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ANALYTICAL SOLUTION OF ADVECTION-DIFFUSION EQUATION: APPLICATIONS IN ENVIRONMENTAL ENGINEERING

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Abstract. *Environmental problems caused by accidents occurring during transportation of chemicals along rivers and lakes are increasing considerably the interest in the study of the dispersion and transport of pollutant in water bodies. In these cases, the most important information obtained from the simulation are the time required for the pollutant to eventually reach the points where the water is collected for treatment and distribution, its corresponding concentration, and the time required for the disposal to leave the corresponding area. The aim of this work is to develop a method to obtain an analytical solution to the two-dimensional advection-diffusion equation which describes the dispersion of pollutant in a water body. The proposed method is based on the application of a differential operator which transforms analytical solutions of a differential equation into new analytical solutions of the same equation. The main advantage of applying this operator is the fact that each new solution has a greater number of arbitrary parameters which allow the solution to satisfy the boundary conditions of the problem in wide regions of the considered domain. We simulate contaminant dispersion in the Guaíba Lake, in the outskirts of Porto Alegre. The results obtained were compared with available data in literature.*

Keywords*. Advection- diffusion equation, pollutant dispersion, Lie symmetries, Bäcklund transformations*

1. Introduction

Environmental problems caused by accidents occurring during transportation of chemicals along rivers and lakes are increasing considerably the interest in the study of the dispersion and transport of pollutant in water bodies. In these cases, the most important information obtained from the simulation are the time required for the pollutant to eventually reach the points where the water is collected for treatment and distribution, its corresponding concentration, and the time required for the disposal to leave the corresponding area. To be effective, such information must be obtained in real time in order to permit implementation of the appropriate emergency procedures, such as to keep certain pumps turned off for some time interval or to eventually confine the disposal in a region far from the collecting points, for further treatment and removal.

The advection diffusion equation that describes mathematically the pollutant dispersion in a water body is given by

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}+kC=\frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right)+Q \qquad (1)$$

where C is the pollutant concentration, t is the time variable, K_x, K_y e K_z are the diffusion coefficients over the respective spatial variables, k is the decay constant, u, v and w are the components of the velocity vector in x, y and z directions, respectively, Q corresponds to the source term.

Several analytical, numerical and hybrid methods which solve Eq. (1) can be found in literature (Zwillinger, 1997), but the analytical solution for some problems of great interest in environmental engineering is not known yet. Alternative methods used to solve Eq. (1) can be compared. The numerical methods based on discrete formulations, such as finite difference and finite elements yield good results (Carnaham, 1972; Ortega et al, 1981; Reali et al, 1984; Greenspan et al., 1988; Bohm, 1990; Rajar et al., 1997; Periáñez, 1998; Yang et al., 1998; Carroll et al, 2000; Bonnet et al, 2001; Drago et al., 2001). Curvilinear grids can be used (Valentine, 1959; Churchill, 1975; Spiegel, 1977; Hauser et al, 1986). Systems based on finite elements have specialized generators of triangular and hexagonal grids that can be adapted to the region geometry (Dhaubadel et al., 1987).

Zabadal (1991) used a variational method (Reddy, 1984) which consisted of a combination of the Petrov-Galerkin formulation and a discretization scheme to simulate the dispersion of coliform and oxygen in Guaíba lake. This formulation produced good results and had an acceptable processing speed for practical purposes.

Using symbolic computation, the systems based on integral transforms yield hybrid numerical analytical solutions to heat and mass diffusion-convection problems. This method consists of transforming the original partial differential equation into a decoupled infinite system of ordinary differential equations (Cotta, 1993).

In 1999, Lersch et al. developed a formulation based on the application of the Fourier transform to obtain approximate solutions in closed form for the two-dimensional advection-diffusion equation. In 2000, Zabadal et al. proposed an extension of the component suppression schemes to obtain a closed form solution for water pollution problems. This method consists of fitting functions of the differential operators in the formal solution by polynomials.

In 2005, Zabadal et al. (2005[a]) proposed a method based on the application of the rules for manipulation of exponential of differential operators in order to obtain a solution for a problem of pollutant dispersion in a water body, assuming that the contaminant does not reach the margins any place of its path and that the velocity field was locally constant and previously known. In the same year, Zabadal et al. (2005[b]) developed an iterative scheme which produced a sequence of analytical solutions for the advection-diffusion equation applied to water pollution problems.

The aim of this work is to develop a method to obtain an analytical solution to the two-dimensional advection-diffusion equation which describes the dispersion of pollutant in a water body. Analytical solutions have several advantages: they are expressed in a closed form, the programs based on this kind of solutions require less processing time, since there is a reduction of the number of operations to be performed, then the amount of memory required to execute the routines decreases significantly. Besides, the source codes based on closed-form solutions are short and easy to depurate. The proposed method is based on the application of a differential operator which transforms analytical solutions of a differential equation into new analytical solutions of the same equation. The main advantage of applying this operator relies on the fact that each new solution has a greater number of arbitrary parameters which allow the solution to satisfy the boundary conditions of the problem in wide regions of the considered domain. We simulate contaminant dispersion in the Guaíba Lake, in the outskirts of Porto Alegre, Brazil. The results obtained were compared with available data in literature.

This article is outlined as follows. In section 2, the mathematical problem is described. In section 3, the two-dimensional advection-diffusion equation describing the process is first transformed into an auxiliary equation with the stream function and the velocity potential of the corresponding inviscid flow as independent variables. In section 4, the results obtained by a simulation in Guaíba Lake are shown. Finally, in section 5, conclusion and recommendations for future work are drawn.

2. Mathematical description of the problem

The problem of pollutant dispersion in a water body can be described as

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}=D\left(\frac{\partial^2 C}{\partial x^2}+\frac{\partial^2 C}{\partial y^2}\right)-kC \tag{2}$$

and the initial state of the system is given by

$$c_0(x,y)=c_c\delta(x-x_c)\delta(y-y_c) \tag{3}$$

where C denotes the pollutant concentration, t is the time variable, D is the diffusion coefficient, k is the decay constant, u e v are the velocity vector components in x and y directions, respectively, the initial condition $c_0(x,y)$ is an impulse with the same mass of the discharge, x_c and y_c are coordinates of the center of the isocurves.

The process of solving the problem described by Eq. (2) and Eq. (3) is showed in the next section.

3. Solution of the advection-diffusion equation

Applying the method of separation of variables, assuming that the velocity field is stationary and that the pollutant degradation is independent of the diffusion and of the advection through the water body,

$$C(x,y,t)=\tau(t)\cdot c(x,y)\,. \tag{4}$$

The substitution of Eq. (4) in Eq. (2) followed by the division of the resulting equation by $\tau(t)\cdot c(x,y)$ yields

$$\frac{1}{\tau}\frac{d\tau}{dt}+k=-u\frac{\partial c}{\partial x}-v\frac{\partial c}{\partial y}+D\left(\frac{\partial^2 c}{\partial x^2}+\frac{\partial^2 c}{\partial y^2}\right)=\lambda\,, \tag{5}$$

where λ corresponds to the separation constant. The system can be written as

$$\frac{1}{\tau}\frac{d\tau}{dt}+k=\lambda\,, \tag{6}$$

$$-u\frac{\partial c}{\partial x}-v\frac{\partial c}{\partial y}+D\left(\frac{\partial^2 c}{\partial x^2}+\frac{\partial^2 c}{\partial y^2}\right)=\lambda\,. \tag{7}$$

Solving Eq. (6) results

$$\tau(t)=\tau_0 e^{-(k-\lambda)t}\,. \tag{8}$$

In equation (8), as $k-\lambda$ corresponds to the value of the decay constant, and hence, λ must be equal to zero, so the system formed by Eq. (6) and Eq. (7) becomes

$$\frac{d\tau}{dt}+k\tau=0 \tag{9}$$

$$u\frac{\partial c}{\partial x}+v\frac{\partial c}{\partial y}-D\left(\frac{\partial^2 c}{\partial x^2}+\frac{\partial^2 c}{\partial y^2}\right)=0\,. \tag{10}$$

The solution of Eq. (9) is given by Eq. (8), considering $\lambda=0$. In order to obtain a solution for Eq. (10) valid for all the domain, a change of variables is performed to rewrite it in terms of new orthogonal coordinates Φ and Ψ. The main goal of the change of variables is to map the water body geometry in a rectangular domain in the new coordinate system.

3.1 Advection-diffusion equation in an orthogonal curvilinear coordinate system

Equation (10) can be expressed in terms of the new variables $\Phi(x, y)$ and $\Psi(x, y)$, which constitute an orthogonal curvilinear system of coordinates, as

$$\begin{aligned}&\left(u\Phi_x+v\Phi_y-D\Phi_{xx}-D\Phi_{yy}\right)\frac{\partial c}{\partial \Phi}+\left(u\Psi_x+v\Psi_y-D\Psi_{xx}-D\Psi_{yy}\right)\frac{\partial c}{\partial \Psi}\\&-D\left(\Phi_x^2+\Phi_y^2\right)\frac{\partial^2 c}{\partial \Phi^2}-D\left(\Psi_x^2+\Psi_y^2\right)\frac{\partial^2 c}{\partial \Psi^2}=0.\end{aligned} \tag{11}$$

Analyzing Eq. (11) and considering the possibility of using a formulation which is independent of the water body geometry, it becomes clear that this equation can be mapped into the target equation

$$\frac{\partial c}{\partial \Phi}=D\left(\frac{\partial^2 c}{\partial \Psi^2}+\frac{\partial^2 c}{\partial \Phi^2}\right), \tag{12}$$

provided that the following auxiliary equations are satisfied:

$$u\Phi_x+v\Phi_y-D\Phi_{xx}-D\Phi_{yy}=1\,, \tag{13}$$

$$u\Psi_x+v\Psi_y-D\Psi_{xx}-D\Psi_{yy}=0\,, \tag{14}$$

$$\left(\Phi_x^2+\Phi_y^2\right)=1 \tag{15}$$

and

$$\left(\Psi_x^2 + \Psi_y^2\right) = 1 . \tag{16}$$

The term of first order in Ψ does not appear in Eq. (11) because the advective transport occurs only along the streamlines. In order to solve Eq. (12) a new formulation to obtain the Lie symmetries admitted by differential equations is employed. This formulation is shown in the next subsection.

3.2 The use of mapping to obtain Lie symmetries

Considering $-\infty < \Phi < +\infty$, $0 < \Psi < +\infty$, the problem described by Eq. (12) and subjected to the boundary condition

$$\left.\frac{\partial c}{\partial \Psi}\right|_{\Psi=0} = 0 \tag{17}$$

and to the restriction

$$c(\Phi_0, \Psi) = c_0(\Psi) \tag{18}$$

can be solved by the application of the differential operator defined by

$$B = p_1(\Phi,\Psi)\frac{\partial}{\partial \Phi} + p_2(\Phi,\Psi)\frac{\partial}{\partial y} + p_3(\Phi,\Psi)I , \tag{19}$$

where I is the identity operator and $p_1(\Phi,\Psi)$, $p_2(\Phi,\Psi)$ and $p_3(\Phi,\Psi)$ are coefficients to be determined. This operator B transforms analytical solutions of a partial differential equation into new analytical solutions of the same equation. Each new solution has a greater number of arbitrary elements which allow this new solution to satisfy a wider set of boundary conditions.

If f_1 is an analytical solution of Eq. (12) whose differential operator can be defined as

$$A = \frac{\partial}{\partial \Phi} - D\left(\frac{\partial^2}{\partial \Phi^2} + \frac{\partial^2}{\partial \Psi^2}\right), \tag{20}$$

then the application of A over f_1 results zero

$$Af_1 = 0 . \tag{21}$$

As B generates new analytical solutions of a partial differential equation

$$Bf_1 = g \tag{22}$$

where g is a new solution of Eq. (12) and consequently

$$Ag = 0 , \tag{23}$$

so it can be written that

$$ABf_1 = 0 . \tag{24}$$

Solving the system formed by Eq. (21) and Eq. (24) the coefficients $p_1(\Phi,\Psi)$, $p_2(\Phi,\Psi)$ and $p_3(\Phi,\Psi)$, which appear in Eq. (19), are determined and this equation can be rewritten as

$$Bc = (\eta_4 - 2\eta_1 \cdot \Psi)\frac{\partial c(\Phi,\Psi)}{\partial \Phi} + (\eta_3 + 2\eta_1 \cdot \Phi)\frac{\partial c(\Phi,\Psi)}{\partial \Psi} + (\eta_2 + \eta_1 \cdot \Psi)c(\Phi,\Psi), \tag{25}$$

where η_1, η_2, η_3 and η_4 are arbitrary constants.

In order to reach the most general solution that can be obtained by the application of this method, we solve

$$Bc = c\ , \tag{26}$$

which produces the invariant solution that can be found when employing operator B.

The solution for Eq. (26) is given by

$$c(\Phi,\Psi) = F1\left(-\eta_2\Phi^2 - \eta_3\cdot\Phi + \eta_4\cdot\Psi - \eta_2\cdot\Psi^2\right)\cdot\exp\left(\frac{2\Phi\sqrt{\eta_2^{\,2}} + (2\eta_1+\eta_4)\arctan\left(\frac{(2\eta_2\Phi+\eta_3)\sqrt{\eta_2^{\,2}}}{\eta_2\sqrt{(-\eta_4+2\eta_2\cdot\Psi)^2}}\right)}{4\sqrt{\eta_2^{\,2}}}\right) \tag{27}$$

where $F1$ denotes an arbitrary function.

The application of the boundary condition represented by Eq. (17) over Eq. (27) produces

$$\begin{aligned} c(\Phi,\Psi) = {} & F1\left(-\eta_2\Phi^2 - \eta_3\cdot\Phi + \eta_4\cdot\Psi - \eta_2\cdot\Psi^2\right)\cdot\exp\left(\frac{2\Phi\sqrt{\eta_2^{\,2}} + (2\eta_1+\eta_4)\arctan\left(\frac{(2\eta_2\Phi+\eta_3)\sqrt{\eta_2^{\,2}}}{\eta_2\sqrt{(-\eta_4+2\eta_2\cdot\Psi)^2}}\right)}{4\sqrt{\eta_2^{\,2}}}\right) \\ & + F1\left(-\eta_2\Phi^2 - \eta_3\cdot\Phi - \eta_4\cdot\Psi - \eta_2\cdot\Psi^2\right)\cdot\exp\left(\frac{2\Phi\sqrt{\eta_2^{\,2}} + (2\eta_1+\eta_4)\arctan\left(\frac{(2\eta_2\Phi+\eta_3)\sqrt{\eta_2^{\,2}}}{\eta_2\sqrt{(-\eta_4-2\eta_2\cdot\Psi)^2}}\right)}{4\sqrt{\eta_2^{\,2}}}\right), \end{aligned} \tag{28}$$

using the concept of reflection at a boundary (Crank, 1975). The restriction given by Eq. (18) determines the arbitrary function F1. In order to write Eq. (28) in the original coordinate system, a suitable combination of stream functions can be used to represent the flow around a given margin and the corresponding velocity potential. For example,

$$\Psi(x,y) = U\cdot y + f(x,y) \tag{29}$$

represents the composition of the stream function for the uniform flow and the stream function for an arbitrary margin. Applying the Cauchy-Riemann equations (Churchill, 1975)

$$\frac{\partial\Phi(x,y)}{\partial x} = \frac{\partial\Psi(x,y)}{\partial y} \tag{30}$$

and

$$\frac{\partial\Phi(x,y)}{\partial y} = -\frac{\partial\Psi(x,y)}{\partial x} \tag{31}$$

it is possible to find an expression for the potential velocity

$$\Phi(x,y) = U\cdot x - \int\frac{\partial f(x,y)}{\partial x}dy + C\ . \tag{32}$$

The substitution of Eq. (29) and Eq. (32) in Eq. (28) yields the solution of Eq. (10) in terms of the original variables and the pollutant concentration described by Eq. (4) in any point of the domain is given by

$$C(x,y) = e^{-kt} c(\Phi(x,y), \Psi(x,y)). \tag{33}$$

4. Results and discussion

In order to illustrate the efficiency of the proposed method, a simulation of a problem of an accident occurred during the transportation of benzene in Guaíba Lake is performed. Figure 1 shows a sketch of this lake which has 70Km of bank extension, its area is 496Km^2 and its length is about 50Km.

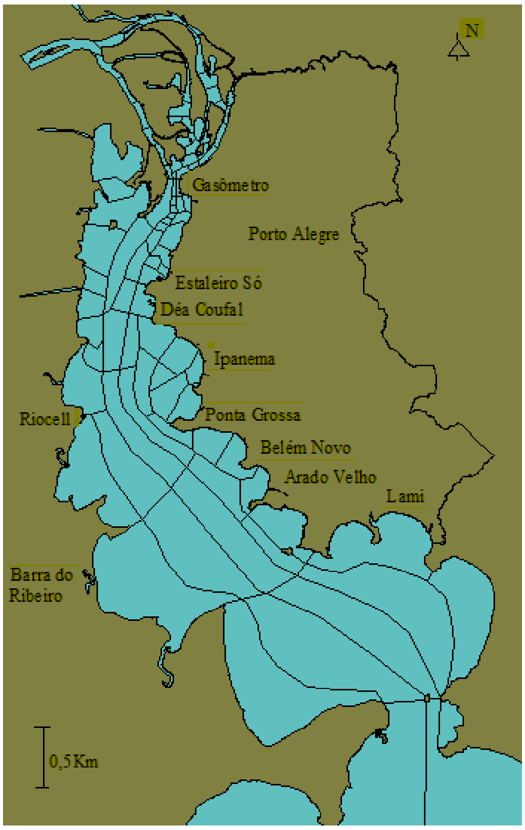

Figure 1: Sketch of Guaíba Lake

In this simulation the expression used to represent the stream function is

$$\Psi(x,y) = U_\infty \cdot y + 800 \cdot \arctan[0{,}01 \cdot (y - f(x))] \tag{34}$$

where U_∞ is the free stream velocity and $f(x)$ corresponds to the function that describes the margin of the considered domain. The velocity potential Φ is calculated by the application of the Cauchy-Riemann equations. The substitution of Φ and Ψ in Eq. (33) gives the solution in Cartesian coordinates. It is considered a discharge of 1.000m^3 of benzene in a region close to Déa Coufal Street. The data used are $U_\infty = 0{,}07$ m/s and $D = 5 \cdot 10^{-4}$ m^2/s, the initial shape of the discharge in orthogonal coordinates is approximated by

$$c(\Phi_0, \Psi) = 2{,}5 \cdot \left(0{,}058\Phi_0{}^2 - 0{,}0047 \cdot \Phi_0 + 0{,}15 \cdot \Psi + 0{,}058 \cdot \Psi^2\right) \cdot \exp(-0{,}5 \cdot \Phi_0) \cdot \\ \exp\left(-1{,}37 \cdot \arctan\left(\frac{(-0{,}116\Phi_0 + 0{,}0047)}{\sqrt{(-0{,}15 - 0{,}116 \cdot \Psi)^2}}\right)\right), \tag{35}$$

and it specifies function $F1$ in Eq. (28).

Figure 2 shows the accident location and the blob's path. It's possible to observe the regions reached by the blob along this path.

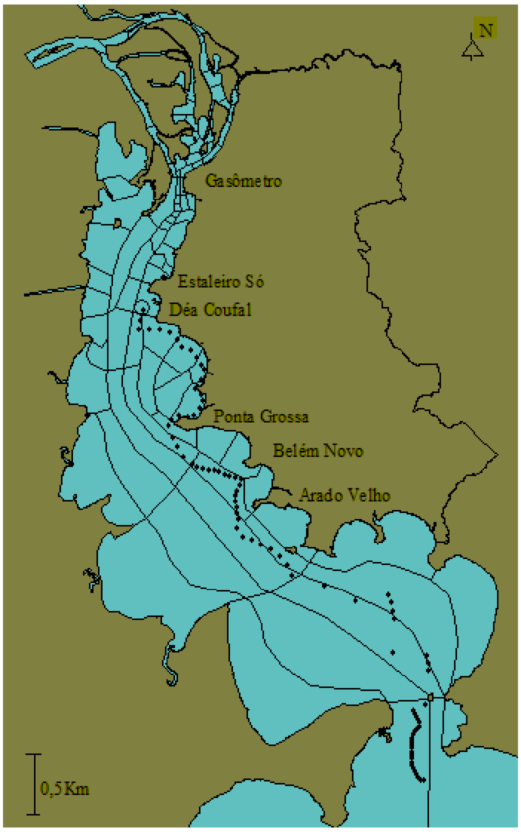

Figure 2: Accident Location close to Déa Coufal Street and blob's path

Figure 3 shows the blob's extension close to the inlet called Ponta do Arado Velho obtained by the proposed method. It took 20 hours for the blob to get to this place.

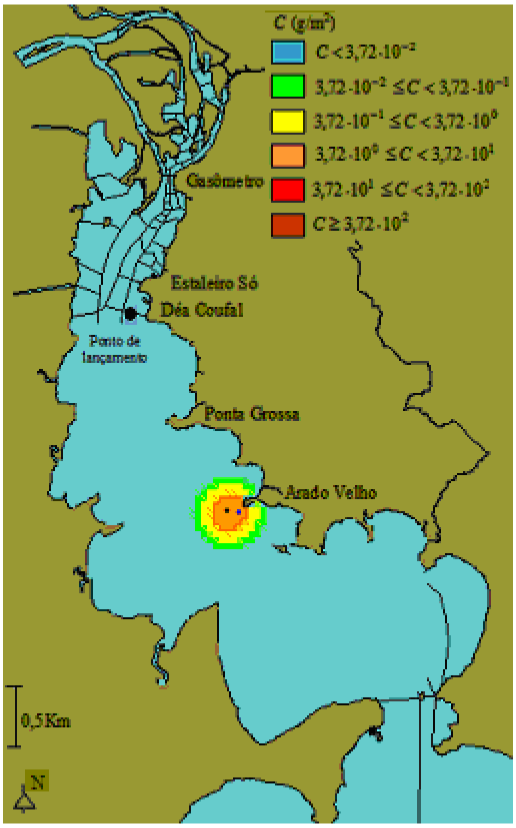

Figure 3: Blob's extension close to Ponta do Arado Velho obtained by the proposed method

Figure 4 shows the blob's extension reported by Zabadal (2000). In both methods the the blob's extension and the time required to reach Ponta do Arado Velho are the same.

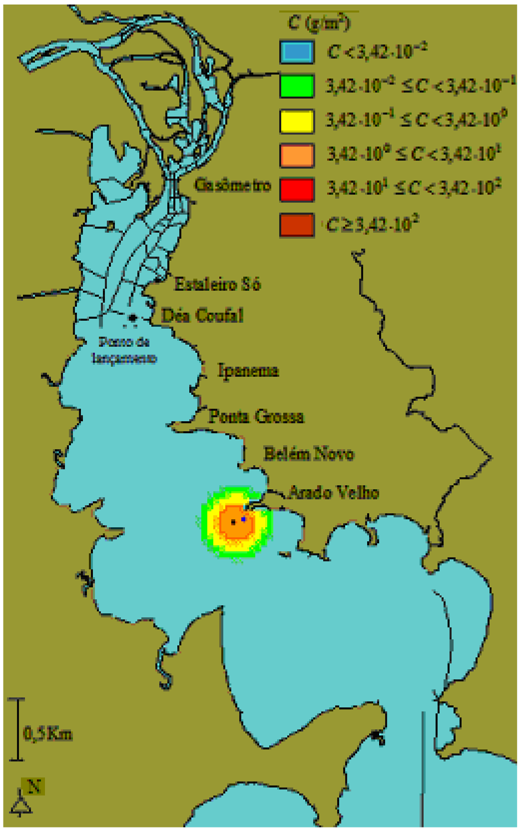

Figure 4: Blob's extension close to Ponta do Arado Velho obtained by Zabadal (2000)

It is important to emphasize that considering the environmental damage caused by the blob, this simulation corresponds to be worst case, because the concentration values are over estimated for pollutant of low solubility, as the collecting points are located 1,2m under the water body surface.

The results were obtained in 10 seconds in microcomputer Semprom 2.4GHZ with 512MB RAM. In the same computer, considering the same scenario the results reported by Zabadal (2000) were generated in 90 seconds.

5. Conclusion

The main advantage of the proposed method relies on the computational features of the corresponding code. The low processing time required to obtain the solutions with Maple V and the small amount of memory needed in most calculations, allow the simulations to be carried out in microcomputers. Obtaining the solution in real time allows advising authorities the regions which will be reached by the blob, in such a way that, emergency procedures, such as turning off certain pumps and confining the disposal in a region far from the collecting points for further treatment or removal, can be performed. The solutions can be implemented in a code written in procedural language, avoiding the use of numerical methods for simulating realistic pollutant dispersion scenarios. The results coincide with data available in literature. The research is currently focused in the formulation of analytical procedures for dealing with the bacteria dispersion in water bodies.

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