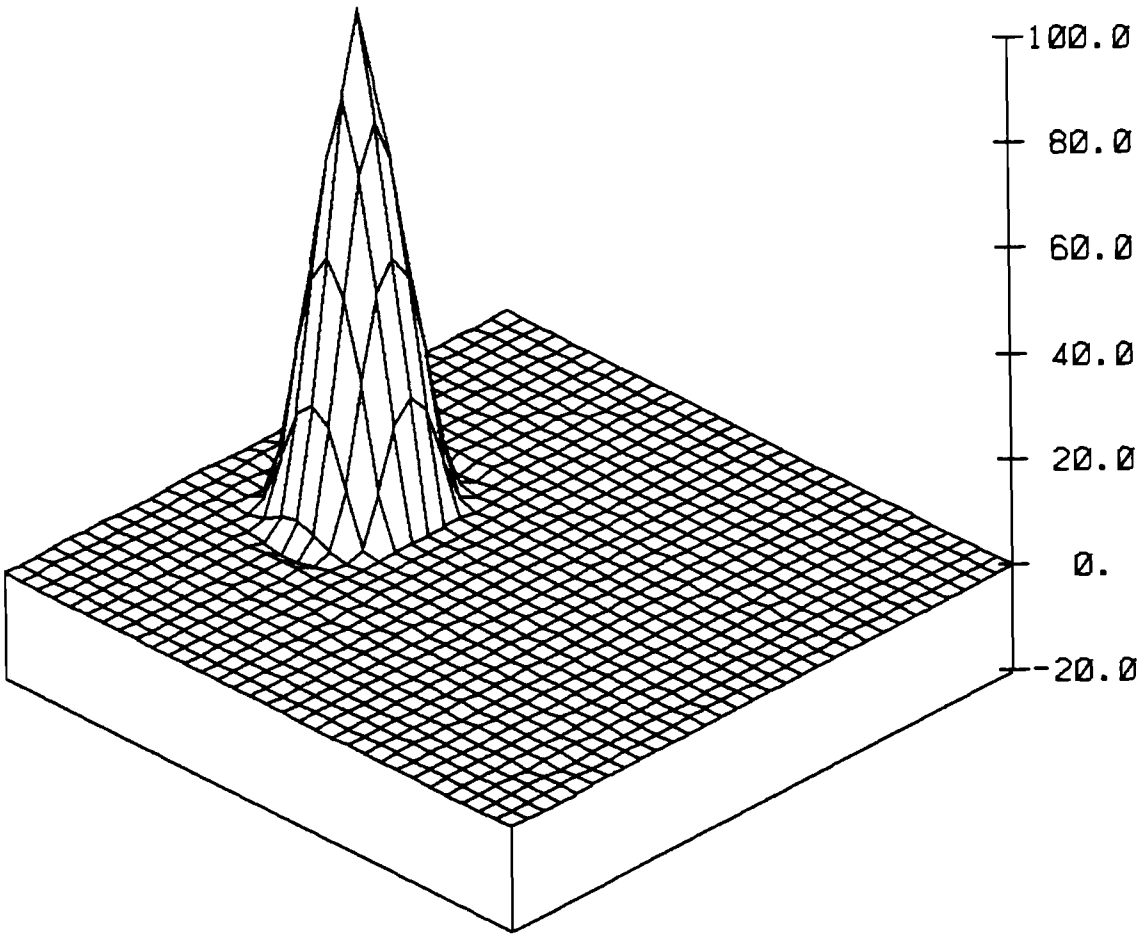

Figure 2c. Shape of the cone after 10 rotations: PS method.

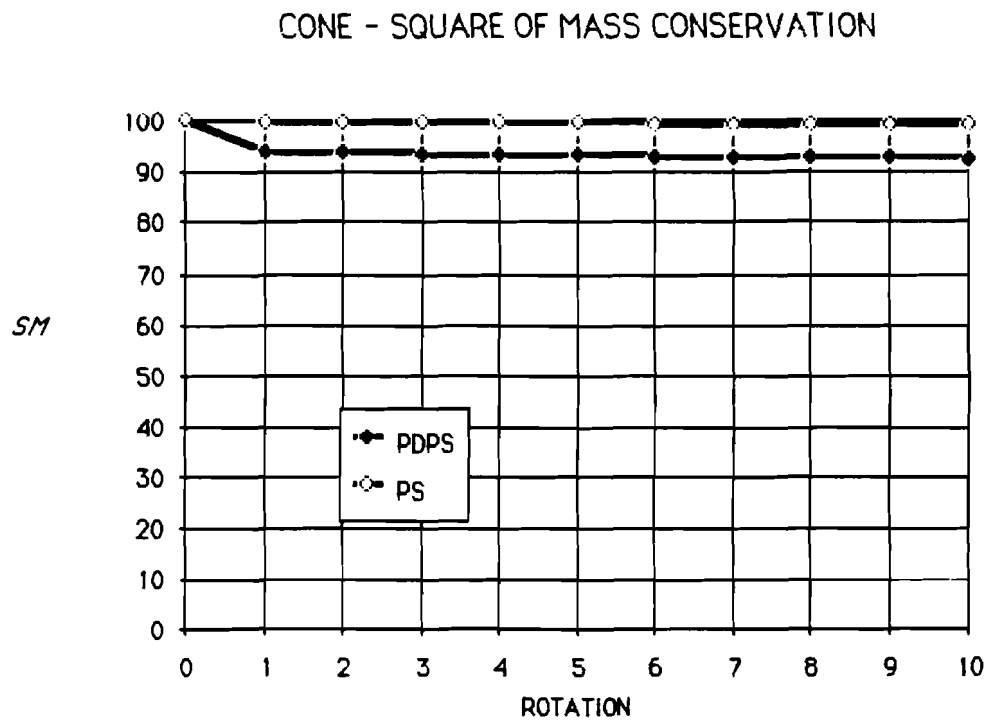

Figure 3. Square of mass conservation, with the cone shape as initial condition.

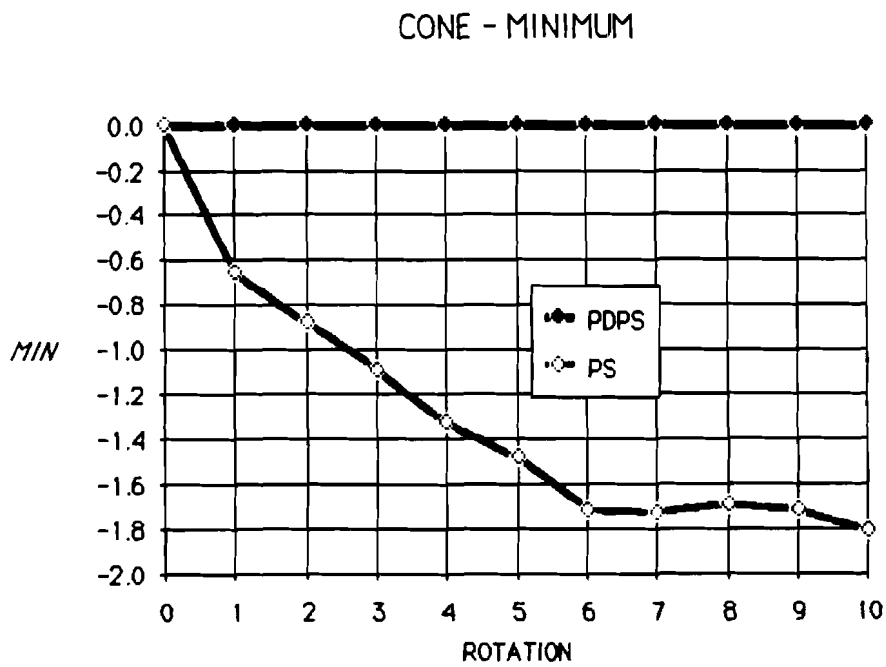

Figure 4. Minimum values for the PDPS and PS methods with the cone shape initial condition.

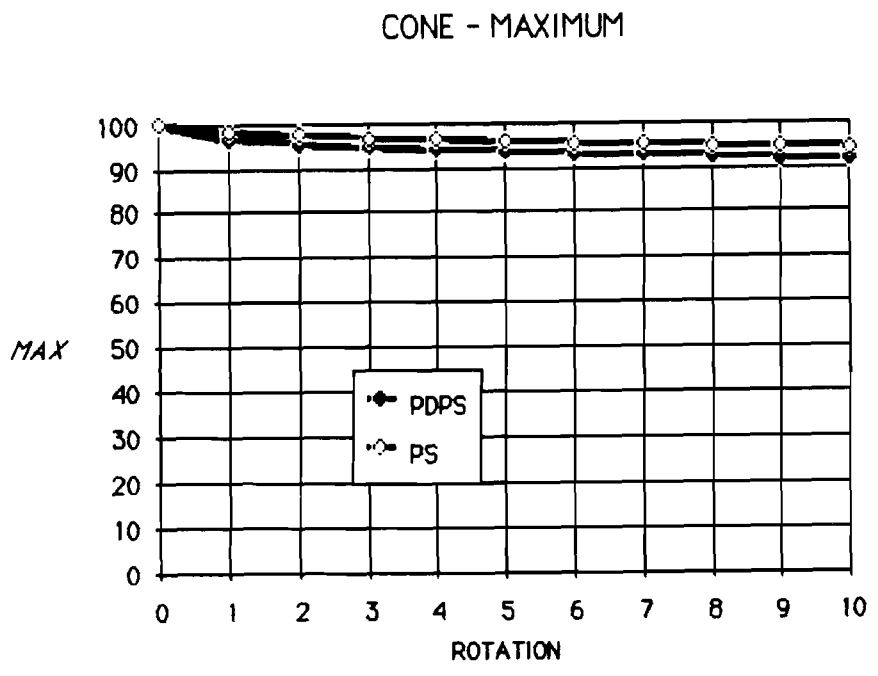

Figure 5. Maximum values for the PDPS and PS methods with the cone shape initial condition.

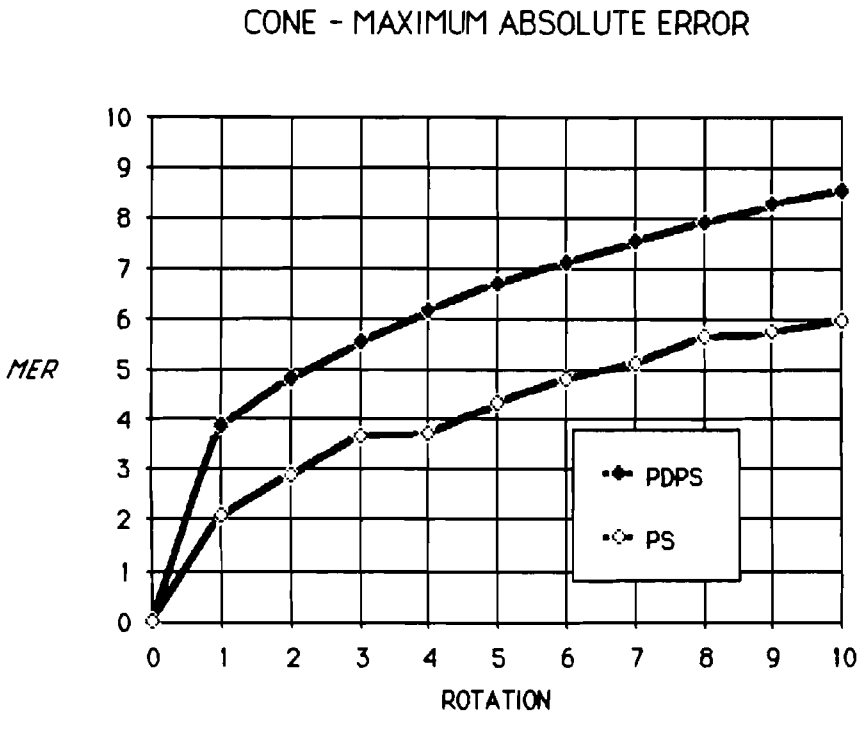

Figure 6. Maximum absolute error for the PDPS and PS methods with the cone shape initial condition.

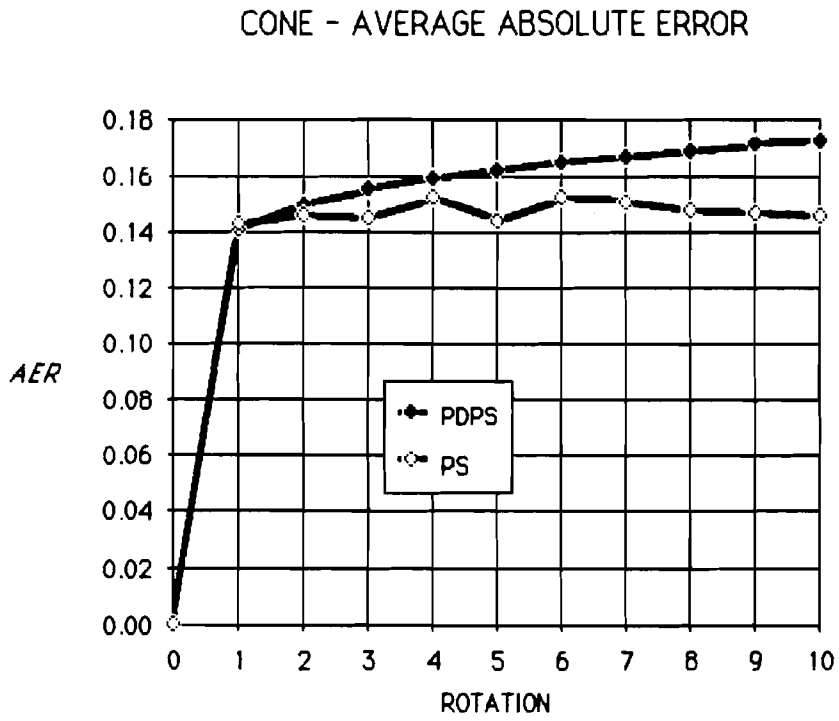

Figure 7. Average absolute error for the PDPS and PS methods with the cone shape initial condition.

The numerical solution after ten rotations is shown in Figure 8b for the PDPS method, and in Figure 8c for the PS method. The difference between the analytical and the numerical solutions is greater than for the cone shape initial condition discussed earlier, but the initial shape is kept quite well. An important advantage of the PDPS method is the absence of shortwave noise, present in the solution given by the PS method.

The square mass is better conserved by the PS method (95% after ten rotations) than by the PDPS method (69.36% after ten rotations). Again, like in the case of the cone shape, the square mass decreases mainly during the first rotation (71.42%) for PDPS, and then remains at the same level 70% (Figure 9).

The minimum for the PDPS method equals to zero during the entire run. For PS it varies from -9.28 after the third rotation to -13.07 after ten rotations (Figure 10). The minimum value produced by the PS method is higher (in absolute value) in case of the rectangular block initial condition than in case of the cone shape initial condition.

The maximum for the PDPS method (Figure 11) increases to 105.6 after the first rotation and then continuously decreases to 101.0 after ten rotations. The maximum for the PS method (Figure 11) is relatively high, reaches 120.16 after the fourth rotation and remains lower afterwards.

The maximum absolute error is much higher compared to the cone shape initial condition, both for PDPS and PS (Figure 12, cf. Figure 6). In case of PDPS the maximum absolute error increases rapidly to 38.91 after the first rotation and then slowly goes to 47.08 after ten rotations. The maximum absolute error increases also in case of the PS method (Figure 12)

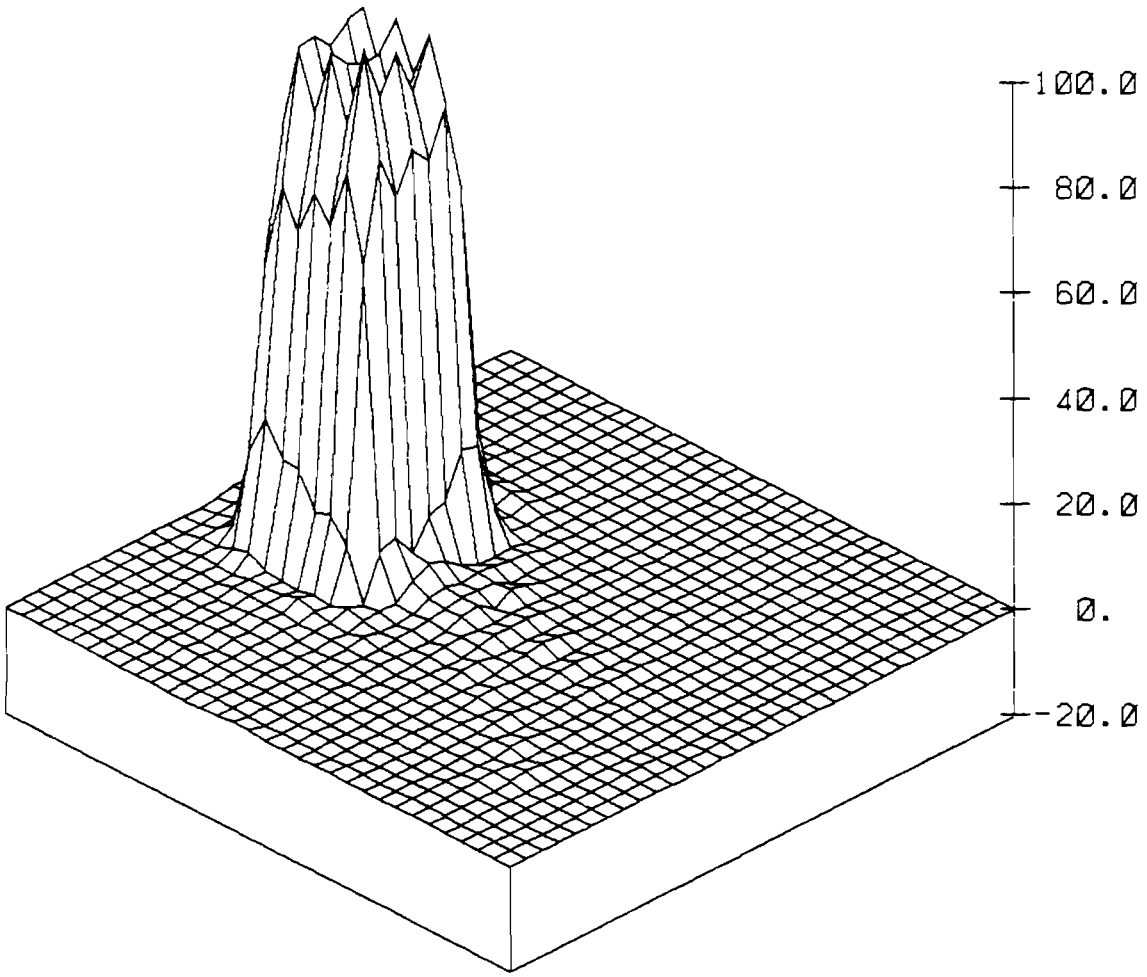

Figure 8b. Shape of the rectangular block after 10 rotations: PDPS method.

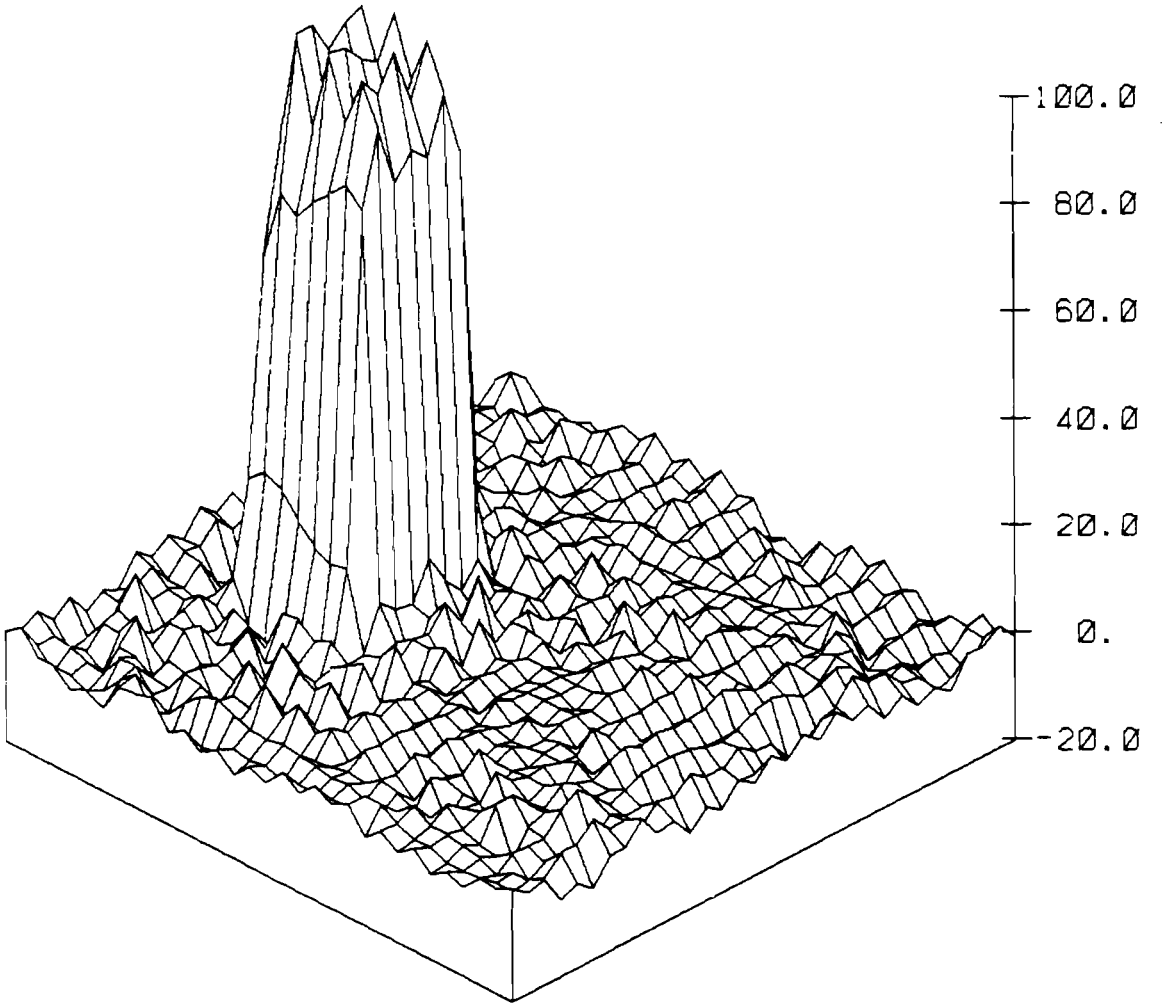

Figure 8c. Shape of the rectangular block after 10 rotations: PS method.

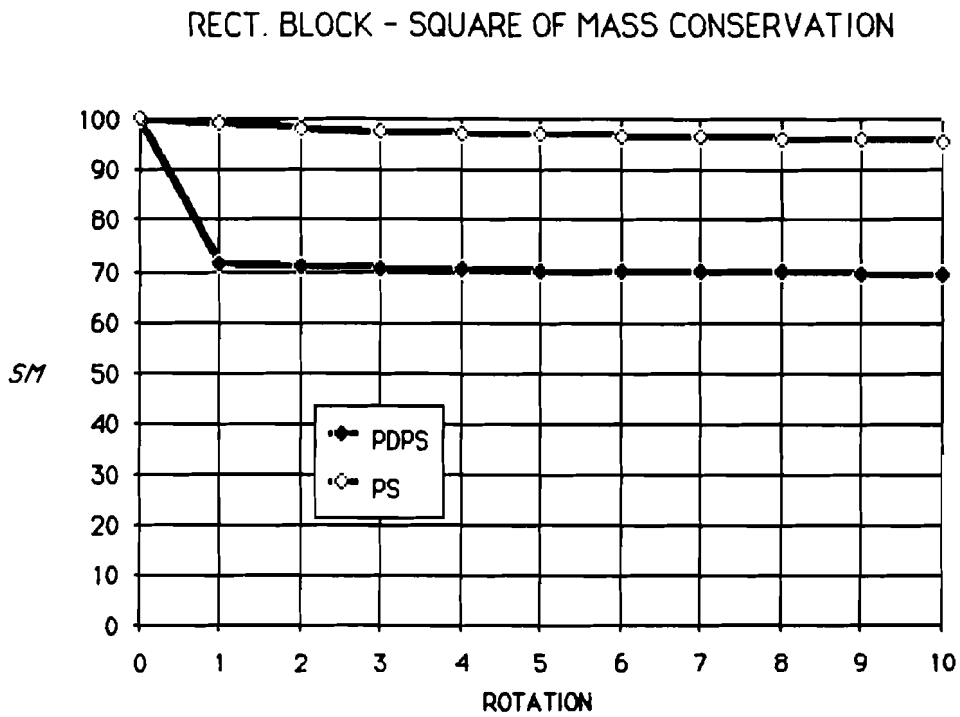

Figure 9. Square of mass conservation, with the rectangular block initial condition.

to 38.8 after seven rotations.

The average absolute error (Figure 13) is about 1.5 times smaller for the PDPS (0.161-0.181) than for the PS method (0.232-0.314).

Compared to the cone initial condition, the rectangular block initial condition is a more critical test for the numerical methods. Differences between numerical and analytical solution are higher and negative numbers are bigger. In the PS solution, there are also short range waves present, which did not occur before. In this case the PDPS method passed the test quite well, and especially, it preserved the numerical maximum close to analytical one and did not produce the shortwave noise, present in PS solution.

3.4. Smooth Initial Condition

Contrary to the two previous cases the last numerical test was performed with the following smooth initial condition:

$$c(i,j) = \begin{cases} 100 \cdot \cos^2(\pi r / 12) & 0 \le r < 6 \\ 0 & 6 \le r \end{cases} \qquad (28)$$

$$r = \sqrt{(i-8)^2 + (j-16)^2} \qquad i,j = 1,\ldots,32$$

The shape of the distribution defined by Equation (28) is shown in Figure 14a.

The numerical solution after ten rotations is shown in Figure 14b for the PDPS method, and in Figure 14c for the PS method. In both cases the differences between the analytical and the numerical solutions are small. In case of the PS method negative values appeared again but shortwaves can not be seen on the grid. The shortwaves are also not present in the PDPS solution.

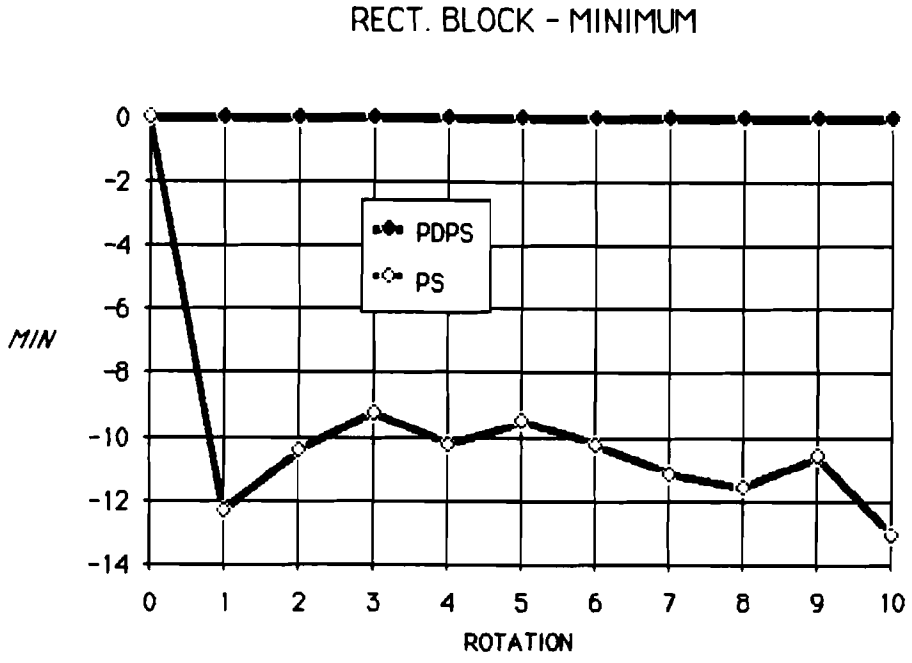

Figure 10. Minimum values for the PDPS and PS methods with the rectangular block initial condition.

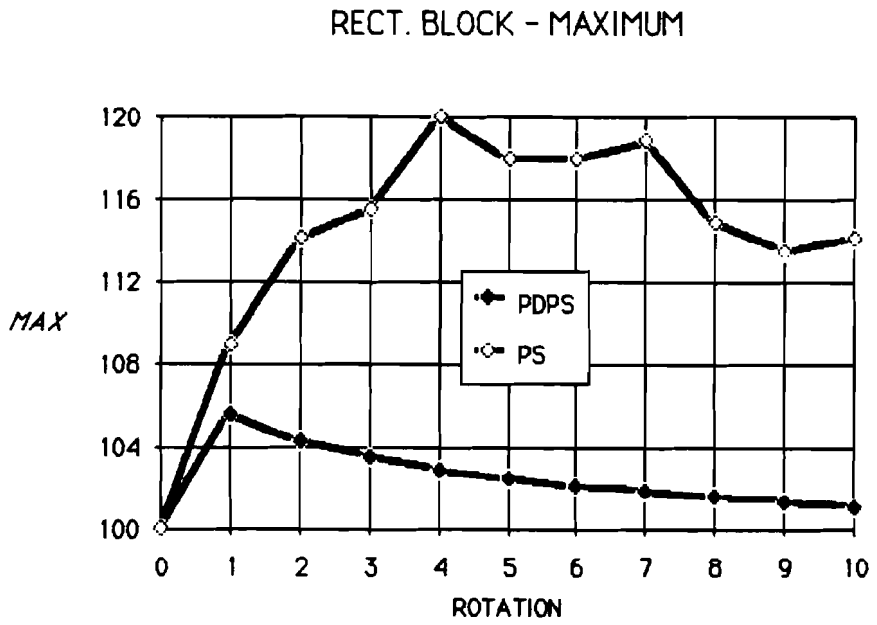

Figure 11. Maximum values for the PDPS and PS methods with the rectangular block initial condition.

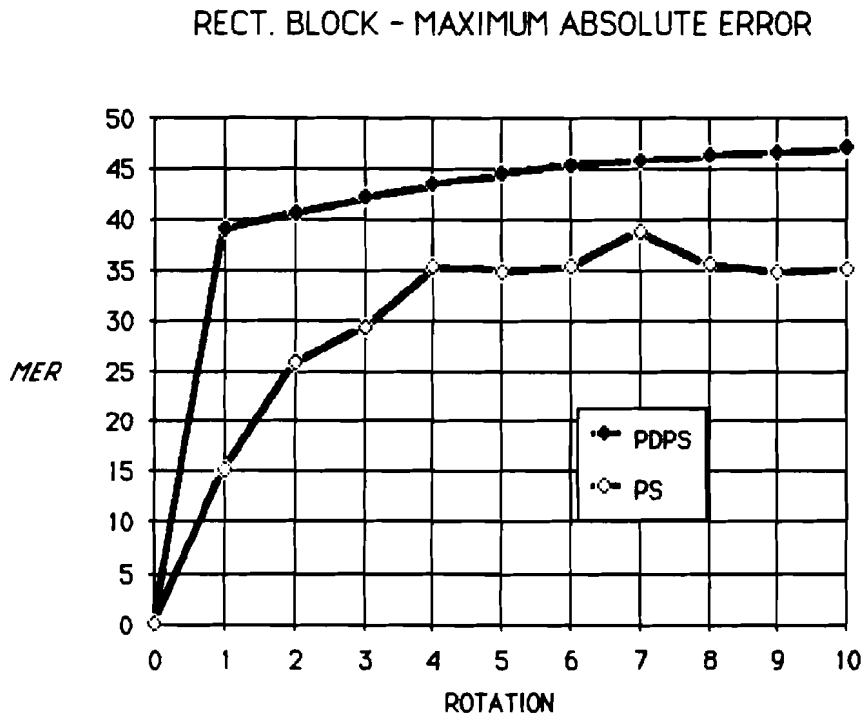

Figure 12. Maximum absolute error for the PDPS and PS methods with the rectangular block initial condition.

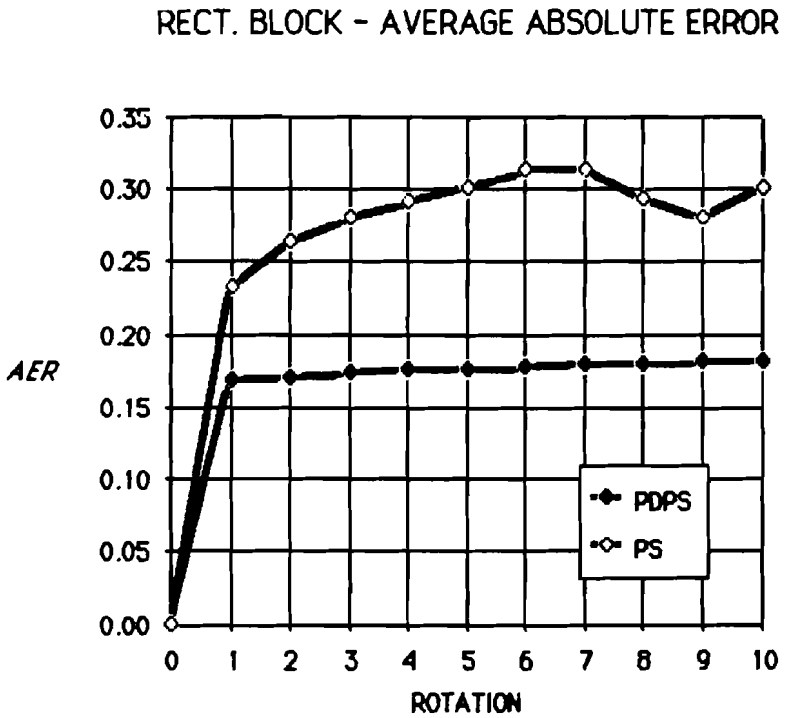

Figure 13. Average absolute error for the PDPS and PS methods with the rectangular block initial condition.

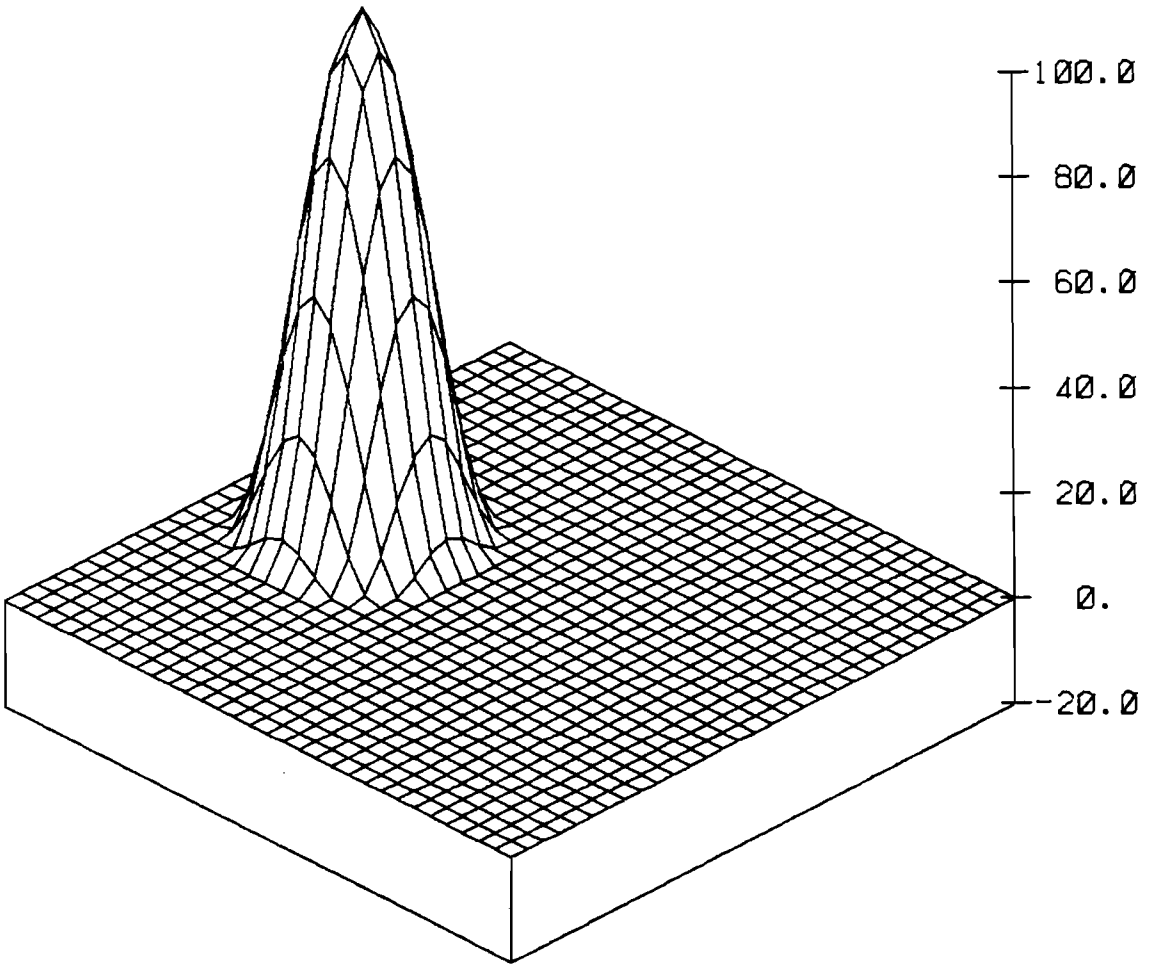

Figure 14a. Smooth shape after ten rotations: analytical solution.

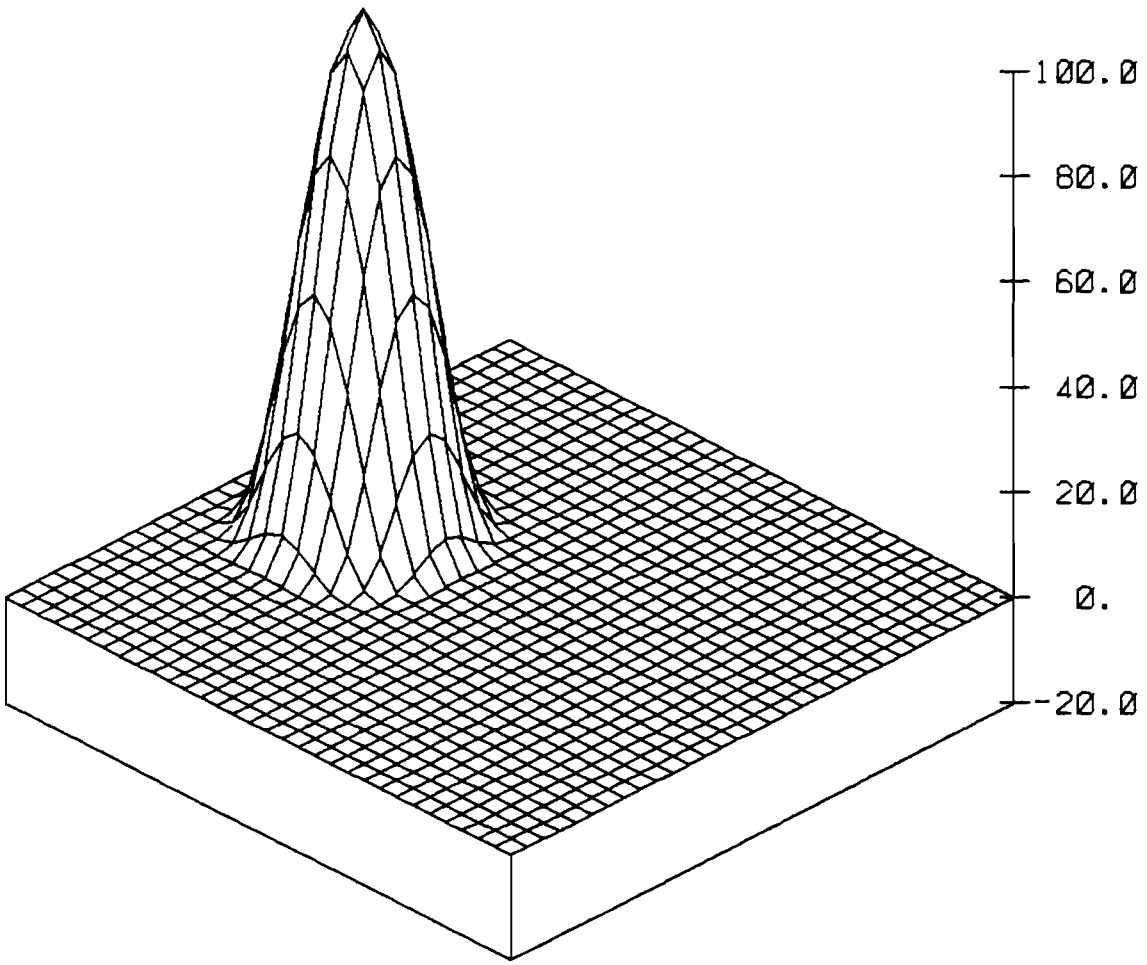

Figure 14b. Smooth shape after ten rotations: PDPS method.

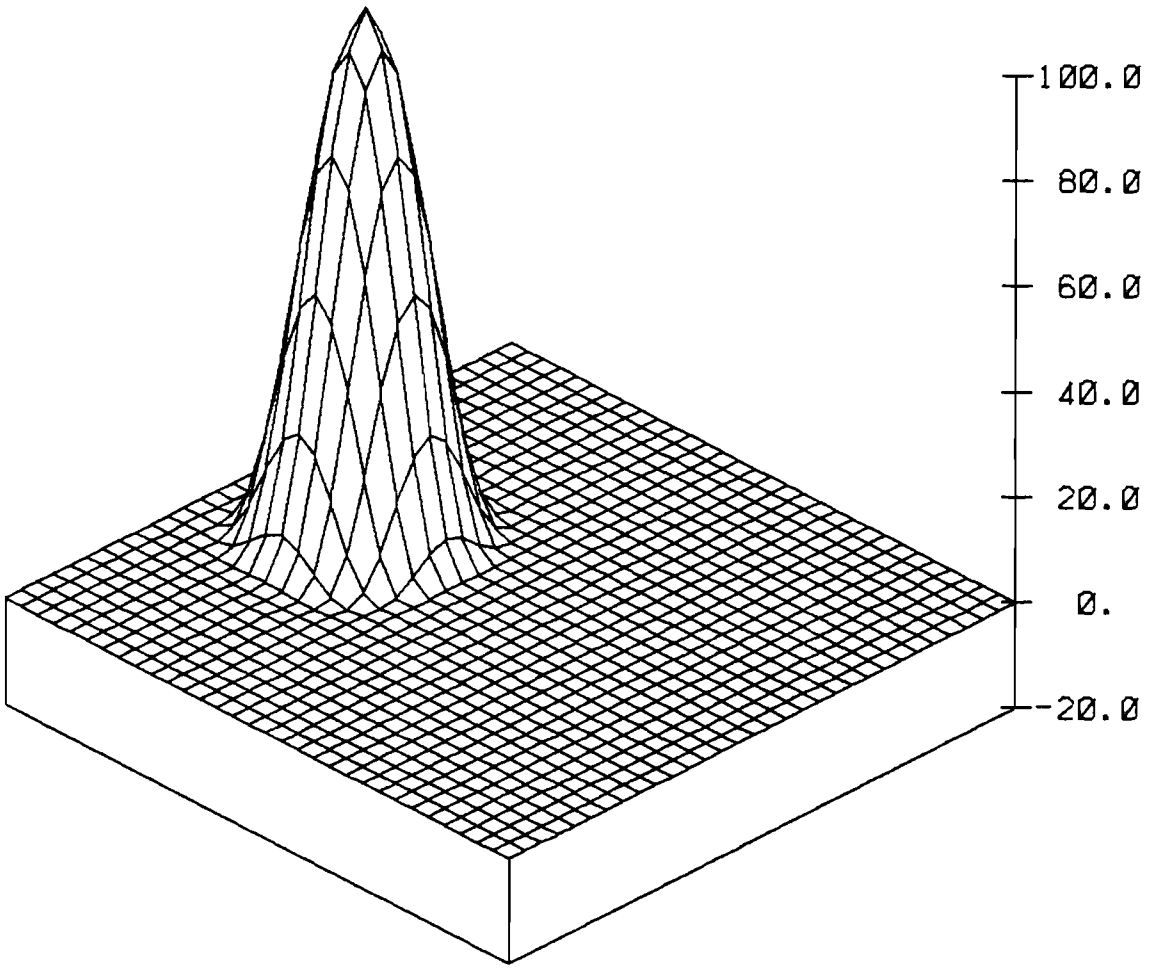

Figure 14c. Smooth shape after ten rotations: PS method.

The square mass, shown in Figure 15, is well conserved by both the PDPS method (98.91% after ten rotations) and the PS method (99.76% after ten rotations). Again, like in both previous cases, the square mass decreases mainly during the first rotations for the PDPS method.

The minimum is zero for the PDPS method during entire run (Figure 16). For PS, it slowly decreases from -0.19 after the first rotation to -0.43 after ten rotations. However, the absolute values of the minimum are rather low compared to the cone shape and rectangular block initial conditions.

The maximum, shown in Figure 16, is very close to the analytical value 100 for both methods. After ten rotations the maximum is equal to 99.32 for the PDPS method and 99.70 for the PS method.

The maximum absolute error (Figure 17) is 0.70 for the PDPS method and 0.69 for the PS, after ten rotations. It increases faster for the PS method (0.27 after the first rotation) than for PDPS (0.53 after the first rotaton).

The average absolute error is practically the same for both methods and it slowly increases from 0.04 after the first rotation to 0.05 after ten rotations.

3.5. Comparison of Different Initial Conditions

The results of the advective test depend both on the numerical method applied to the advection equation and on the shape of the initial condition. For each of the three different initial conditions the PDPS and PS methods conserve initial mass with an accuracy better than 0.001%. Also, for all of them, the PDPS method does not produce negative values and this is the most important feature of the method. However, the values of the other

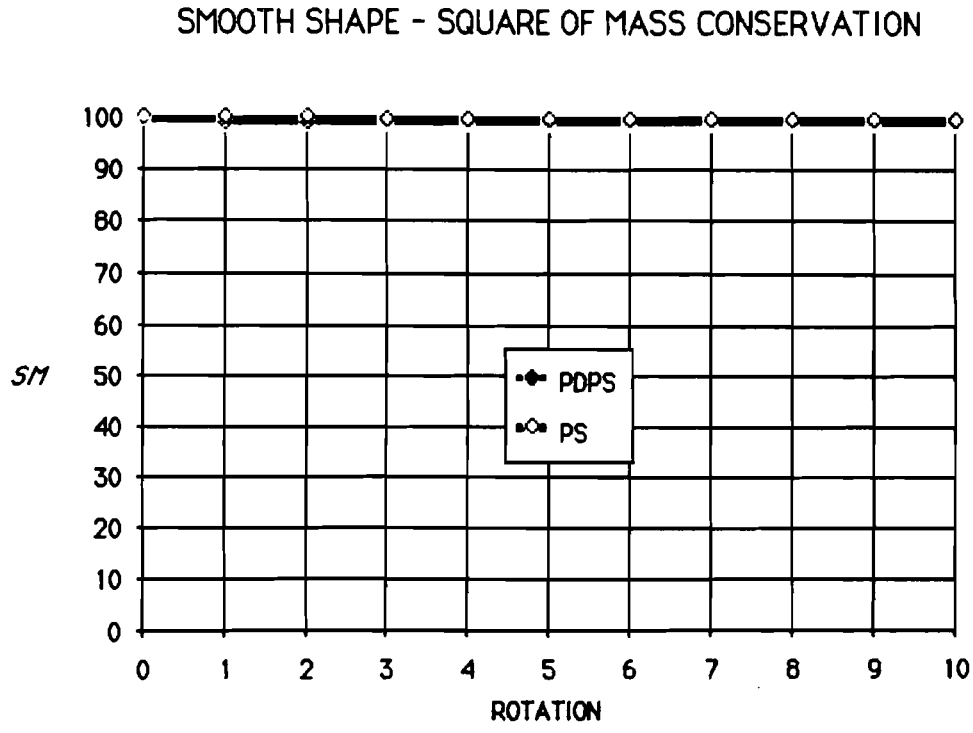

Figure 15. Square of mass conservation: smooth initial condition.

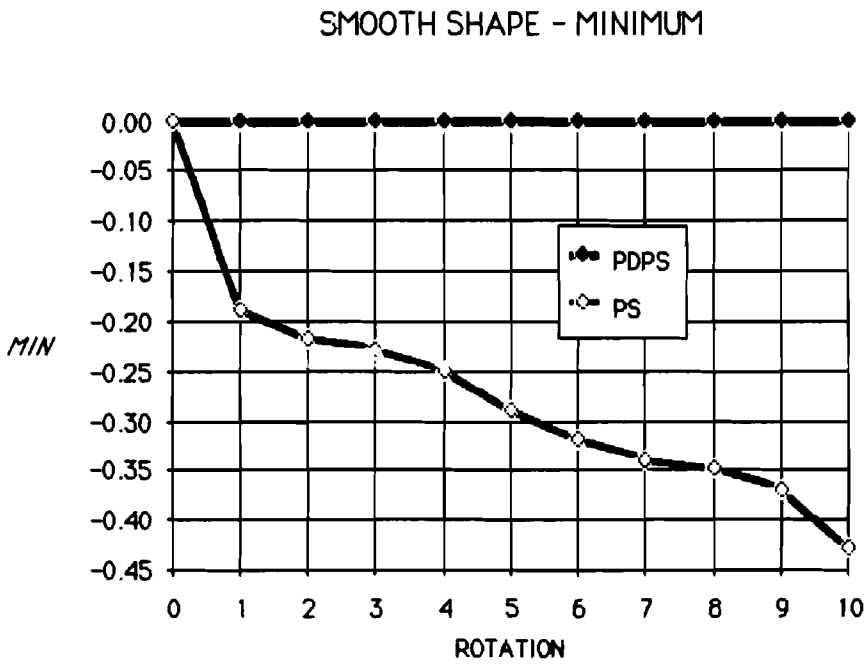

Figure 16. Minimum values for the PDPS and PS methods with the smooth initial condition.

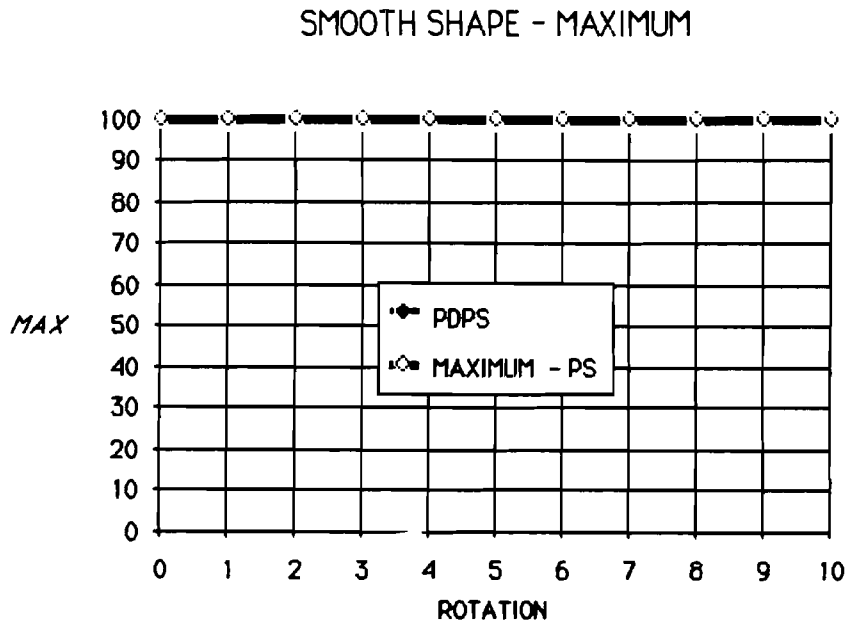

Figure 17. Maximum values for the PDPS and PS methods with the smooth initial condition.

measures (*SM*, *MIN* for the PS method, *MAX*, *MER* and *AER*), defined in Section 3.1, depend on the shape of initial condition.

The square mass is better conserved (Figure 15) for the smooth shape than for the cone shape (Figure 3) and the rectangular block (Figure 9). After ten rotations, only 0.46% of the square mass is lost in the PS solution and 1.09% in the PDPS solution. For the rectangular block the square mass decrease after ten rotations is: 4.28% for PS and 30.64% for PDPS. The corresponding numbers for the cone initial conditions are: 0.93% for PS and 7.33% for PDPS.

The minimum values generated by the PS method are smaller (Figure 16), -- in absolute units -- for the smooth shape (-0.43 after seven rotations) than for the rectangular block (-13.07 after ten rotations), and for the cone (-0.181 after ten rotations).

Similarly, the maximum for both methods is closer to the analytical solution in case of the smooth shape (99.32 for PDPS, 99.70 for PS; Figure 17) than in case of the rectangular block (101.00 for PDPS, 114.04 for PS), and the cone shape (91.45 for PDPS, 94.02 for PS).

The maximum absolute error after ten rotations (Figure 18) is also smaller for the smooth shape (0.70 for PDPS, 0.69 for PS) than for the rectangular block (47.08 for PDPS, 35.08 for PS) and the cone (8.55 for PDPS, 5.98 for PS).

Finally, the average absolute error (Figure 19) is slightly higher for the smooth shape (0.05 for PDPS and PS, after ten rotations) than for the cone shape (0.172 for PDPS, 0.146 for PS) and the rectangular block (0.181 for PDPS, 0.301 for PS).

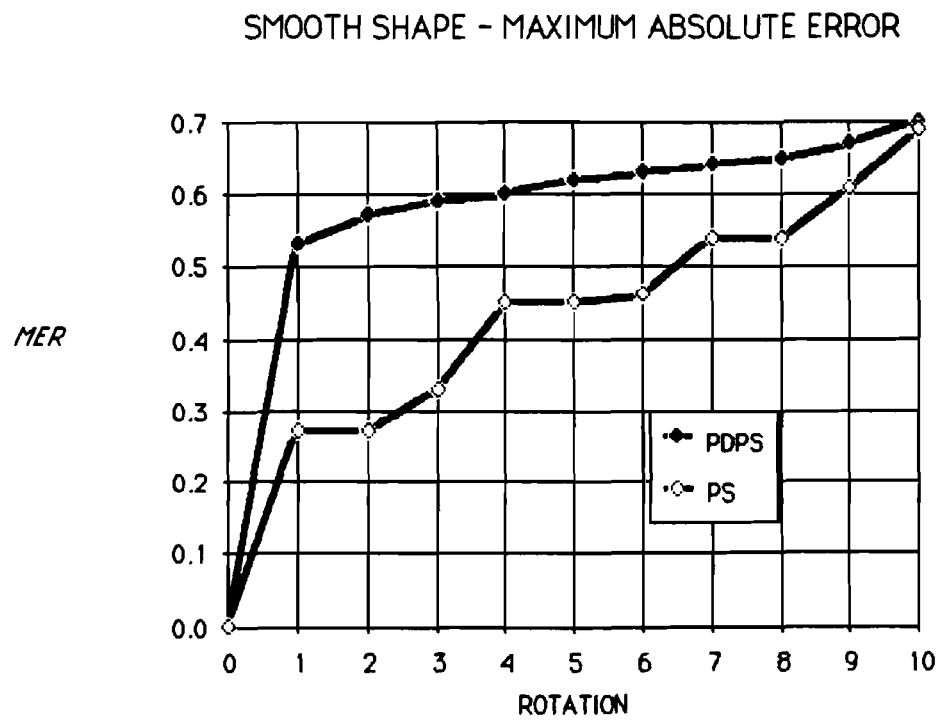

Figure 18. Maximum absolute error for the PDPS and PS methods with the smooth initial condition.

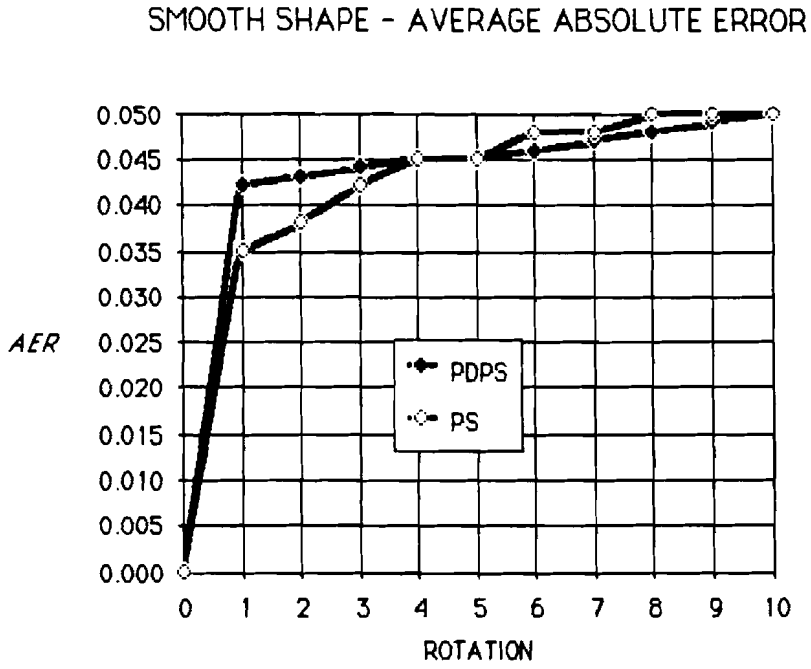

Figure 19. Average absolute error for the PDPS and PS methods with the smooth initial condition.

Comparing different intial conditions, it seems that the rectangular block shape is the most critical test for the numerical methods. It is also confirmed by the generation of the artificial shortwave noise, with the high amplitude for the rectangular block initial condition (Figure 8b-c), smaller for the cone initial condition (Figure 2b-c) and practically invisible for the smooth initial condition (Figure 14b-c).

4. CONCLUSIONS

The PDPS method presented in this paper is simple and comprehensive both in mathematical formulation and in practical application. It does not produce negative values and conserves initial mass with 100% accuracy. The method consists of two basic parts: (1) The pseudospectral solution, and (2) the filtering procedure. Compared to the pseudospectral approach the additional computer-time for the PDPS method is only about 10% higher. The multidimensional filtering procedure is general enough to be combined with methods other than PS, and especially with explicit time integration algorithms. The PDPS method can also be applied to the advection-diffusion equation in the same way as to the advection equation.

From the numerical tests, performed with the PDPS and PS methods in the rotational velocity field, it seems that -- for both methods -- results depend on the initial condition. The most commonly used cone shape gives relatively good results concerning accuracy and shortwave noise. From the three different conditions tested, the most critical one is the rectangular block shape with very steep gradients. In this case, the magnitude of the negative values generated by the PS method is larger (Figure 10) than for the other initial conditions (Figures 8c and 14c). Also the amplitude of the

shortwaves on the entire grid system is larger (Figure 8c). Both, negative values and shortwaves noise (except some small disturbances close to the rectangular block) are not present in the PDPS solution.

Also the average absolute error is smaller for the PDPS method, except in the cone case, when it is slightly higher compared to the PS solution.

Summarizing, the accuracy of the PDPS method is very close to the PS one. The advantage of PDPS is a complete elimination of negative values from the solution and therefore its possible application to non-linear problems (e.g. chemical reactions during the transport). An additional advantage of PDPS is the absence of shortwaves, typical for the PS solution, in case of steep gradients in the concentration field.

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