# AN IMPLICIT NUMERICAL SCHEME FOR THE ATMOSPHERIC POLLUTION

A. G. Bratsos[1], T. Papakostas[2], I. Th. Famelis[1], A.I. Delis[3] and D. G. Natsis[1]

**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.

**Index Terms**

Advection-Diffusion; Finite-difference Method; Turbulence; Atmospheric pollution.

*AMS* — 76B60, 76F05, 86-08, 65M06.
*PACS*— 92.60.Hp, 92.60.hk, 47.27.tb.

## I. INTRODUCTION

THE concentration of air pollutants have in general been steadily increasing during the last two decades. To correctly gauge the impact of various sources of pollutants requires careful modeling the complex physical processes associated with the advection and diffusion of air pollution. These models are computationally demanding and require the use of stable and accurate numerical schemes, [12], [11], [13], [15]. By considering only passive pollutants in an air pollutant transport model the advection–diffusion system of equations can drive the dynamical evolution of the pollutant concentration in a similar way that this is done, for example, in water flows [1], [5], [7], [5].

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 $\mu/h$. Then the concentration-density $c$ can be described from the following $3D$ advection-diffusion (AD) 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. Therefore

$$\boldsymbol{\nabla}\cdot(\boldsymbol{K}\otimes\boldsymbol{\nabla}\,c)=\frac{\partial}{\partial x}\left(K_x\,\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\,\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\,\frac{\partial c}{\partial z}\right), \tag{1.2}$$

where the factors $K_x$, $K_y$ and $K_z$ can be evaluated using various methods such as to have constant values or to calculated in the numerical weather model etc.

For the unstrained term $S$ it can be assumed that either $S=q(t)$ (locally) or the source $S$ follows a Gaussian distribution, which depends from the distance $d$ of the local source and expands to the grid cells as follows

$$S(d)=\frac{\partial c}{\partial t}(d)=\frac{q(t)}{2\pi\sigma_n^2 H}\ e^{-\frac{d^2}{2\,\sigma_n^2}}, \tag{1.3}$$

where $H$ is the vertical expansion of the smog and $\sigma_n^2$ is the horizontal area of the grid cell that includes the source.

The velocity field can be available in hour intervals but a numerical scheme for Eq. $(1.1)$ is going to need time steps in $s$, therefore in order to have the velocity field for all the necessary time steps there could be a linear interpolation in time.

Eq. $(1.1)$ for the one-dimensional problem, where $c=c(x,t)$, $v=v(x)$, $K=K_x=K(x)$, $\boldsymbol{\nabla}c=c_x i$,

$$\boldsymbol{\nabla}\cdot(\boldsymbol{K}\otimes\boldsymbol{\nabla}\,c)=\frac{\partial}{\partial x}\left(K\,\frac{\partial c}{\partial x}\right)=\frac{\partial K}{\partial x}\frac{\partial c}{\partial x}+K\,\frac{\partial^2 c}{\partial x^2}$$

and

$$\boldsymbol{\nabla}\cdot(c\,\boldsymbol{v})=\frac{\partial c}{\partial x}v+c\frac{\partial v}{\partial x},$$

[1]Department of Mathematics, Technological Educational Institution (T.E.I.) of Athens, GR-122 10 Egaleo, Athens, Greece. E-mail: bratsos@teiath.gr, ifamelis@teiath.gr and natsisd@otenet.gr
[2]Department of Natural Resources and Environment, Technological Educational Institution (T.E.I.) of Crete, Branch of Chania, GR-731 33 Crete, Greece. E-mail: taxiar@chania.teicrete.gr
[3]Department of Sciences, Division of Mathematics, Technical University of Crete, Chania 73100, Crete, Greece. E-mail: adelis@science.tuc.gr

reads to the following diffusion-advection equation

$$\frac{\partial c}{\partial t}+\frac{\partial c}{\partial x}v+c\frac{\partial v}{\partial x}=\frac{\partial K}{\partial x}\,\frac{\partial c}{\partial x}+K\frac{\partial^2 c}{\partial x^2}+S\,;\;\; x\in(L_0,\,L_1)\;\text{ and }\; t>0. \tag{1.4}$$

Eq. $(1.4)$ when

$v=0$, $K$ constant without the source $S$ reduces to the classical diffusion equation

$$\frac{\partial c}{\partial t}=K\frac{\partial^2 c}{\partial x^2}\,;\;\; x\in(L_0,\,L_1)\;\text{ and }\; t>0, \tag{1.5}$$

$v=\mu$ constant and $K=1/Re$, $Re$ being the Reynolds number leads to

$$\frac{\partial c}{\partial t}+\mu\,\frac{\partial c}{\partial x}=\frac{1}{Re}\,\frac{\partial^2 c}{\partial x^2}+S\,;\;\; x\in(L_0,\,L_1)\;\text{ and }\; t>0. \tag{1.6}$$

Initial conditions are assumed to be of the form

$$c\,(x,0)=f(x), \tag{1.7}$$

while boundary conditions

$$c\,(L_0,t)=g(x)\;\text{ and }\; c\,(L_1,t)=\tilde{g}(x)\,;\; t>0 \tag{1.8}$$

with $f$, $g$ and $\tilde{g}$ known functions.

## II. The numerical method

Finite difference schemes is a common choice for advection-diffusion equations see, for example, [9], [13], [11], [6], [2], [3], [4]. Explicit in time schemes are restricted by the well known CFL like stability restrictions that reduce substantially their computational efficiency. Our scope here is to present an implicit scheme that highly relaxes this restriction.

### A. Grid and solution vector

For the numerical solution the region $\Omega=[L_0<x<L_1]\times[\,t>0\,]$ with its boundary $\partial\Omega$ consisting of the lines $x=L_0$, $x=L_1$ and $t=0$, is covered with a rectangular mesh, $G$, of points with coordinates $(x,t)=(x_m,t_n)=(L_0+mh,nl)$ with $m=0,1,...,N+1$ and $n=0,1,...$, so that $h=(L_1-L_0)\,/\,(N+1)$. The solution of Eq. $(1.4)$ at the typical mesh point $(x_m,t_n)$ is $c\,(x_m,t_n)$ which may be denoted, when convenient, by $c_m^n$. The solution of an approximating difference scheme at the same point will be denoted by $C_m^n$, while for the purpose of analyzing stability, the numerical value of $C_m^n$ actually obtained (subject, for instance, to computer round-off errors) will be denoted by $\tilde{C}_m^n$.

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

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

### B. The finite-difference scheme

Eq. $(1.4)$ using central-difference approximations for the space partial derivatives, when applied to the general mesh point $(x_m,t_n)$ of the grid $G$, leads to the following system of ordinary differential equations

$$\begin{aligned}\frac{d\,C_m^n}{d\,t} \;=\; & -\frac{1}{2\,h}\left(C_{m+1}^n-C_{m-1}^n\right)v_m-\frac{1}{2\,h}\left(v_{m+1}-v_{m-1}\right)C_m^n\\ & +\frac{1}{4\,h^2}\left(K_{m+1}-K_{m-1}\right)\left(C_{m+1}^n-C_{m-1}^n\right)\\ & +\frac{1}{h^2}\left(C_{m+1}^n-2C_m^n+C_{m-1}^n\right)K_m+S_m^n\end{aligned}$$

for $m=1,2,...,N$, which can be written in a matrix-vector form as

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

where $D=\text{diag}\left\{d/d\,t\right\}$ matrix of order $N$ and $A$, $B$ are tridiagonal matrices of order $N$ given by

$$A=\begin{bmatrix} 0 & 1 & & & & \\ -1 & 0 & 1 & & & \\ & . & . & . & & \\ & & & -1 & 0 & 1 \\ & & & & -1 & 0 \end{bmatrix}, \tag{2.3}$$

$$B=\begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & & . & . & . & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{bmatrix} \tag{2.4}$$

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

$$\begin{aligned}\mathbf{b}^n &= [b_1^n,\, b_2^n,\, ...,\, b_N^n]^T \left[\left\{\frac{1}{2\,h}\,v_1-\frac{1}{4\,h^2}\,(K_2-K_0)+\frac{1}{h^2}K_1\right\}C_0^n\right. \\ &\left. ,0,...,0,\ \left\{-\frac{1}{2\,h}\,v_N+\frac{1}{4\,h^2}\,(K_{N+1}-K_N)\ +\frac{1}{h^2}K_N\right\}C_{N+1}^n\right]^T \end{aligned} \tag{2.5}$$

the vector of the boundary conditions also of order $N$.

Using the recurrence relation

$$\mathbf{C}\,(t+\ell)=\ e^{\ell\,D}\ \mathbf{C}\,(t)\,,\ \ t=\ell,\,2\,\ell,... \tag{2.6}$$

in which the matrix-exponential term is replaced with the $(1,0)$ Padé approximant of the form

$$e^{\ell\,D}\ \approx(I-\ell\,D)^{-1}\,, \tag{2.7}$$

where $I$ the identity matrix of order $N$, finally leads to

$$(I-\ell\,D)\ \mathbf{C}\,(t+\ell)=\mathbf{C}\,(t)\,. \tag{2.8}$$

Let $r=\ell/h$ and $p=\ell/h^2$. Eq. $(2.8)$ using Eq. $(2.2)$ leads to the following linear system

$$\begin{aligned}&\left[I+\frac{r}{2}\text{diag}\,\{v_m\}\,A+\frac{r}{2}\text{diag}\,\{v_{m+1}-v_{m-1}\}\right.\\ &\left.-\frac{p}{4}\text{diag}\,\{K_{m+1}-K_{m-1}\}\,A-p\,\text{diag}\,\{K_m\}\ B\right]\mathbf{C}(t+\ell)\\ &-\ell\,\mathbf{S}^{n+1}-\ell\,\mathbf{b}^{n+1}=\mathbf{C}(t),\end{aligned} \tag{2.9}$$

which, when the notation of the grid $G$ is used, gives

$$\begin{aligned}&\left[\frac{r}{2}\,v_m-\frac{p}{4}\,(K_{m+1}-K_{m-1})-p\,K_m\right]\ C_{m+1}^{n+1}+\left[1+\frac{r}{2}\,(v_{m+1}-v_{m-1})+2\,p\,K_m\right]\ C_m^{n+1}\\ &+\left[-\frac{r}{2}\,v_m+\frac{p}{4}\,(K_{m+1}-K_{m-1})-p\,K_m\right]\ C_{m-1}^{n+1}-\ell\,S_m^{n+1}-\ell\,b_m^{n+1}=C_m^n\end{aligned} \tag{2.10}$$

for $m=1,2,...,N$.

### *C. The stability analysis*

Following the Fourier method of analyzing stability it is considered a small error of the form

$$Z_m^n=C_m^n-\tilde{C}_m^n \tag{2.11}$$

with

$$Z_m^n=e^{\alpha n\ell}e^{i\beta mh}\ \ ;\ \ i=\sqrt{-1}, \tag{2.12}$$

where $\alpha$ is complex number and $\beta$ is real. Then the von Neumann necessary criterion for stability requires the following condition to be satisfied

$$\left|e^{\alpha\,\ell}\right|\leq1+\ell\,\mathcal{S}, \tag{2.13}$$

where $\mathcal{S}$ a non negative constant independent of $\ell$ and $h$.

Let

$$\mathcal{S}=\max_{m=1,2,\ldots,N}\ S_m^n\ ;\ \ n=0,1,... \tag{2.14}$$

Then $\mathcal{S}$ obviously satisfies the required condition for the constant on the right-hand side of In. $(2.13)$. Eq. $(2.10)$ when the last two terms on the right-hand side, because of $(2.13)$, are omitted, otherwise the problem is without a source, using Eqs. $(2.11)$-$(2.12)$ after canceling both sides by $e^{\alpha n\ell}e^{i\beta mh}$ leads to

$$\Big\{\Big[\frac{r}{2}\,v_m - \frac{p}{4}\,(K_{m+1}-K_{m-1}) - p\,K_m\Big]\;e^{i\beta h}\;+1+\frac{r}{2}\,(v_{m+1}-v_{m-1})$$
$$+2\,p\,K_m + \Big[-\frac{r}{2}\,v_m\;+\frac{p}{4}\,(K_{m+1}-K_{m-1}) - p\,K_m\Big]\;e^{-i\beta h}\Big\}\,e^{\alpha\ell}=1$$

otherwise

$$\Big\{i\;\Big[r\,v_m^n - \frac{p}{2}\,(K_{m+1}-K_{m-1})\Big]\;\sin\beta h + 1\;+\frac{r}{2}\,(v_{m+1}-v_{m-1}) + 2\,p\,K_m\,(1-\cos\beta h)\Big\}\,e^{\alpha\ell}=1$$

and finally to the following *stability* equation

$$\Big\{i\;\Big[r\,v_m - \frac{p}{2}\,(K_{m+1}-K_{m-1})\Big]\;\sin\beta h + 1\;+\frac{r}{2}\,(v_{m+1}-v_{m-1}) + 4\,p\,K_m\sin^2\frac{\beta h}{2}\Big\}\;\xi=1, \tag{2.15}$$

where $\xi = e^{\alpha\ell}$ is the amplification factor.

- Eq. $(2.10)$ for the diffusion problem given by Eq. $(1.5)$ becomes

$$\xi = \left(1+4\,p\,K\sin^2\frac{\beta h}{2}\right)^{-1}. \tag{2.16}$$

  Since $p$, $K>0$, condition $(2.7)$ is always satisfied, so the method is unconditionally stable.
- Eq. $(2.10)$ for the advection-diffusion problem given by Eq. $(1.6)$ becomes

$$\xi = \left(i\,\mu\,r\,\sin\beta h + 1 + \frac{4\,p}{Re}\sin^2\frac{\beta h}{2}\right)^{-1}. \tag{2.17}$$

  so

$$\left|\xi^2\right| \;=\; \frac{Re^2}{(2\,p+Re-2\,p\cos\beta h)^2+\mu^2\,r^2\sin^2\beta h} \le \left(1+\frac{4\,p}{Re}\right)^{-2}. \tag{2.18}$$

  Then condition $(2.7)$ is always satisfied and the scheme is, again, unconditionally stable.

## III. Numerical results

In this section, numerical results are presented based on the scheme presented above. In all the test problems presented below free outflow boundary conditions are implemented.

The first test problem has an analytical solution with $S=0$. The analytical solution is that of a Gaussian pulse of unit height centered at $x_0 = 1$m in a region bounded by $0\le x\le 6$ and is given by

$$C(x,t) = \frac{1}{\sqrt{4t+1}}\;e^{-\frac{(x-x_0-ut)^2}{K(4t+1)}}, \tag{2.19}$$

where $u$ is the velocity and $K$ the (constant) diffusion coefficient in the $x$ direction. The values of the various parameters used are $D = 5\cdot 10^{-3}m^2/s$ and $u = 0.8m/s$. 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.

For the next test problem we assume an area of length $L=200m$ and we impose a constant velocity $u=1m/s$ with the diffusion coefficient $K=5\cdot 10^{-2}m^2/s$. The value of $h=0.1m$ and $l=0.2$s. A pollutant source is placed at $x=50m$ with a constant emission rate $S=u_s q_s$, where $u_s=20m/s$ the gas exit speed and $q_s=0.1\mu g/m^3$ the source concentration rate. The results are presented in Fig.2 where the advection of the pollutant can be seen at four different times.

For the same problem we assume initially that $u=0$ for the first 50s and that $K=5\cdot 10^{-1}m^2/s$. After 50s the (wind) velocity changes to $u=1m/s$ in the positive direction. In Fig. we can see the effect of diffusion for the first 50s, the concentration is increased locally and spreads in both directions. Then it is advected in the positive direction.

In the next problem we assume the existence of two sources located at $x=150m$ and $x=300m$ respectively in an area of 1000m. The second source has now $q_s=.05\mu g/s$. We use $K=0.1m^2/s$, $h=0.2m$ and $l=0.01s$ In Fig.4 we can see the evolution of concentration in the domain, by time $t=180s$ the two source have contributed to an increase in the concentration to a maximum value of $3\mu/m^3$ which gradually propagates in the rest of the domain.

For the last test case a more realistic case is presented. Assuming a domain of $L=50km$ with $u=1m/s$ and $K=10^3m^2/s$ (a typical value of the daily atmospheric boundary layer). A source is placed at $x=25km$ based on Eq. (1.3) with $H=1m$, $\sigma_n=h$ and $q(t)=2\mu/m^3$. The computational parameters used where $h=25m$ and $l=1s$. The effect of the diffusion can be clearly seen in Fig.5 as it is dominant in this case. The concentration hasn't reach its peak value even after five hours but has spread in all the half domain in the positive direction.

We point out that in all computations the value of the time step is highly increased when compared to other explicit schemes usually presented in the literature.

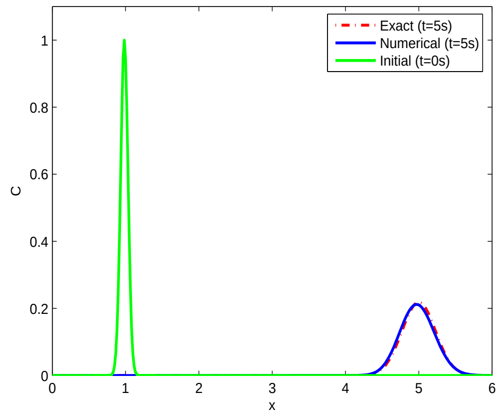


Fig. 1. Test Problem 1: Evolution of a Gaussian pulse (comparison with exact solution))

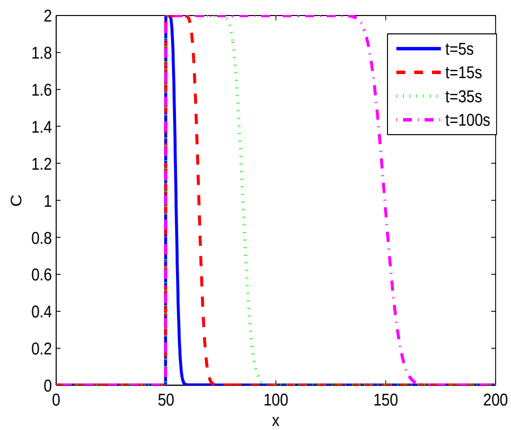


Fig. 2. Test Problem 2: Evolution of pollutant concentration from a source ($u = 1$ and $K = 5 \cdot 10^{-2}$)

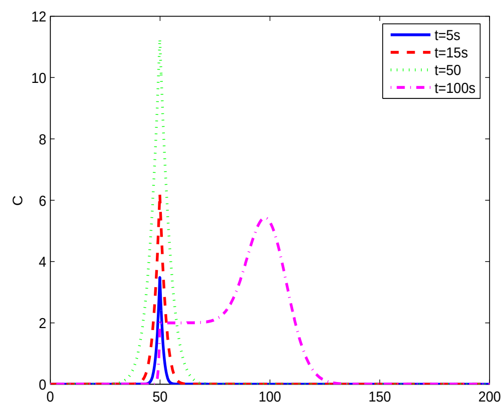


Fig. 3. Test Problem 3: Evolution of pollutant concentration from a source ($u = 0$, for the first 50s, and $K = 5 \cdot 10^{-1}$)

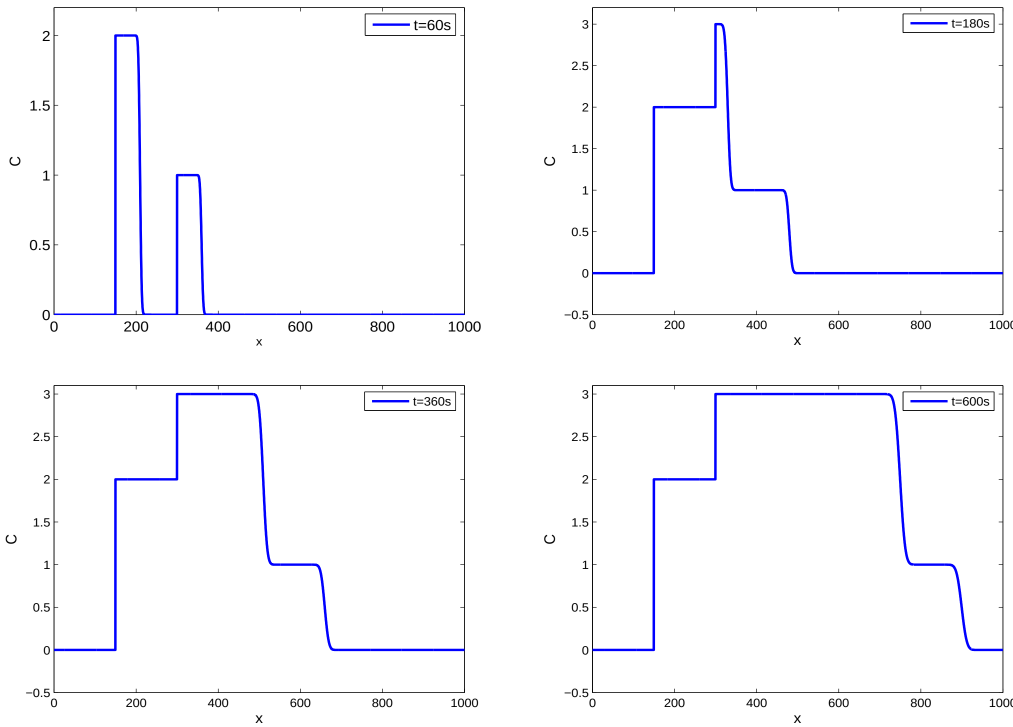


Fig. 4. Test Problem 4: Evolution of pollutant concentration from two sources

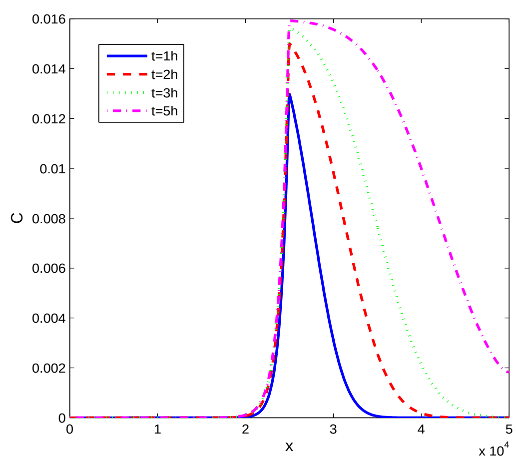


Fig. 5. Test Problem 4: Evolution of pollutant concentration from a source ($K = 10^3 m^2/s$)

## Acknowledgements

Authors Papakostas and Delis for this research were co-funded 75% by E.U. and 25% by the Greek Government under the framework of the Education and Initial Vocational Training Program - Archimedes, Technological Educational Institution (T.E.I.) Crete and authors Bratsos, Famelis and Natsis under the same Program - Archimedes, Technological Educational Institution (T.E.I.) Athens project "*Computational Methods for Applied Technological Problems*".

## References

[1] Chatwin, P.C., Allen, C.M. (1985), "Mathematical models of dispersion in rivers and estuaries", Ann. Rev. Fluid Mech., Vol. 17, pp. 119-149.
[2] Dehghan, M. (1999), "Fully implicit finite difference methods for two-dimensional diffusion with a non-local boundary condition", J. Comput. Appl. Math., Vol. 106, pp. 255-269.
[3] Dehghan, M. (2002), "Fully explicit finite difference methods for two-dimensional diffusion with an integral condition", Nonlinear Anal. Theory Methods Appl., Vol. 48, pp. 637-650.

[4] Dehghan, M. (2004), “Numerical solution of the three-dimensional advection-diffusion equation”, Appl. Math. Comput., Vol. 150, pp. 5-19.
[5] Guvanasen, V., Volker, R.E. (1983), “Numerical solutions for solute transport in unconfined aquifers”, Int. J. Numer. Methods Fluids, Vol. 3, pp. 103-123.
[6] Hindmarsh, A.C., Gresho, P.M., Griffiths, D.F. (1984), “The stability of explicit Euler time-integration for certain finite difference approximations of the advection-diffusion equation”, Int. J. Numer. Methods Fluids, Vol. 4, pp. 853-897.
[7] Holly, F.M., Usseglio-Polatera, J.M. (1984), “Dispersion simulation in two-dimensional tidal flow”, J. Hydraul. Eng., Vol. 111, pp. 905-926.
[8] Lax, P.D., Wendroff, B. (1964), “Difference schemes with high order of accuracy for solving hyperbolic equations”, Commun. Pure Appl. Math., Vol. 17, pp. 381-398.
[9] Mitchell, A.R., Griffiths, D.F. (1980), *The Finite Difference Methods in Partial Differential Equations*, T. Wiley.
[10] Pasquill, F. (1974), *Atmospheric Diffusion*, John Wiley and Sons, New York.
[11] Rivin, G., Voronina, P.V. (1997), “Aerosol transfer in the atmosphere: selection of a finite difference scheme”, Atmos. Oceanic Opt., Vol. 10, No. 6, pp. 386-392.
[12] Sokol, Z., “Comparison of several numerical schemes applied to advection equations”,Quartely of the Royal Meteorological Sosciety, Vol.123, pp.213-224.
[13] Twizell, E.H. (1984), *Computational Methods for Partial Differential Equations*, Ellis Horwood, Chichester, UK.
[14] Warming, R.F., Hyett, B.J. (1974), “The modified equation approach to the stability and accuracy analysis of finite-difference methods”, J. Comput. Phys., Vol. 14, No. 2, pp. 159-179.
[15] Zlatev, Z., Berkowicz, R., Prahm, L.P. (1984), “Implementation of a variable stepsize variable formula in the time-integration part of a code for treatment of long-range transport of air pollutants”, J. Comput. Phys., Vol. 55, pp. 278-301.