An implicit numerical scheme for the atmospheric pollution

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Abstract— **The model relates the concentration of a polluter in the atmosphere with the field vector of wind velocity, the turbulent diffusivity vector and the rate of mass diffusion of the polluter. An implicit finite-difference method is proposed for the numerical solution of this one-dimensional advection-diffusion model.**

Keywords—**Advection-Diffusion; Finite-difference Method; Turbulence; Atmospheric pollution.**

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I. Introduction

Let $c(x, y, z, t)$ $\mu g/m^3$ be the concentration-density of a passive polluter in the atmosphere, $\mathbf{v} = [v_x, v_y, v_z]^T$ m/s be the vector field of the velocity of the wind, which is given from a numerical model of weather data forecast, $\mathbf{K} = [K_x, K_y, K_z]^T$ be the turbulent diffusivity tensor and S $\mu g/m^3 s$ be the source of the polluter with mass release rate $q(t)$ in μ/h. Then the concentration-density c can be described from the following $3D$ advection-diffusion equation

$$\frac{\partial c}{\partial t} + \boldsymbol{\nabla} \cdot (\boldsymbol{v}\, c) = \boldsymbol{\nabla} \cdot (\boldsymbol{K} \otimes \boldsymbol{\nabla}\, c) + S(q(t)). \tag{1.1}$$

In Eq. (1.1) in order to simplify the quantity $\boldsymbol{K} \otimes \boldsymbol{\nabla}\, c$ only the diagonal terms were used. For the unstrained term S it can be assumed that either $S = q(t)$ (locally) or the source S follows a Gaussian distribution.

Eq. (1.1) for the one-dimensional problem, where $c = c(x, t)$, $v = v(x)$ and $K = K_x = K(x)$, leads to the following diffusion-advection equation

$$\frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} v + c \frac{\partial v}{\partial x}$$

$$= \frac{\partial K}{\partial x}\frac{\partial c}{\partial x} + K \frac{\partial^2 c}{\partial x^2} + S\,;\;\; x \in (L_0,\, L_1) \text{ and } t > 0. \tag{1.2}$$

Eq. (1.2) when $v = 0$, K constant without the source S reduces to the classical diffusion equation $c_t = K\, c_{xx}$, while when $v = \mu$ constant and $K = 1/Re$, Re being the Reynolds number leads to

$$\frac{\partial c}{\partial t} + \mu\, \frac{\partial c}{\partial x} = \frac{1}{Re}\, \frac{\partial^2 c}{\partial x^2} + S\,;\;\; x \in (L_0,\, L_1) \text{ and } t > 0. \tag{1.3}$$

Initial conditions are assumed to be of the form $c\,(x, 0) = f(x)$ while boundary conditions $c\,(L_0, t) = g(x)$ and $c\,(L_1, t) = \tilde{g}(x)$ for $t > 0$ with f, g and $\tilde{g}$ known functions.

II. The numerical method

For the numerical solution the region $\Omega = [L_0 < x < L_1] \times [\,t > 0\,]$ with its boundary $\partial\Omega$ is covered with a rectangular mesh of points with coordinates $(x, t) = (x_m, t_n) = (L_0 + mh, nl)$ with $m = 0, 1, ..., N + 1$ and $n = 0, 1, ...$ The solution of an approximating difference scheme at the same point will be denoted by C_m^n.

Let the solution vector at time level $t = t_n = n\ell$ be

$$\mathbf{C^n} = \mathbf{C}\,(t_n) = [C_1^n, C_2^n, ..., C_N^n]^T\,. \tag{2.1}$$

Using central-difference approximants for the space partial derivatives Eq. (1.2), when applied to the general mesh point (x_m, t_n), leads to a system of the form

$$\begin{aligned} D\,\mathbf{C}(t) \;\; = \;\; & -\frac{1}{2\,h}\text{diag}\,\{v_m\}\; A\,\mathbf{C}(t) \\ & -\frac{1}{2\,h}\text{diag}\,\{v_{m+1} - v_{m-1}\}\; \mathbf{C}(t) \\ & +\frac{1}{4\,h^2}\text{diag}\,\{K_{m+1} - K_{m-1}\}\; A\,\mathbf{C}(t) \\ & +\frac{1}{h^2}\text{diag}\,\{K_m\}\; B\,\mathbf{C}(t) + \mathbf{S}^n + \mathbf{b}^n, \end{aligned} \tag{2.2}$$

where $D = \text{diag}\,\{d/d\,t\}$ matrix of order N and A, B are tridiagonal matrices of order N with appropriate entries,

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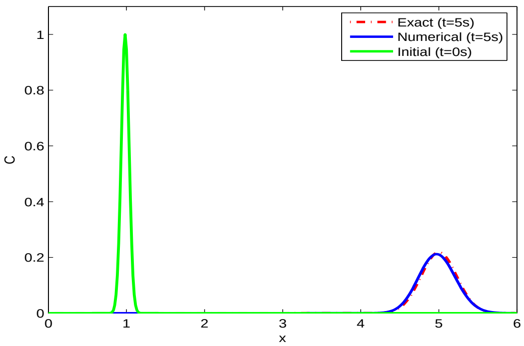

Fig. 1. Test Problem 1: Evolution of a Gaussian pulse (comparison with exact solution))

$\mathbf{C}^n = [S_1^n, S_2^n, ..., S_N^n]^T$ a vector of order N and $\mathbf{b}^n$ the vector of the boundary conditions also of order N.

Using the recurrence relation $\mathbf{C}(t+\ell) = \exp(\ell D)\,\mathbf{C}(t)$; $t = \ell,\, 2\,\ell, ...$ with the $(1,0)$ Padé Eq. (2.2) finally leads to

$$(I - \ell D)\;\mathbf{C}(t+\ell) = \mathbf{C}(t)\,, \tag{2.3}$$

where I the identity matrix of order N.

III. Numerical results

Extended numerical experiments based on the scheme (2.3) are given at the following paper. One of them in which it is assumed that $S = 0$ and the analytical solution is that of a Gaussian pulse of unit height centered at $x_0 = 1$m in a region bounded by $0 \leq x \leq 6$ given by

$$C(x,t) = \frac{1}{\sqrt{4t+1}} \exp\left\{-\frac{(x - x_0 - ut)^2}{K(4t+1)}\right\}, \tag{2.4}$$

where u is the velocity and K the (constant) diffusion coefficient in the x direction is examined here. The values of the various parameters used are $D = 5 \cdot 10^{-3} m^2/s$ and $u = 0.8 m/s$. The space step and time step are taken to be $h = 0.02m$ and $l = 0.01s$ respectively. The distribution of the Gaussian pulse at $t = 5$s is computed using the presented numerical scheme and compared with the concentration distribution obtained using the exact solution in Fig. 1, where we can see that the numerical solution follows very closely the exact one.

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