TESTING OF NUMERICAL ADVECTION SCHEMES AND SPLITTING TECHNIQUES USED IN POLLUTION DISPERSION MODELING ON AN ANALYTIC SOLUTION

Dimiter Atanassov, Tatiana Spassova
National Institute of Meteorology and Hydrology, 66, Tsarigradsko chaussee, 1784 Sofia, Bulgaria

INTRODUCTION

Before being validated on field data, a numerical dispersion model could be tested on the exact analytic solution of the problem, if such could be obtained. This is a wide spread practice in development of numerical advection schemes. Usually, the advection peculiarities of the schemes are considered. In the real nature the advection of the pollutants is accompanied by their simultaneous release in (emission) and removal from (dry and wet deposition) the atmosphere. In dispersion modelling, however, these processes are considered separately, one after another within a time step. Usually, they are in the order emission (E)–advection (A) – deposition (D) repeated at each time step. This procedure was first formulated clearly by *Marchuk* (1975). It is known as "time splitting". Some specific errors are associated with the splitting procedure. Their origin is illustrated in Figure 1. Within a time step, the air pollution concentration in a grid cell is varying after each operator, differing considerably from the exact analytic value. The error could be generated at least in two ways. The model's output concentration is usually taken after one of the operators. In this way it could be significantly wrong. The often applied procedure of averaging over time (from several time steps up to months and years) does not improve the result if the concentration at each considered time step is taken after one and the same operator. A solution to this problem could be to average the concentration after each operator within the time steps. The other error is due to one and the same order of operators at each time step. For instance, the deposition is always taken from the air concentration established after advection and never from the concentration established after emission, which is not realistic. The wide applied solution of this problem is to change the operators' order in the next time step. This approach will be assessed hereafter.

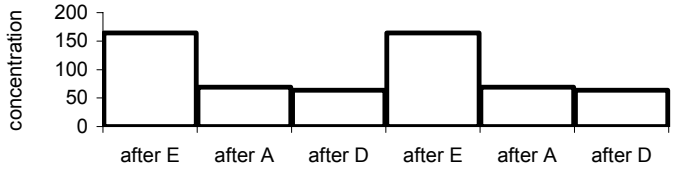

Figure 1. Mechanism of error generation. The air pollution concentration after emission (E), after advection (A) and after dry deposition (D) in a grid cell for two consecutive time steps. The results are from the Bott's scheme; The advection is caused by 1D wind of speed of 0.5 relative units, space and time steps =1; E is 100 relative units per time step. The deposition is 0.075 of the air concentration per time step. The exact analytic concentration is 99.0.

The idea of the present study is to compare the numerical results to the exact (analytic) solution of the advection equation with incorporation of emission and deposition. The goal is to outline a "technology" for testing of numerical advection schemes, including different techniques of incorporating of emission and removal.

Two types of numerical advection schemes are considered: the typical flux Eulerian scheme of *Bott* (1989) and the semi-Lagrangian one of Egan and Mahoney (*Atanassov et all.*,1997).

ANALYTIC SOLUTION

The concentration *C(x,t)* of a passive air pollutant advected along the x axis, is described by the following differential equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = Q - \alpha C \ , \tag{1}$$

where Q [kg/m^{2}s] is the emission rate per unit space area; αC is the loss of air pollutant per unit area per unit time (total dry and wet deposition); the coefficient α [s^{-1}] is the removal rate. The stationary solution of (1) is obtained for different complex distributions of source and sink regions (intervals) along *x* axis (*Atanassov et all*.,1996). Hereafter, $u(x)$ = const is assumed.

Unlike the stationary analytic solution, the numerical one includes a non-stationary transition period, after which a stationary concentration distribution at some distance downwind the emission sources should be established and the deposition per time step should become constant with time. In the following tests, the numerical schemes have been run long enough (300 time steps), so the stationary numerical solution is established over the considered space domain. The numerical deposition is defined as the mean value in the last 20 steps.

Equation (1) gives the concentration continuously at each point along the *x* axis, while the numerical schemes give the average concentration in a numerical grid cell. For more precise comparison, the analytic solution is averaged over the grid cells (*Atanassov et all.,* 1996). A numerical grid step $dx = 1$ and a time step $dt = 1$ have been assumed; the wind speed is equal to the Courant number in this case.

INCORPORATION OF THE DEPOSITION IN NUMERICAL SCHEMES

In the idealized case considered here, it does not matter what reason causes the removal of pollutants from the air - chemical transformation, dry deposition or washout by rain. In a numerical scheme, the classic way to calculate deposition *D* per time step Δt is

$$D = C\alpha\Delta t \, , \tag{2}$$

where the coefficient α could be a rather complex function of the parameterisation of the deposition process. An alternative to (2) could be the following equation:

$$D = C\left(1 - e^{-\alpha\Delta t}\right), \tag{3}$$

expressing the gradual decrease of pollutant mass during the time interval Δt .

SPLITTING TECHNIQUES – MODEL'S VERSIONS

In addition to the simplest way to split the processes mentioned in the introduction, other splitting techniques could be used. Several possibilities are considered in the present study, defining in this way different versions of the numerical models. Another way to formulate model's version, is to calculate the deposition according to (2) or (3) - see Table 1.

The same model versions have been build with the advection scheme of Egan & Mahoney; their notation starts with letter "E" instead of "B". In models' notation, the usage of (2) is denoted by the letter "c" (classic) and the usage of (3) by the letter "f" (fine-time deposition). Versions "1"

and "2" are the two simplest possibilities to split the processes. Versions "3" and "4" are a manner to change the operators' order from one time step to the next. Versions "5" are another approach, first proposed in (*Atanassov et all.,* 1996); the deposition is taken from mean value of the air concentration after emission and after advection.

Table 1. Model versions with Bott's scheme and some their main peculiarities. In the operators' order sequence E stands for emission, A for advection and D for deposition.

Model notation	Calculation of D formula:	Concentration - subject of deposition	Operators' order Time steps 1	2	3	4	5	6
B1c, f	(2) or (3)	after A	E A D	E A D	E A D	E A D	…	
B2c, f	(2) or (3)	after E	E D A	E D A	E D A	E D A	…	
B3c, f	(2) or (3)	after A, after D	E A D	D A E	E A D	D A E	…	
B4c, f	(2) or (3)	after E, after A	E D A	A D E	E D A	A D E	…	
B5c, f	(2) or (3)	(after E+ after A) / 2	E A D	E A D	E A D	E A D	…	

A SET OF TESTS

The model versions listed above have been run for different configurations of emission and deposition areas along x-axis. They are briefly described on Table 2.

Table 2. A set of tests used in the study. All tests are performed for 3 values of the wind speed, namely u=0.1, 0.5 and 0.9.

Test	Situation
1-00-2-*u*	1) Single cell emission = 100 2) Uniform deposition rate α = 0.075
1-00-5-*u*	1) Single cell emission=600 2) The deposition rate α is a complex function of x
3-00-2-*u*	1) Complex sharp emission distribution $Q(x)$ =(100,20,100, ...20,100,20) 2) Uniform deposition rate α = 0.075
5-33-2-*u*	1) Complex sharp emission distribution $Q(x)$ =(300,60,600, ... 60,600,60) 2) Uniform deposition rate α =.075 + precipitation =(.5, .5, .3, .3, .3, .8, .8)

STATISTICAL ASSESSMENTS AND RESULTS

All model versions and tests are evaluated in terms of deposition by the following relative error:

$$RR_k = \frac{D_k^{numerical} - D_k^{analytic}}{D_k^{analytic}} 100\% \qquad \text{and} \qquad RR = \sum_k \left| RR_k \right|, \quad \text{(4a,b)}$$

where k is the grid cell index.

The models turn to have quite different behavior for different wind speed - see the model's B1c results in Figure 2. For that reason, three wind speed values are considered for each test. The averaged over them error is presented in the shaded columns of Table 3 (see also Fig.4). Version B2c always overestimates the deposition in the emitting grid cell(s), because the deposition is taken after the release and before the advection.

All the models B3c,f, B4c,f, E3c,f and E4c,f show a strange behavior for big Courant numbers (Figure 3) that causes the significant errors in the case u=0.9 (see Table3). The reason is the

double advection without emission between them. The released quantity is advected too far away from the source cell by the second advection operator before the occurrence of the next release. When the next release happens, a local minimum of the concentration appears between the new released quantity and the old one. The deposition is proportional to the concentration and also posses such nonrealistic shape.

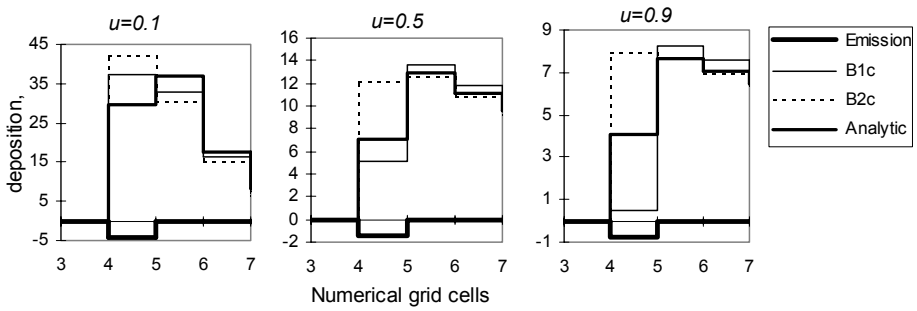

Figure 2. Deposition per time step according to model versions B1c and B2c; test 1-00-2. Analytic solution is the bold line; emission is presented on the negative side of the y axis.

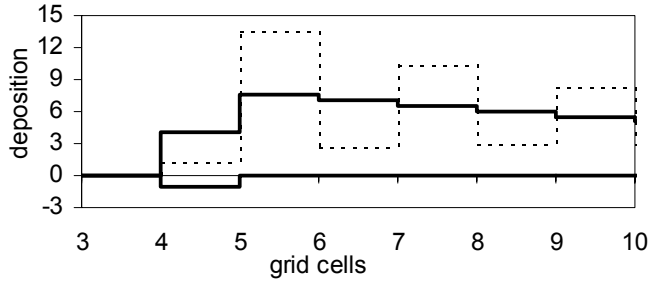

Figure 3. Deposition per time step according to version B3c (dashed line); test 1-00-2-9; u=0.9. The bold line is the analytic solution.

The errors are considered over two areas: 1) the whole area (excluding where $D_k^{analytic} < 1$) and 2) the area (grid cells) where there is emission. The results for the whole area for version "c" are presented in Table 3. The last column on the right is the averaged over the all test errors.

CONCLUSIONS

A complex of reasons causes the errors presented on Table 3. Part of them is due to shortcoming of the advection scheme itself – this part is illustrated in a comparison of Bott's and Egan&Mahoney's results. The sensitivity to the splitting technique is demonstrated by a comparison of different models versions. There are errors depending on some factors, not subservient to investigators, like the wind speed and the space (and time) configuration of emission and deposition rate. The error for *u*=0.1 (excluding those of model's versions "3" and "4" for *u*=0.9) are usually bigger. The errors in the case of complex emission and deposition configuration are substantially bigger – compare test 5-33-2 with others. The errors over the emission area are considerably bigger compared to areas without emission–see Figure 4.

Table 3. The relative error RR % averaged over the whole area where $D_k^{analytic} > 1.0$.

Test	1-00-2-u				1-00-5-u				3-00-2-u				5-33-2-u				All
Model	u=.1	u=.5	u=.9	all u	u=.1	u=.5	U=.9	all u	u=.1	u=.5	u=.9	all u	u=.1	u=.5	u=.9	all u	tests
B1c	15.8	4.0	6.7	8.8	9.5	4.4	4.5	6.1	13.7	4.9	6.6	8.4	39.0	57.5	60.2	52.2	18.9
B2c	23.6	10.3	7.9	13.9	13.2	7.3	5.4	8.6	18.9	10.0	8.6	12.5	45.6	69.5	71.0	62.0	24.3
B3c	19.5	5.0	28.5	17.7	11.0	5.0	20.3	12.1	16.1	4.8	20.7	13.9	41.1	57.3	74.9	57.8	25.4
B4c	19.8	6.7	29.1	18.5	11.0	5.1	25.0	13.7	16.1	6.5	21.2	14.6	42.5	47.4	77.6	55.8	25.7
B5c	14.6	2.3	0.1	5.7	9.7	1.2	0.1	3.7	13.2	1.8	0.2	5.1	38.2	14.2	2.8	18.4	8.2
E1c	7.5	4.6	6.7	6.3	10.4	4.6	4.4	6.5	6.4	4.7	6.5	5.9	14.5	48.1	56.5	39.7	14.6
E2c	12.6	8.7	7.8	9.7	12.3	6.7	5.3	8.1	11.1	9.1	8.7	9.6	27.1	64.4	68.3	53.3	20.2
E3c	8.2	2.7	27.3	12.7	10.7	3.9	22.7	12.4	6.9	3.5	11.8	7.4	18.2	44.2	67.1	43.2	18.9
E4c	8.9	2.8	28.1	13.3	10.8	3.9	21.7	12.1	7.5	4.2	12.3	8.0	22.1	48.3	64.5	45.0	19.6
E5c	3.7	0.9	0.3	1.6	4.5	0.9	0.2	1.9	2.8	0.9	0.2	1.3	14.1	20.8	7.2	14.0	4.7

The present study aims to show the way for testing, but some recommendations could also be drown. The often used approach to change the operators' order from one time step to the next (versions "3" and "4", here) should be applied carefully, because the repeated application of one the same operator could cause significant errors. The approach used in version "5" should be definitely preferred.

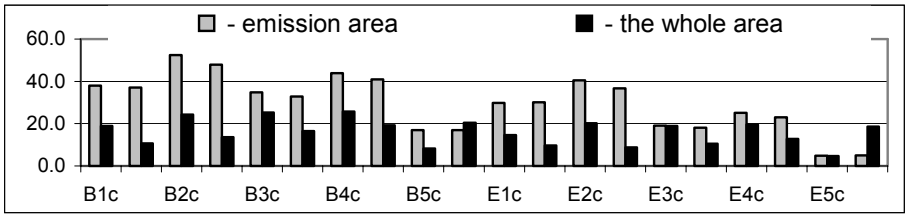

Figure 4. The relative errors RR % averaged over all wind speeds and over all tests. The errors for all models' versions, "c" and "f", are presented separately for the whole area where $D_k^{analytic} > 1.0$ and for the area where there is emission .

There are many possibilities to split the processes in numerical modeling. Probably only few of them have been considered here. Knowledge on the model itself is very important in its testing, analysis and possible improvements, and consequently, the model's author is the right person to perform the testing. A set of exact analytic solutions is available on request to anyone wishing to test his model.

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