SIMULATION OF ATMOSPHERIC POLLUTION DISPERSION

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Abstract. The aim of this paper is to provide a solution to the atmospheric advection-diffusion equation (ADE) and to describe its properties from the stability and the accuracy point of view. We suggest how to solve the problem by an approximation of the ADE with the system of ordinary differential equations and we state the theoretical limitations of a discretization steps both in time and space. We have done series of tests that prove the theoretical assumptions. The advantage of our approach with respect to other approaches such as strict finite differencing schemes, finite element methods and different kinds of methods of characteristics is knowledge of its theoretical bounds, simplicity and the ease of extensibility.

1 Introduction

The modeling of atmospheric pollution has a great importance in the case of prediction of pollutant behavior throw the atmosphere. It has gone big journey in the last century as is stated in [1]. One of the first models was so called Gaussian plume model which was first proposed by Pasquille and others in sixties of 20th century. It was firstly used for modeling pollution dispersion from a point source, however, it was soon applied to line and area sources as well. It matched with the observations and became a standard in every industrial country. The concern shifted to studying of dispersion phenomena, namely dry dispersion. It means that the pollutant behavior above the ground and a study of its causalities had been in the area of interest. Consequently, a new full form of diffusion equation was formulated, which contains diffusivity, advection, deposition, emission and chemistry terms. Since that time no new general model was proposed and it is focused until now to solute the full atmospheric equation.

In our paper, we are concentrated to a model consisting of advection, diffusion and deposition terms [4]. The steady state form of this kind of equation is of the form:

$$u_x \frac{\partial C}{\partial x} = D_y(x)\frac{\partial^2 C}{\partial y^2} + D_z(x)\frac{\partial^2 C}{\partial z^2} + W\frac{\partial C}{\partial z} \tag{1}$$

where the C is concentration in space domain (x, y, z), u_x is a wind size in x direction, D_y and D_z diffusion coefficients in appropriate axes and W is a deposition rate or deposition velocity. The equation (1) does not include the chemical and emissivity terms which are neglected. The appropriate boundary conditions are stated in next section - equations (2a-e).

The paper is structured as follows. In Section 2, the dispersion model of unsteady source is proposed and a stability analysis is performed. The experiments with stability criterions as well as the critical accuracy place are shown in Section 3. At the end the final conclusion and remarks are stated.

2 Unsteady dispersion model

The steady state form of the ADE is, however, not sufficient form for modeling of the pollutant dispersion under real conditions. Therefore, the other properties such as variable wind directions and forces, natural/artificial obstacles etc. should be taken into account in our model.

$$\frac{\partial C}{\partial t} = -u_x\frac{\partial C}{\partial x} + D_y(x)\frac{\partial^2 C}{\partial y^2} + D_z(x)\frac{\partial^2 C}{\partial z^2} + W\frac{\partial C}{\partial z} \tag{2}$$

$$C(0,0,y,z) = \frac{Q}{u}\delta(y)\delta(z-H) \tag{2a}$$

$$C(t,x,-\infty,z) = 0, C(t,x,+\infty,z) = 0 \tag{2b-c}$$

$$C(t,-\infty,y,z) = 0, C(t,+\infty,y,z) = 0 \tag{2d-e}$$

$$C(t,x,y,+\infty) = 0 \tag{2f}$$

$$\left[D_z\frac{\partial C}{\partial z} + WC\right]_{z=0} = [vC]_{z=0} \tag{2g}$$

Therefore, the equation (1) must be used in its more general form including the time variable and boundaries that respect terrain and obstacles (2). The symbols in equation (2) has the same meaning as in equation (1) except that C is a function of time-space domain (t, x, y, z). The initial condition (2a) defines the concentration of the pollutant in a source of pollution (source with strength of Q), which lies in height H. The boundary conditions (2b-f) show that the concentration reached zero far away from the source in x, y and z directions. Finally, the last boundary condition (2g) expresses how the rate of concentration changes close to the terrain ground. Here v means the deposition velocity and it is influenced by various pollutant, atmosphere and terrain properties.

2.1 Model approximation

There are many possibilities how obtain solution to the partial differential equation (2). Since the analytical solution is not known, the numerical approach must be used. Again, many numerical methods have been developed in the past few decades. The finite differences approach belongs between widely used as well as finite element method and different kinds of method of characteristics. The first one is a classical approach where the approximated part is the partial differential equation itself. The partial derivatives and time derivatives are substituted by finite differences. The accuracy of that kind of solution depends on an order of finite differences – the number of Taylor terms used. On the other hand in the case of finite element method, the solution equation is approximated directly most often by weighted linear function [5]. In the method of characteristics, the hyperbolic PDE is transformed from a time domain to the domain of characteristic curves that contains the information about the solution. In some simple cases, it can be applied directly, otherwise it is applied numerically [7].

In our work we have chosen a method of lines as a method for solving PDE because its simplicity, the derivable limitations and ease of extensibility. It is based on finite differences where the variables (spatial) are discretized except for one (time variable). This procedure gives us a system of ordinary differential equations (ODE), which can be solved by numerous explicit or implicit methods such as Euler, Runge-Kutta and others. After applying of central differences in space of second order to equation (2), we get:

$$\begin{aligned}\frac{dC(t,x,j,k)}{\partial t} &= -\frac{u_x}{2\Delta x}(C(t,i+1,j,k)-C(t,i-1,j,k))+\\ &+\frac{D_y(x)}{\Delta y^2}\cdot(C(t,i,j+1,k)-2C(t,i,j,k)+C(t,i,j-1,k))+\\ &+\frac{D_z(x)}{\Delta z^2}\cdot(C(t,i,j,k+1)-2C(t,i,j,k)+C(t,i,j,k-1))+\\ &+\frac{W}{2\Delta z}\cdot(C(t,i,j,k+1)-C(t,i,j,k-1))\end{aligned} \tag{3}$$

with appropriate initial and boundary conditions (the partial derivative in condition (2g) is approximated by second order forward difference operator):

$$\begin{aligned}&C(0,0,0,H)=\frac{Q}{u_x\Delta y\Delta z} \\ &C(0,i,j,k)=0 \text{ otherwise}.\end{aligned}\quad \begin{aligned}&C(t,0,j,k)=0.\\ &C(t,N_i,j,k)=0.\\ &C(t,x,0,k)=0.\\ &C(t,x,N_j,k)=0.\\ &C(t,x,j,N_k)=0.\end{aligned}\quad C(t,x,j,0)=\frac{D_z(4C(t,x,j,1)-C(t,x,j,2))}{2\Delta z(v-W)+3D_z}. \tag{3a-g}$$

2.2 Stability analysis

In order to analyze the stability of the equation (3), the von Neumann stability analysis was made. It analyzes theoretical bounds of coefficients in the discretized domain of a linear equation [2]. Let us do this procedure for a case, when the explicit Euler method is used for solving the system of ODE (3). This is equivalent to the well known forward time and central space method (FTCS).

Let advection terms, c_x and c_z, diffusion terms, d_y and d_z, and a transformation are defined as:

$$c_x=\frac{u_x\Delta t}{2\Delta x},\ c_z=\frac{W\Delta t}{2\Delta z},\ d_y=\frac{D_y\Delta t}{\Delta y^2},\ d_z=\frac{D_z\Delta t}{\Delta z^2},\ C(t,i,j,k)=U^t e^{I(\Theta i+\Phi j+\Psi k)} \tag{4}$$

Then, after substituting terms (4) into equation (3) and applying von Neumann stability analysis, we obtain:

$$U^{t+1}=[1+2d_y(\cos\Phi-1)+2d_z(\cos\Psi-1)-I(2c_x\sin\Theta-2c_z\sin\Psi)]\cdot U^t=G\cdot U^t \tag{5}$$

where

$$\Theta=k_x\Delta x,\ \Phi=k_y\Delta y,\ \Psi=k_z\Delta z,\ I^2=-1$$

As far as the amplification factor G is a complex number, then for numerical stability following condition must be satisfied:

$$|G|^2 = [1 + 2d_y(\cos\Phi - 1) + 2d_z(\cos\Psi - 1)]^2 + (2c_x \sin\Theta - 2c_z \sin\Psi)^2 \le 1 \tag{6}$$

After simple manipulation of inequality (6) we get:

$$d_y \cos\Phi + d_z \cos\Psi - (d_y + d_z) + \left[d_y \cos\Phi + d_z \cos\Psi - (d_y + d_z)\right]^2 \le -(c_x \sin\Theta - c_z \sin\Psi)^2 \tag{7}$$

The left side of the inequality (7) is a quadratic function of the form $f(x)=x^2+x$ and its right side is always negative. From these facts following condition must be satisfied:

$$-1 \le d_y \cos\Phi + d_z \cos\Psi - (d_y + d_z) \le 0 \tag{8}$$

Second inequality of (8) is satisfied for every d_y and d_z assuming that they are non-negative – it is true according to their definitions (4). First inequality, and thus the whole condition for every Φ and Ψ, holds for:

$$d_y + d_z \le \frac{1}{2} \tag{9}$$

Next, the absolute value of the right hand side of inequality (7) is maximal for Θ=π/2 and Ψ=3π/2 and it is a limiting case:

$$(d_y + d_z - d_y \cos\Phi)(-d_y - d_z + d_y \cos\Phi + 1) \ge (c_x + c_z)^2 \tag{10}$$

From the fact that left hand side of inequality (10) corresponds to function $f(x)=-x^2+x$, then it has a maximum of ¼ and new condition must be at least:

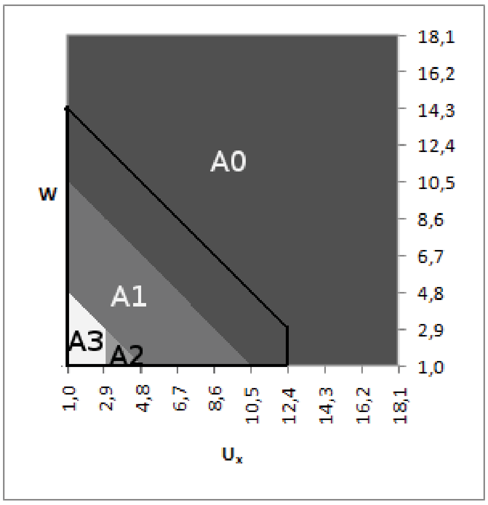
$$c_x + c_z \le \frac{1}{2} \tag{11}$$

However, it is not satisfied for every cases of left side of equation (10). Since the condition (9) holds, the left side of (10) is minimal for cos Φ=1 and then the final condition is:

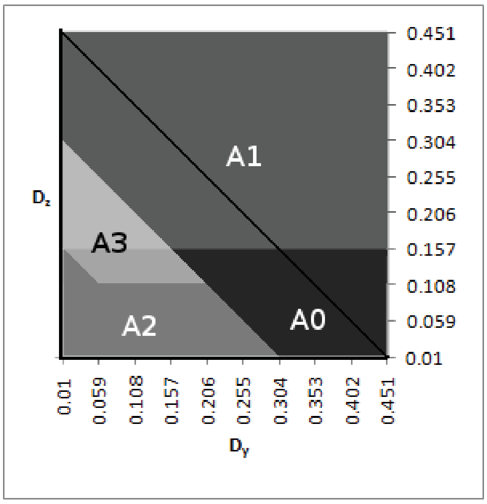
$$c_x + c_z \le (1 - d_z)d_z \tag{12}$$

3 Current results

We have tested our solution with simple case when the source is steady state and the ground is flat everywhere. The analytical solution is known for this simplified equation [4]. Moreover, we compared the theoretical stability conditions that are derived in previous section with experiments.



a



b

Figure 1. The areas of stability for variable advection number (a) and diffusion number (b).

Figure 1 shows the areas where the solution is stable or not. The particular areas are marked with color of different grey level. In Figure 1a the advection numbers, defined in (4), are varying according to the sizes of W and u_x coefficients and thus the stability space is altered appropriately. The condition (11) bounds the area of A1 as a stable, therefore A0 is unstable. However, after applying of (12) the stable area is further reduced into A2, in which all stability criterions are satisfied. The experiments fit to the area of A3 which is a part of A2, thus the theoretical requirements are correct.

In Figure 1b the various diffusion numbers, defined in (4), are investigated. Here, the coefficients in the area of A1 satisfy condition (12) and the coefficients of A2 satisfy (9). The intersection of these areas A1 and A2 has the brightest color and is a little smaller than the area of A3, which was obtained by the experiments. Again it corresponds with each other up to some numerical errors. In both Figures 1a and 1b the areas bordered with black line belong to stable space of solutions where the 4^{th} order Runge-Kutta method was used. It is obvious that the area of stability is much larger than in case of FTCS method.

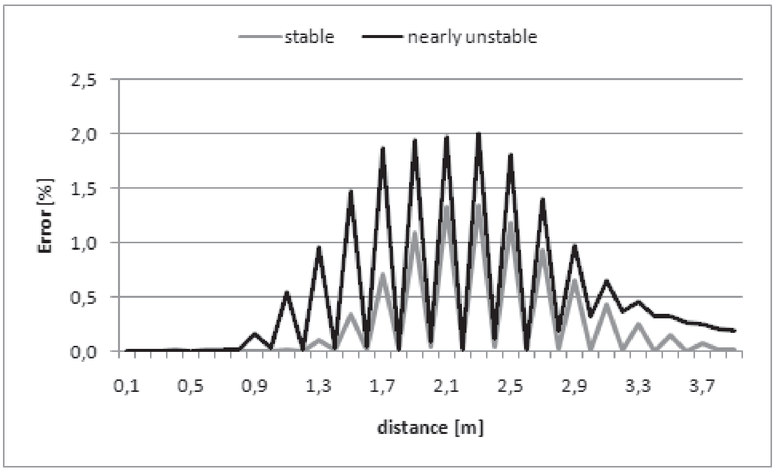


Figure 2. The mean error propagation along a wind direction.

The accuracy is clearly another important property of the approximation. The larger errors are arisen near the source when the steady state equation is approximated [3]. This is caused due to the fact that source strength is only approximated and a large gradient appears there. However, when the time derivative is added this kind of error disappears during a time. The second place where the error was relatively large is near the ground, where the boundary condition (3g) is applied (Figure 2). The solution have tendency to oscillate around the proper value. It is seen in Figure 2, where two cases are shown. The error is expressed in absolute value. While in a case of a stable solution the oscillations are damped in further distance, in a case of an almost unstable solution (near the border of stability) the error remains far away from the source.

4 Conclusion

The method of lines was successfully used to approximate of the solution to the advection-diffusion equation with deposition term. The stability analysis for the case of FTCS algorithm was carried out and it was supported by experiments. The method is very accurate up to approximation of boundary conditions.

The problem of oscillation of numerical solution is well known and thus the many propositions have been made. In recent years the generalized characteristics method that combines Eulerian (time-space domain) and Lagrangian (domain of characteristics) methods is being developed for transport-disperse problems [6]. It turns out that it greatly reduces the numerical anomalies and it can incorporate the boundary conditions naturally within its definition. Therefore it can be inspiring for further development of this work.

The investigation of possible incorporation of reaction terms into ADE as well as testing of non-constant coefficients will be other stages of the project. The latter is especially important in this field, because every physical variable in equation (2) is changing during time and space in the real world.

5 References

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