PRELIMINARY STUDY OF USING ELLAM FRAMEWORK FOR SOLUTION OF ATMOSPHERIC ADVECTION-DIFFUSION-REACTION EQUATION

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Abstract

This paper deals with the numerical solution of the specific atmospheric equation called advection-diffusion-reaction equation (ADR). This equation describes the behaviour of the pollutant that was released to the atmosphere, namely a change of its concentration during time. The ADR equation is rather complicated, because of the highly variable coefficients with respect to time and space. The common technique to simplify the solution is to use the approach of operator splitting, where the ADR equation is divided into two or three parts that contain advection, diffusion or reaction part, sometimes two of them together. Then the special methods are used to solve each part of it. This paper contains the results of experiments where the Walcek [1] and ELLAM methods were compared with each other through various tests that refer to the pure advection equation. The slightly adapted ELLAM method has turned out to be the more accurate and the more stable in these tests.

Keywords: contaminant dispersion, atmospheric pollution, advection-diffusion-reaction equation, ELLAM framework

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1 Introduction

The area of pollutant dispersion is nowadays exposed to vivid research interest of scientific community and close attention is given to the modeling of this phenomenon. The dispersion model is described by a specific partial differential equation (PDE) called advection-diffusion-reaction (ADR) equation. The advection part denotes the transport of the material, which is caused mostly by a wind in the atmosphere or by a stream in a water environment, such as lakes, seas or rivers. The diffusion part of the equation is linked to a process that is natural for molecules in a liquid state or in a gaseous state. For this kind of molecules, the forces between them are weaker and when the substance/pollutant penetrates such environment it can reach an equilibrium state and it leads to a uniform dispersion throughout the environment. The last reaction part includes the chemical reactions of the pollutant in the atmosphere which result mostly in sinking of the contaminant concentration.

The dispersion model is described by the the PDE that is very complex and only its special cases can be solved analytically. Therefore, the numerical methods are used to acquire the solution. The splitting operator technique is used to simplify the solution by splitting equation into smaller parts corresponding to advection, diffusion and reaction. Although the special simple methods can be used to solve the separate parts, the error due to splitting, which is often neglected, arises [2].

The Walcek method [1] was successfully tested and compared against up to its date best methods that solve the pure advection part of the ADR equation. Consequently, another method, more precisely the framework, for solution of advection dominated pollutant dispersion model was being developed. Although the ELLAM is much more complicated than the Walcek's method, it has the advantage of incorporating of the other part, diffusion or reaction. The ELLAM has many variants that were mostly adapted to water fluid environments were the behaviour of the flows is different from the atmospheric turbulent flows. Therefore, in this paper the slightly modified version of ELLAM was compared with the Walcek method in appropriate various tests.

The paper is organized as follows. In the second section Walcek's method is presented. The ELLAM method is described and discussed in the third section. The fourth chapter contains the declaration of the test methodology and the particular tests are presented. The overall conclusion is then stated in the last section.

2 Advection equation and its solution

The advection part of the ADR equation in one dimension has the form

$$\frac{\delta c}{\delta t} = -\frac{\delta(Vc)}{\delta x} \tag{1}$$

where c is a concentration, t means time, V is the velocity and x is the spatial variable. The velocity field is often very complex and therefore, no analytical solution exists and numerical approximations are used instead. The simplest numerical approximations cause the inaccuracies and artificial artefacts to the solution. The long term research that has taken several last decades has lead to the numerical methods that try to hold several properties. These are mass conservation, monotonicity (peak and minima preservation with no spurious peaks calculated) algorithm simplicity, and a small number of calculations per time step. Various methods were developed to meet one or more properties, however the trade-off was required. Bott [3] suggested one of the algorithm that yielded the many of the desirable properties, however, it is complicate to implement. Walcek followed their research and proposed an algorithm that satisfies the properties and is relatively easy to implement.

2.1 Walcek's method

For many applications, fluid density is not constant, i.e. when advection is calculated in two- or three-dimensional flows. Therefore, the mixing ratios are used instead of concentrations:

$$\frac{\delta(q\rho)}{\delta t} = -\frac{\delta(V\rho q)}{\delta x} \tag{2}$$

where $q = c/\rho$ is the mixing ratio and ρ is the fluid density. The mixing ratio of a substance in grid cell "*i*" at time $t + \delta t$ can be initially estimated using a forward-time approximation to the "*t*" derivative in equation 2, and evaluating the spatial derivative at the initial time:

$$q_i^{guess} = \left[q_i^t D_{d-1} - \frac{F_{i+1/2}}{\delta x_i} + \frac{F_{i-1/2}}{\delta x_i} \right] \Big/ D_d \tag{3}$$

where the D_{d-1} and D_d terms are the dimensionally dependent fluid densities at the beginning and end of the time step or dimensional step in a multi-dimensional calculation.

Simple upwind schemes assume that concentrations within each grid cell are constant, however the reasonable distribution of the mixing ratios between grid cells can be supposed. The higher order polynomials were succesfully used to prevent artificial numerical diffusion [4]. In Walcek scheme the dual-linear functions are used to approximate the distributions inside each cell, which leads to the less complicated scheme in opposite to schemes preserving the advantages of higher order polynomials schemes.

It is reasonable to limit the concentration at edges of neighbouring cells to prevent unrealistic concentrations. The concentration at the edge of two cells must be in range of concentration of each of them. It is physically impossible to gain another level of concentration. Since the Walcek scheme assumes the Courant number $Cour = V\Delta x/\Delta t$ less than 1 due to the method stability, the next limitation type can be set. The mixing ratio in the cell where the fluid is advected into must be less than the highest mixing ratio in the upwind cell initially.

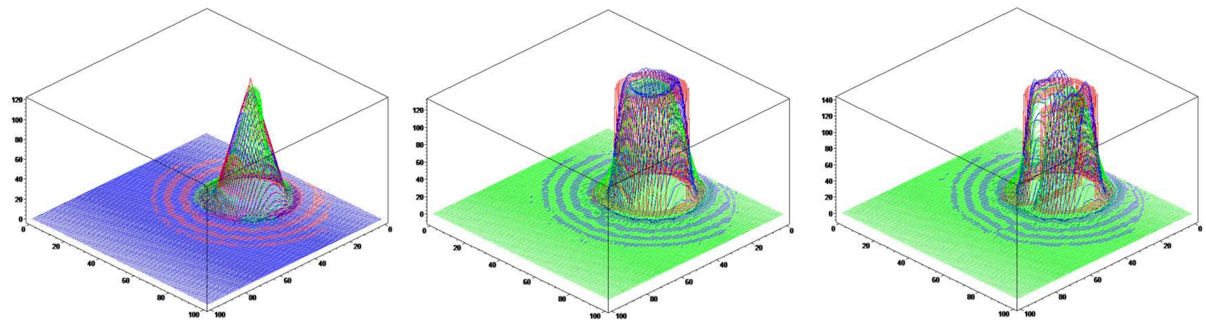

Fig. 1 Rotating test results performed to cone (left), cylindrical (middle) and slotted cylindrical (right) initial conditions. The exact solution is red, the result of the Walcek method is green and the ELLAM is blue.

2.2 ELLAM framework

ELLAM method is based on a philosophy of algebraic theory by Herrera [5]. In this theory, the test functions are used to define the weak form of the governing equation. To develop the ELLAM framework, the following advection-diffusion equation in one space dimension will be used as a model:

$$\frac{\partial c}{\partial t} + V\frac{\partial c}{\partial x} - D\frac{\partial^2 c}{\partial x^2} = f(x,t), \qquad 0 < x < L, \quad t > 0, \tag{4}$$

where c is the concentration, V is the wind, D is the diffusion and λ is the retardation coefficient. $f(x,t)$ is a source term. For simplicity, it is assumed that the coefficients are constants. The ELLAM idea uses general concepts of localized adjoint methods [28,29] to define test functions based on specific solutions to the homogeneous adjoint equation associated with the governing equation 4. The following weak form of the governing equation is further used [6]:

$$\int_{\Omega_t}\int_{\Omega_x}\left(\frac{\partial c}{\partial t} + V\frac{\partial c}{\partial x} - D\frac{\partial^2 c}{\partial x^2}\right) w(x,t)dxdt = \int_{\Omega_t}\int_{\Omega_x} f(x,t)w(x,t)dxdt. \tag{5}$$

The $w(x,t)$ is the test function. The problem is to find the solution such as the equation 5 holds. The advantage is that we can choose the test function freely. Integration by parts in both space and time yields the adjoint operator, and the test function is chosen to satisfy the homogeneous version of the adjoint equation:

$$-\frac{\partial w}{\partial t} - V\frac{\partial w}{\partial x} - D\frac{\partial^2 c}{\partial x^2} = 0. \tag{6}$$

The test function $w(x,t)$ that satisfy the equation 6 is [6]:

$$w_i^{n+1}(x,t) = \begin{cases} \frac{x - x_{i-1}}{\Delta x} + V\frac{t^{n+1}-t}{\Delta x}, \\ \quad x_{i-1}^* \le x \le x_i^*, \\ \quad t^n < t < t^{n+1} \\ \frac{x_{i+1} - x}{\Delta x} + V\frac{t^{n+1}-t}{\Delta x}, \\ \quad x_i^* \le x \le x_{i+1}^*, \\ \quad t^n < t < t^{n+1} \\ 0, \quad \text{all other } x, t, \end{cases} \tag{7}$$

where x_{i-1}^*, x_i^* a x_{i+1}^* are space positions of points x_{i-1}, x_i a x_{i+1} in time t^n lying on a characteristics curve $\frac{dx}{dt} = V$. The property of the weak form of equation is that it can be divided into parts by integrating by parts. Then the terms are dealt with separately. The advantage of the ELLAM framework is its ability to integrate the boundary conditions. They simply appear as other integral terms in the equation.

The important part of the ELLAM scheme is the accurate characteristics tracking of the points. The problem of characteristics tracking is described by the ordinary differential equations, thus the solution can be obtained by various numerical methods. The crucial is to set the size of integration step and together the speed of calculation. In our case we choose the tracking by Runge-Kutta 4th order method with the constant step size. The tests showed us that it turned out to be the proper method among others like Euler or lower order R-K methods.

3 The performed experiments

The experiments come out from these presented by Walcek and they refer to the advection part of the governing equation 4. In case of ELLAM the diffusion coefficient was set nearly to zero to simulate the advection equation only. The test were performed in two dimensions, where the rotating and divergent wind fields were used.

The experiment settings was as follows. All tests were done in a squared space which was divided into 100 x 100 points. The diameters of the initial shapes was set to 15 points for all tests. The time steps were set such as the Courant number would be less than one in case of Walcek algorithm. On the other hand the time step was set to 8^{th} and 24^{th} multiple of Walcek setting in case of ELLAM. The step size of ELLAM algorithm was choose in this way to reach the approximately same calculation time as in case of Walcek scheme.

3.1 Error measures

For the experiment evaluation the following error measures were chosen. The first one relates to law of mass conservation. That is the final mass distribution of the experiment should be the same as at the beginning.

The relative root mean square error (RMS) is the second measure. The differences between the exact and calculated solution are normalized by the difference between peak and minimum concentration levels. The result is the number bigger or equal to zero where one means 100 percent error with respect to concentration interval between initial peak and initial zero levels:

$$Err_{RMS} = \frac{\sqrt{\sum_{i=1}^{100}\sum_{j=1}^{100}(Calc_{i,j} - exact_{i,j})^2/100^2}}{Peak_0 - Min_0}, \tag{8}$$

where i and j are indexes of points in the domain, $Calc_{i,j}$ and $exact_{i,j}$ is the calculated and exact concentration of point with coordinates $[i, j]$, $Peak_0$ and Min_0 is the peak and minimum concentration in the initial time.

The next error measure is the peak error represented by equation of the form:

$$Err_{peak} = 1 - \frac{Peak_c - Min_c}{Peak_0 - Min_0}, \tag{9}$$

where $Peak_c$ and $Peak_0$ is the calculated and initial peak of the concentration, Min_c and Min_0 is the calculated and initial minimum of the concentration level.

The last error measure is referred as mass distribution ratio. It represents shape preservation without reference to the advected shape. The algorithm can for example nicely preserve shapes but it shift the position of the shape to wrong position. Thus its RMS error would be relatively high. On the other hand the distribution error would be pretty smaller. The distribution error is defined as:

$$Err_{dist} = 1 - \frac{\sum_{i\in\Omega_i}\sum_{j\in\Omega_j} Calc_{i,j}}{\sum_{i\in\Omega_i}\sum_{j\in\Omega_j} exact_{i,j}}, \tag{10}$$

where the Ω_i and Ω_j refers to domain where $Calc_{i,j}$ and $exact_{i,j}$ differs from Min_0.

3.2 Rotating wind

The rotating wind fields serve as reference test where the error can be easily measured. At the beginning the concentrations distribution is set and it is used as initial conditions to the equation. Then the suitable time steps are chosen and the time of the simulation is set to multiples of the whole rotations.

The experiments were performed with three different initial conditions. The shape of the distribution was set to cone, cylinder and slotted cylinder. The results of the 60 rotations are shown in Fig. 1.

In Fig. 1 it is seen that the Walcek algorithm distorted the solution slightly - it is obviously seen especially for the cone case at the peak of the shape. The similar results are for the cylindrical shapes where the Walcek algorithm gets the shape thinner - its mostly like a truncated cone.

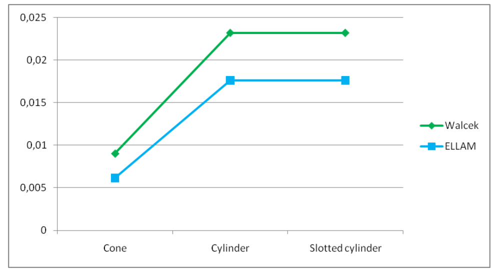

Fig. 2 The resulting mass mean error of rotating tests of Walcek and ELLAM solutions. The cases of cone, cylinder and slotted cylinder are shown.

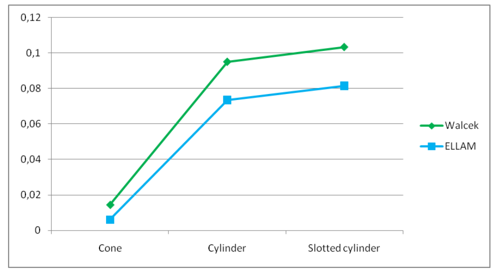

Fig. 3 The resulting root mean square error of rotating tests of Walcek and ELLAM solutions. The cases of cone, cylinder and slotted cylinder are shown.

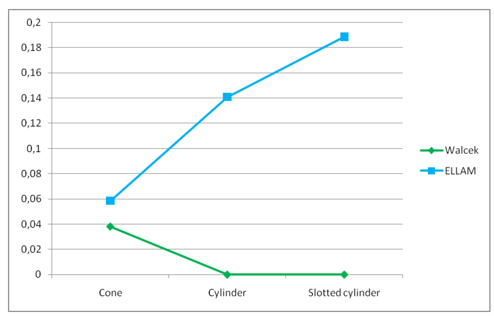

Fig. 4 The resulting peak error of rotating tests of Walcek and ELLAM solutions. The cases of cone, cylinder and slotted cylinder are shown.

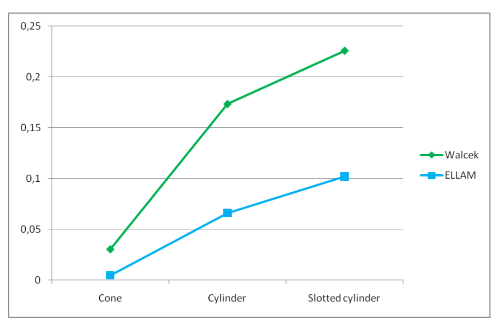

Fig. 5 The resulting distribution error of rotating tests of Walcek and ELLAM solutions. The cases of cone, cylinder and slotted cylinder are shown.

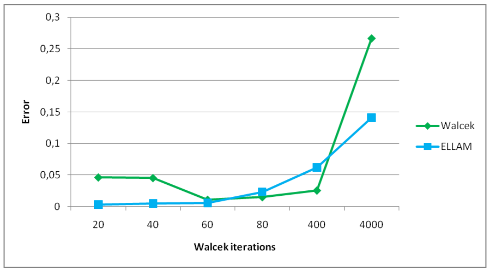

Fig. 6 The mass mean error propagation during divergent wind test of Walcek and ELLAM solutions.

In Fig. 2, 3, 4 and 5 one can see the error measurement for the overall rotating wind tests that was performed. The tests include the 1, 6 and 60 rotations, where the first two cases represents the short term and the last the long-term simulations. It is obvious that both algorithms conserve mass, however, the ELLAM gained less errors. RMS and distribution errors are much less in case of ELLAM algorithm, which corresponds with the images in Fig. 1. The only error in which the Walcek algorithm dominates is the peak error. It is caused by slight oscillations near the peak of concentration.

3.3 Divergent wind

The divergent wind test simulates the atmospheric non-uniform wind field. In this case the space is divided into several areas where the wind is rotating separately. The initial non-zero concentration is placed between two central areas. The expected result of long-term simulation can be described as follows. The contaminant concentration started to disperse to local wind areas. Then it begins to follow the wind velocities. The final distribution of concentration should be the uniform concentration mostly in the two central areas.

The consecutive states of the simulation are shown in Fig. 7. The concentration distributions of the particular states agree for both Walcek and ELLAM algorithms. However, in the final state of the simulation the distribution is expected as uniform and the Walcek algorithm calculated an uneven concentration top. In case of ELLAM the evenness is much higher. This agrees with the final mass error, which is shown in Fig. 6.

4 Conclusion and future work

The preliminary tests were done for the use of ELLAM scheme to ADR equation that describes the pollutant behaviour in the atmosphere. From the performed experiments it is obvious that the ELLAM successfully past the tests and in majority of cases it overcame the state of the art method for solution of the advection equation.

The performed experiments dealt with the cases where the wind fluid was artificially generated. The complex wind experiments should come after. The advantage of the ELLAM method is its natural ability to incorporate boundary conditions. Therefore, the tests of different deposition models that model the dispersion of the con-

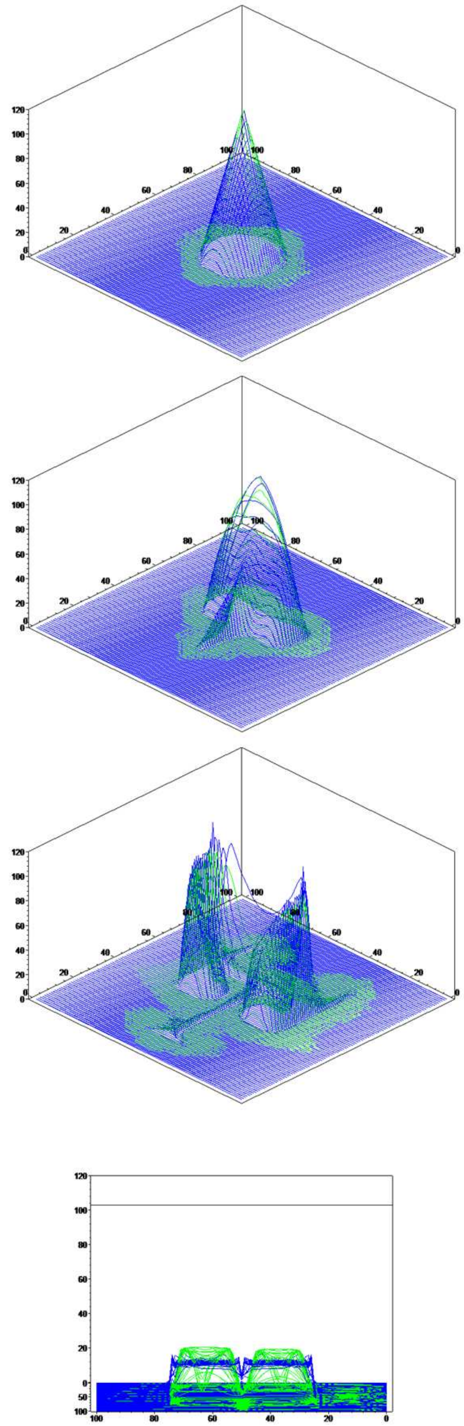

Fig. 7 Divergent test results performed to cone placed in the middle of the space. The result of the Walcek method is green and the ELLAM is blue.

taminant near the ground should be considered. We are planning both in the near future.

5 Acknowledgements

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