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Closed form solutions for water pollution problems – II

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Abstract

In the last decades, the interest in studying pollutant dispersion in water bodies has increased as a consequence of the environmental problems caused by the industrial and technological development. This work proposes a new analytical method for solving the two-dimensional advection-diffusion equation describing the dispersion of bacteria and chemicals in lakes and rivers. The method is based on an iterative scheme that provides a sequence of exact solutions with an increasing number of arbitrary functions and parameters, thereby avoiding the a priori knowledge of any of the Lie symmetries admitted by the equation. The arbitrary components are ultimately specified by the application of appropriate boundary conditions to the problem. A simulation was made of the pollutant propagation problem in the Guaíba Lake in the outskirts of Porto Alegre, Brazil, for Departamento Municipal de Águas e Esgotos (DMAE), the county's water treatment and sewage disposal authority, and the results were compared with available experimental data. The main advantages of the method rely on the low processing time and on the analytical character of the solutions obtained.

Keywords: pollutant dispersion, advection-diffusion equation, Lie symmetries, auto-Bäcklund transformations

1 Introduction

The increase of the number of people living in areas close to rivers and lakes and the industrial and technological development cause environmental problems, such as water and air pollution. As a consequence, there is a great interest in studying the pollutant dispersion in water and in the atmosphere. Presenting a closed form solution to the two-dimensional advection-diffusion equation that describes the pollutant dispersion in a water body is the motivation of this paper.

The solution of the advection-diffusion equation in two and three-dimensional domains with arbitrary geometry is usually an expensive task from the computational point of view. Numerical

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Notation

D	Pollutant diffusion coefficient in the medium
k	Pollutant decay constant
Q	Source term
t	Time variable
u	Component of the velocity vector in x direction
v	Component of the velocity vector in y direction
V	Magnitude of the velocity vector
Ψ	Stream function
Φ	Potencial velocity

methods employed to carry out the simulation of fluid flows often require long processing times, even when working with relatively coarse grids [2,4,8,9,11,13,16,20–22,25] . Moreover, for most practical problems, the irregular shape of the boundaries imposes a lower bound for the mesh density at the margins. The finite element represents well complex geometries because it allows variations in the size of the elements of the mesh and the boundary conditions can be easily implemented [23].

In the last thirty years, a number of hybrid formulations using conformal mappings were proposed in order to reduce the processing time of finite-differences based schemes [3, 7, 18, 24, 27]. These methods generate curvilinear adaptive grids for two-dimensional problems and have been successfully applied for simulating viscous fluid flows in heat exchangers and turbomachineries. These formulations are, however, restricted to particular geometries for which there exist conformal transformations eventually available in specialized tables [5, 14]. In 1999, a formulation based on the application of the Fourier transform was used in order to obtain closed form approximate solutions to the two-dimensional advection-diffusion equation [15]. In 2004, Zabadal et al. simulated bidimensional viscous flows around bodies of arbitrary geometry. They solved Helmholtz equation using rules for manipulation of differential operators in order to obtain a closed form solution to the vorticity [29]. Also in 2004, Zabadal et al proposed a hybrid method for solving steady bidimensional diffusive problems in water pollution in water bodies of arbitrary geometry [26]. In 2005, Zabadal et al. [28] 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.

There are practical situations, e.g. those involving real time simulation of emergency scenarios, for which the processing speed is a crucial feature. Examples are accidents occurring during transportation of chemicals along rivers and lakes. In these cases, the most important information obtained from simulation are the time required for the pollutant to eventually reach the points where 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 need for a high speed processing system capable of simulating real time emergency scenarios has, thus, motivated the present development.

In this work a new analytical method for solving steady and unsteady water pollution problems is presented. The method consists in an iterative scheme based on symbolical computation which provides exact solutions for the two-dimensional advection-diffusion equation. Pollutant concentrations are obtained in terms of the stream function (Ψ) and velocity potential (Φ), taken as the independent variables in these (assumed) inviscid flows. The use of such variables allows the solution to be obtained as for a rectangular region problem, independent from the geometry of the considered domain. The method is useful in simulations involving pollutant releases in real time (i.e. within seconds) in microcomputers. It has been employed to simulate dispersion scenarios in regions whose complex geometry usually requires large amounts of memory and very high processing times to obtain numerical and closed form expressions for the pollutant concentration distributions.

This article is outlined as follows. In section 2, the essential elements of Lie group theory needed for the solution of this class of problems is introduced, which allows converting an exact solution of a given differential equation into another containing more arbitrary elements - parameters and functions - employed to match the desired boundary conditions. The concept is next applied to the dispersion problem of interest. 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 considered water element as independent variables. Exact solutions of the resulting auxiliary equation can then be obtained according to the number of symmetries of a continuous transformation group under which the equation is invariant. The set of these so-called Lie symmetries can be determined by means of the infinitesimal invariance criteria [17], but the number of floating point operations needed to perform such calculation is usually high, what may restrict its application. An alternative iterative scheme which does not imposes the a priori knowledge of any of the Lie symmetries is thus proposed where, at each iteration, a new exact solution is obtained. This iterative scheme is employed, in section 3, to simulate a real environmental scenario, and the results are compared with available experimental data. Finally, in section 4, conclusions and recommendations for future work are drawn.

2 Theoretical foundations

The Lie symmetries of a given differential equation consist in changes of variables that leave the equation invariant [6, 10, 12]. For instance, the heat equation for unitary thermal diffusivity,

given by

$$\frac{\partial f}{\partial t} = \frac{\partial^2 f}{\partial x^2}, \tag{1}$$

admits symmetry of the type $[X + 2ct, T, F\exp(-cx + c^2 t)]$. In other words, the transformation

$$x \rightarrow X + 2ct\ , \quad t \rightarrow T\ , \quad f \rightarrow Fe^{-cx+c^2 t}, \tag{2}$$

with c an arbitrary parameter and the upper case letters denoting the new transformed variables, does not change Eq. (1). This can be readily verified by direct substitution in the equation with the aid of the chain rule.

The most important feature of the Lie symmetries arises as a direct consequence of the above property. Since the change of variables $[x \rightarrow \alpha\ , t \rightarrow \beta\ , f \rightarrow \phi]$ does not alter the differential equation, any known solution $f(x,t)$ can be converted into a new solution $\phi(\alpha, \beta)$ which may contain more arbitrary elements (parameters and functions), and thus satisfy more comprehensive boundary conditions eventually applied to the problem. In order to clarify this argument, the function

$$f = c_0 + c_1 x + c_2 t + \frac{c_2}{2}x^2, \tag{3}$$

obtained directly by inspection, is an exact solution of Eq. (1), although its application for physical problems is considerably restricted. This function can, however, be employed to generate another exact solution by means of the above-mentioned change of variables. Thus, substituting x by $X + 2ct$, t by T and f by $F\exp(-cX - c^2 T)$ in Eq. (3), yields

$$F = [c_0 + c_1(X + 2cT) + c_2 T + \frac{c_2}{2}(X + 2cT)^2]\left[e^{cX+c^2 T}\right], \tag{4}$$

which satisfies $\partial F/\partial T = \partial^2 F/\partial X^2$ and a wider set of initial/boundary conditions than the former solution. Successive applications of other known symmetries over Eq. (4) produce other exact solutions to the problem. Eventually, a general solution is obtained which is invariant with respect to all Lie symmetries admitted by the differential equation. The set of Lie symmetries can be determined by means of the infinitesimal invariance criteria [17] in a process which is usually time consuming, especially if the number of symmetries is large. Fortunately, for most practical purposes, the general solution needs not to be obtained. It is often sufficient to find a particular solution that admits a certain number of symmetries and matches, at least locally, the specific conditions prescribed to reproduce a given physical scenario.

From what has been said, the use of Lie symmetries based mappings depend on the knowledge of, a priori, at least a particular solution of the differential equation and some suitable changes of variables which keep the equation unchanged. Sometimes it is first necessary to transform the original equation into another whose particular solutions and symmetries are known. These transformations may, however, lead to auxiliary equations that are more difficult to solve than the original one.

In this work, the advection-diffusion equation for the pollutant concentration f in a medium,

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} + v\frac{\partial f}{\partial y} - D\left(\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}\right) + kf = 0, \tag{5}$$

where u and v are the components of the velocity vector (assumed constant), D is the pollutant diffusion coefficient in the medium and k its decay constant, is first decomposed in two uncoupled partial differential equations, assuming separation of variables, as

$$\frac{\partial f}{\partial t} + kf = 0 \tag{6}$$

$$u\frac{\partial f}{\partial x} + v\frac{\partial f}{\partial y} - D(\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}) = 0, \tag{7}$$

where the separation constant was taken as zero in order to obtain Eq. (6), the well known pollutant kinetics decay equation. This system presents several applications in water pollution problems, such as planning sewer lines and evaluating environmental damages due to industrial disposals. Loadings in the former application are usually represented by source terms in the right hand side of Eq. (7), in generating steady solutions for those problems. In this work the steady solution is obtained by solving an auxiliary transient problem in which the loading is assumed to be the initial condition. In order to construct the steady-state concentration profile, a time convolution is performed over the transient solution. The time variable, in this case, is expressed as a Lagrangian coordinate defined in terms of the components of the velocity vector, as

$$t = {}^1\!/_2 \int \left[{}^{dx}\!/_u + {}^{dy}\!/_v \right]. \tag{8}$$

While the solution of Eq. (6) is known, Eq. (7) is next expressed in terms of new variables $a(x, y)$ and $b(x, y)$, employing the chain rule, as

$$\begin{aligned}&[ua_x + va_y - D(a_{xx} + a_{yy})]\tfrac{\partial f}{\partial a} - D(a_x^2 + a_y^2)\tfrac{\partial^2 f}{\partial a^2} + [ub_x + vb_y - D(b_{xx} + b_{yy})]\tfrac{\partial f}{\partial b} - \\ &D(b_x^2 + b_y^2)\tfrac{\partial^2 f}{\partial b^2} - 2D(a_x b_x + a_y b_y)\tfrac{\partial^2 f}{\partial a \partial b} = 0.\end{aligned} \tag{9}$$

This expression can be simplified if we assume that the new variables constitute an orthogonal curvilinear system of coordinates, $\nabla a \cdot \nabla b = 0$:

$$[ua_x + va_y - D(a_{xx} + a_{yy})]\frac{\partial f}{\partial a} - D(a_x^2 + a_y^2)\frac{\partial^2 f}{\partial a^2} + [ub_x + vb_y - D(b_{xx} + b_{yy})]\frac{\partial f}{\partial b} - D(b_x^2 + b_y^2)\frac{\partial^2 f}{\partial b^2} = 0. \tag{10}$$

The next step consists in choosing particular functions a and b which simplify the solution of the resulting equation. A suitable choice of these new coordinates, for most practical purposes in environmental engineering, consists in taking $a = \Psi$ (the stream function) and $b = \Phi$ (the velocity potential) for inviscid flows. Eq. (10) is now written as

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

Taking into account that, for potential flows,

$$\begin{aligned} u\Psi_x + v\Psi_y &= 0 \\ \Psi_x^2 + \Psi_y^2 &= V^2 \\ u\Phi_x + v\Phi_y &= V^2 \\ \Phi_{xx} + \Phi_{yy} &= 0 \\ \Phi_x^2 + \Phi_y^2 &= V^2, \end{aligned} \tag{12}$$

where V is the magnitude of the velocity vector, Eq. (11) reduces to

$$-D(\Psi_{xx} + \Psi_{yy})]\frac{\partial f}{\partial \Psi} - DV^2\frac{\partial^2 f}{\partial \Psi^2} + V^2\frac{\partial f}{\partial \Phi} - DV^2\frac{\partial^2 f}{\partial \Phi^2} = 0. \tag{13}$$

This expression can be further simplified by recalling that the Laplacian of the stream function vanishes for potential flows. Thus

$$\frac{\partial^2 f}{\partial \Psi^2} + \frac{\partial^2 f}{\partial \Phi^2} = \frac{1}{D}\frac{\partial f}{\partial \Phi}. \tag{14}$$

This equation states that while the diffusion is isotropic, the advective transport occurs only along the streamlines, i.e., there is no flow in the direction normal to the main stream. It can be readily verified that the viscous effects due to the boundary layer are still present in this equation. Indeed, when $f = \omega$ (vorticity) and $D = \nu$ (kinematics viscosity), these effects arise due to the second derivative with respect to the stream function, whose corresponding physical mechanism consists in propagating the vorticity by diffusion along the direction transverse to the main flow. This mechanism is responsible for the development of the boundary layer at a given interface.

2.1 The auto-Bäcklund transformation

In order to obtain an analytical solution to Eq. (14), this work proposes a method based on a sequence of non-homogenous splits for which the source terms appearing in the corresponding systems of differential equations can be obtained from any particular solution of the original equation. An iterative scheme is obtained, in such a way that each iteration produces a new exact solution that satisfies a wider set of boundary conditions.

Consider the equation

$$Lf = 0, \tag{15}$$

where L is a linear differential operator, which can be written as

$$L = A - B, \tag{16}$$

where the inverse of A is known. Then, Eq. (15) can be rewritten as

$$Af = Bf, \tag{17}$$

or, as non-homogeneous system of differential equations

$$Af = Q \tag{18}$$

and

$$Bf = Q \tag{19}$$

where the source term must be determined. Applying operator B over Eq. (18), it yields

$$BAf = BQ, \tag{20}$$

and applying operator A over Eq. (19), it produces

$$ABf = AQ. \tag{21}$$

Assuming that the operators are linear, the subtraction of Eq. (20) from Eq. (21) yields

$$[A, B]\, f = AQ - BQ, \tag{22}$$

when $[A, B] = 0$, the source term Q and f obey the same differential equation. The former result allows carrying out an iterative scheme which can be described as

$$Af_{k+1} = f_k \tag{23}$$

and

$$Bf_{k+1} = f_k. \tag{24}$$

This system can be solved directly. Starting with any particular function f_0 of the original equation, Eq. (23) can be solved and the result is

$$f_{k+1} = A^{-1} f_k + h_A, \tag{25}$$

where h_A corresponds to any function belonging to the null space of A. The substitution of Eq. (25) into Eq. (24) results

$$f_{k+1} = BA^{-1} f_k + Bh_A. \tag{26}$$

Equation (26) is often solved for the arbitrary elements contained in h_A. In some situations, this equation must be split, producing another system of non-homogeneous differential equations, whose solution is obtained by applying the same procedure again.

The new solution obtained is then replaced on the right side of Eq. (23) and Eq. (24) and the process is repeated. It is important to emphasize that each iteration produces an exact solution. The process is stopped when the solution obtained has enough arbitrary elements to satisfy the initial and boundary conditions imposed in a given domain. It means that the number and nature of the arbitrary elements (constants or functions) in the solution will determine the extension of the subdomain in which the solution remains valid. The number of iterations define if the solution will be used in the whole domain or in a sub region of it. In the case when A and B do not commute, the proposed method is modified, by defining the g-commutator,

$$[A,B]_g = AgB - BgA, \tag{27}$$

where g is an unknown function. As in the former case, it is easy to show that when g-commutator is null an analogous iterative scheme can be performed:

$$Af_{k+1} = \frac{f_k}{g} \tag{28}$$

and

$$Bf_{k+1} = \frac{f_k}{g}. \tag{29}$$

Multiplying Eq. (28) and Eq. (29) by g, it yields

$$gAf_{k+1} = f_k \tag{30}$$

and

$$gBf_{k+1} = f_k. \tag{31}$$

Applying operator B over Eq. (30) and A over Eq. (31), it results

$$BgAf_{k+1} = Bf_k \tag{32}$$

and

$$AgBf_{k+1} = Af_k. \tag{33}$$

Finally, the subtraction of Eq. (33) from Eq. (32) produces

$$[A,B]_g f_{k+1} = Af_k - Bf_k. \tag{34}$$

In order to guarantee the "g-commutativity" between A and B, the function g must satisfy some auxiliary differential equations which are often simpler than the original one to be solved. For most practical purposes, it is possible to map the original equation in a way that $[A, B] = 0$, and even when the operators do not commute there are infinite solutions for the auxiliary equations which comes from the condition $[A, B]_g = 0$.

2.2 Obtaining a set of particular solutions

Equation (14) is solved by the described formulation considering that $[A, B] = 0$. Despite the existence of hybrid methods for solving this equation (for instance, integral transforms), a set of exact solutions can be readily obtained if we express it in terms of a non-homogeneous system in the form

$$\begin{cases} \frac{1}{D}\frac{\partial f}{\partial \Phi} = Q(\Psi, \Phi) \\ \frac{\partial^2 f}{\partial \Psi^2} + \frac{\partial^2 f}{\partial \Phi^2} = Q(\Psi, \Phi) \end{cases}, \tag{35}$$

where Q plays the role of a source function which must be specified. Each source function admitted by the system produces a particular solution for Eq. (14). It will be shown that an iterative analytical scheme can be applied in order to obtain a set of exact solutions to this problem, without knowing any of its Lie symmetries.

In order to produce a sequence of particular solutions for $Af - Bf = 0$, or for the system

$$\begin{cases} Af = Q \\ Bf = Q \end{cases}, \tag{36}$$

two conditions are assumed:

a) the operators A and B commute, i.e., $[A, B] = 0$; and

b) equations $Af = Q$ and $Bf = Q$ can be solved analytically.

The commutative requirement implies that the source term Q obeys the same differential equation satisfied by function f. Indeed, applying operator B over $Af = Q$ and operator A over $Bf = Q$, yields

$$\begin{cases} BAf = BQ \\ ABf = AQ \end{cases}. \tag{37}$$

Subtracting the resulting equations, the following condition is obtained

$$AQ - BQ = ABf - BAf = [A, B]f, \tag{38}$$

which means the source term must also satisfy the original differential equation if $[A, B] = 0$. In this case, it is possible to construct a sequence of exact solutions employing the iterative scheme

$$\begin{cases} Af_{k+1} = f_k \\ Bf_{k+1} = f_k \end{cases}, \tag{39}$$

starting from any available particular solution. In this work, a sequence was obtained using the trivial solution as starting point. Thus, initially,

$$\begin{cases} \frac{1}{D}\frac{\partial f}{\partial \Phi} = 0 \\ \frac{\partial^2 f}{\partial \Psi^2} + \frac{\partial^2 f}{\partial \Phi^2} = 0. \end{cases} . \tag{40}$$

This system is solved in three steps:

i) direct integration of the first equation that yields

$$f = g\left(\Psi\right); \tag{41}$$

ii) replacement of the solution obtained into the second equation:

$$\frac{\partial^2 \left[g\left(\Psi\right)\right]}{\partial \Psi^2} + \frac{\partial^2 \left[g\left(\Psi\right)\right]}{\partial \Phi^2} = 0; \tag{42}$$

iii) solution of the second equation.

Equation (22) can be rewritten as

$$\frac{d^2 \left[g\left(\Psi\right)\right]}{d\Psi^2} = 0; \tag{43}$$

whose solution is

$$g\left(\Psi\right) = c_1\Psi + c_2. \tag{44}$$

Therefore after the first iteration, an exact solution arises:

$$f_1 = c_1\Psi + c_2. \tag{45}$$

The second iteration consists of replacing the source term by the new solution given by Eq. (45):

$$\begin{cases} \frac{1}{D}\frac{\partial f}{\partial \Phi} = c_1\Psi + c_2 \\ \frac{\partial^2 f}{\partial \Psi^2} + \frac{\partial^2 f}{\partial \Phi^2} = c_1\Psi + c_2. \end{cases} \tag{46}$$

Solving the system defined by Eq. (46), we get a new exact solution for the problem. Integrating the first equation, we obtain

$$f = c_1 D\Phi\Psi + c_2 D\Psi + g(\Psi). \tag{47}$$

The replacement of the Eq. (47) into the second equation defined by (46) gives

$$\frac{d^2g}{d\Psi^2} = c_1\Psi + c_2, \tag{48}$$

whose solution is

$$g(\Psi) = c_1\frac{\Psi^3}{6} + c_2\frac{\Psi^2}{2} + c_3\Psi + c_4. \tag{49}$$

The substitution of Eq. (49) into Eq. (47) yields the solution for the second iteration:

$$f_2 = c_1\left(D\Psi\Phi + \frac{\Psi^3}{6}\right) + c_2\left(D\Phi + \frac{\Psi^2}{2}\right) + c_3\Psi + c_4. \tag{50}$$

Each new solution obtained is replaced in the source term, and the process is repeated. The iterative scheme stops when the particular solution contains a number of arbitrary parameters that satisfy, at least locally, the prescribed boundary conditions.

It is important to emphasize that when we define the proposed method as iterative, we do not mean that each iteration produces an approximation for the exact solution, as the classical definition of an iterative process. Instead, it means that each iteration yields a new exact solution for the problem. These iterations are performed in order to add arbitrary constants to the solution. These arbitrary parameters will satisfy the boundary conditions of the problem in wider regions of the considered domain. In some cases, the iterative process can even dispense the domain discretization.

3 Results and discussion

The solutions obtained were employed to simulate the propagation of conservative and non-conservative pollutants in water bodies. The boundary condition imposed at the soil-water interface is given by

$$\frac{\partial f}{\partial \Psi} + \alpha f = 0, \tag{51}$$

which takes into account the pollutant retention at the margins. In this equation, the parameter α is obtained by estimating the normal derivative at some points chosen along the margins. The normal derivative is approximated by a central finite difference based on two concentration measurements, taken at the margin and into the mainstream, and separated by distances of about 3m.

Table 1 presents values of k, D and α used in the simulation of Scherichia Coli dispersion resulting from loads occurring at different locations along the Guaíba Lake, in the outskirts of Porto Alegre city, Brazil. Figure 1 shows a sketch of this lake.

Table 1: Basic parameters – Pollutant propagation simulation (source: [1])

Parameter	Nomenclature	Value
Decay constant (s^{-1})	k	$3.0\ 10^{-5}$
Diffusion coefficient (m^2/s)	D	$2.0\ 10^{-4}$
Numerical parameter (m^2/s)	α	$3.0\ 10^{-4}$

Figure 1: Sketch of Guaíba Lake

Table 2 presents load concentrations (assumed continuous) at selected points inside the lake.

Table 2: Scherichia Coli load concentration at selected positions (source: [1])

$x(m)$	$y(m)$	$C(org/100\ ml)$
170924	671270	$1.45\ 10^{2}$
170924	665831	$4.99\ 10^{4}$
172533	669202	$1.10\ 10^{5}$
174678	658859	$3.22\ 10^{3}$
177589	655105	$1.12\ 10^{3}$
177819	658093	$9.49\ 10^{2}$

Table 3 shows typical values of the local velocity field at selected points inside the lake.

Table 3: Local water velocity field at selected positions (source: [1])

$x(m)$	$y(m)$	$u(m/s)$	$v(m/s)$
191615	638811	-6.47 10^{-3}	-3.24 10^{-2}
187322	642263	3.19 10^{-1}	-8.71 10^{-2}
185640	647353	2.82 10^{-1}	-1.73 10^{-1}
184755	648239	2.84 10^{-1}	-1.69 10^{-1}
174353	649965	8.06 10^{-2}	-5.75 10^{-2}
175946	653240	8.51 10^{-1}	-1.01 10^{-2}
180196	657622	-1.33 10^{-2}	-5.34 10^{-2}
175539	662876	-4.43 10^{-2}	-7.60 10^{-2}
174130	668879	-4.01 10^{-2}	-1.02 10^{-1}
175307	669572	-3.18 10^{-1}	-9.09 10^{-2}

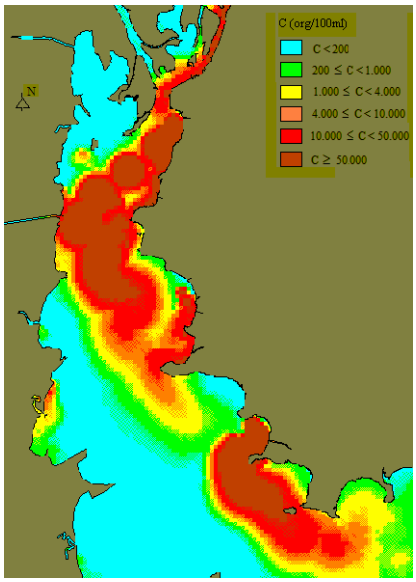

Figure 2: Concentration of Escherichia Coli along the Guaíba Lake (org/100ml)

The steady state pollutant concentration map, obtained using the exact solutions corresponding to 5 iterations in Eq. (35), is shown in Figure 2. The solutions were obtained using Maple V and implemented in Visual Basic 6.0, in order to generate the concentration map. The results were compared with experimental data provided by Departamento Municipal de Águas e Esgotos (DMAE), the county's water treatment and sewage disposal authority [1]. The total processing time of the resulting code was about 20 min in an AMD K6II - 300MHz computer, and the mean square deviation between the numerical results and experimental data was about

20%, as shown in Table 4. This deviation is of the same order as the uncertainty verified during experimental data acquisition, arising from fluctuations in the velocity field and load composition. Despite of using a 2-D model the results agree with experimental data, therefore there is no need of simulating a 3-D model. There are no experimental data to perform comparisons to the latter.

Table 4: Calculated versus experimental results

$x(m)$	$y(m)$	f_{calc}	$f_{\exp}$
171805	668878	$2.9\ 10^5$	$2.3\ 10^5$
174752	671140	$4.1\ 10^5$	$3.8\ 10^5$
172559	665451	$1.3\ 10^5$	$9.9\ 10^4$
175438	663121	$1.1\ 10^4$	$8.6\ 10^3$
175095	660585	$4.8\ 10^3$	$5.0\ 10^3$
175575	656267	$8.3\ 10^2$	$7.2\ 10^2$
179345	655033	$7.1\ 10^2$	$5.9\ 10^2$
184348	648316	75	66
189969	647562	40	31
192231	642353	99	80

Figure 3 shows the results obtained by a method based on the application of rules for manipulation of exponential of differential operators that appear on the formal solution of the advection-diffusion equation [19]. These results agree qualitatively with the ones shown in Fig. 2 resulted from the proposed method.

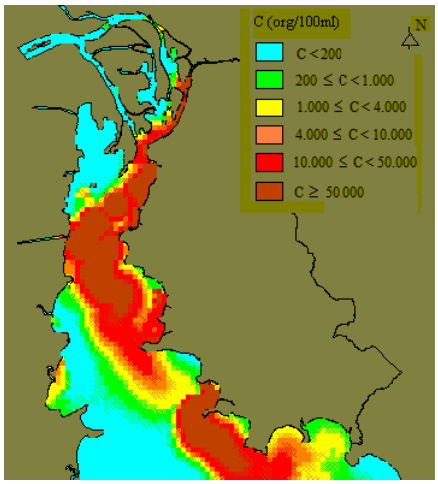

Figure 3: Concentration of Escherichia Coli along the Guaíba Lake using formal solutions

4 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 closed-form solutions with Maple V (about 1 min for five iterations) and the small amount of memory needed in most calculations, allow the simulations to be carried out in low performance microcomputers. 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 research is currently focused in the formulation of analytical procedures for dealing with non-commutative differential operators, in order to extend the application of the method to other areas of interest in transport phenomena.

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References

[1] L. Böhm. Dmae technical report. Technical Report 38, 1990.

[2] M. Bonnet and K. Wessen. Elmo, a 3-d water quality model for nutrients and chlorophyll: first application on a lacustrine ecosystem. *Ecological Modeling*, 141:19–33, 2001.

[3] J. Carnaham. *Applied Numerical Methods*. McGraw-Hill, 1972.

[4] R. Carroll, J. Warwick, K. Heim, J. Bonzongo, J. Miller, and W. Lyons. Simulation of mercury transport and fate in the carson river. *Ecological Modeling*, 125:255–278, 2000. Nevada.

[5] R. Churchill. *Complex Variables and Applications*. McGraw-Hill, 1975.

[6] G. Dattoli, L. Gianessi, M. Quattromini, and A. Torre. Exponential operators, operational rules and evolution problems. *II Nuovo Cimento*, 113:699–710, 1998.

[7] R. Delaney. Time-marching analysis of steady transonic flow in turbomachinery cascades using the hopscotch method. *Journal of Engineering for Power*, 105:272–279, 1983.

[8] M. Dhaubadel, J. Reddy, and D. Tellionis. Finite-element analysis of fluid flow and heat transfer for staggered bundles of cylinders in cross flow. *International Journal for Numerical Methods in Fluids*, 7:1325–1342, 1987.

[9] M. Drago, B. Cescon, and L. Iovenitti. A three-dimensional numerical model for eutrophication and pollutant transport. *Ecological Modeling*, 145:17–34, 2001.

[10] G. Emanuel. *Solution of Ordinary Differential Equations by Continuous Groups*. Chapman & Hall/CRC, 2001.

[11] D. Greenspan and V. Casuli. *Numerical Analysis for Applied Mathematics, Science and Engineering*. Addison-Wesley Publishing Co., 1988.

[12] N. Ibragimov. *Handbook of Lie Group Analysis of Differential Equations*. CRC Press, 1995.

[13] A. Jameson, W. Schmidt, and E. Turkel. Numerical solution of the euler equations by finite volume methods using runge-kutta time-stepping schemes. In *AIAA 14th Fluid and Plasma Dynamics Conference*, 1981.

[14] H. Kober. *Dictionary of Conformal Representations*. Dover Publications, 1944.

[15] E. Lersch, C. Hoffman, and J. Zabadal. Sistema híbrido de simulação de propagação de poluentes. *Ecos Pesquisa*, 2:7–38, 1999.

[16] R. Periá nez. A three dimensional σ-coordinate model to simulate the dispersion of radionuclides in the marine environment: application to the irish sea. *Ecological Modeling*, 114:59–70, 1998.

[17] P. Olver. *Applications of Lie Groups to Differential Equations*. Springer, 2000.

[18] J. Ortega and W. Poole. *Numerical Methods for Differential Equations*. Pitman Publishing, 1981.

[19] C. Poffal and J. Zabadal. Solving the advection diffusion equation using formal solutions: simulation of pollutant dispersion in water bodies. In *XXVII Iberian Latin American Congress on Computational Methods in Engineering*, 2006.

[20] R. Rajar and C. Matjaz. Hydrodynamic and water quality modeling: an experience. *Ecological Modeling*, 101:195–207, 1997.

[21] M. Reali, R. Rangogni, and V. Pennati. Compact analytic expressions of two-dimensional finite difference forms. *International Journal for Numerical Methods in Engineering*, 20:121–130, 1984.

[22] J. Reddy. *Applied Functional Analysis and Variational Methods in Engineering*. McGraw-Hill, 1986.

[23] J. Silvestrini, E. Schettini, and N. Rosauro. Efad: Código numérico para resolver problemas de tipo advecção-difusão pelo método dos elementos finitos. In *6 Encuentro Nacional de Investigadores y Usuários Del Métodos de Elementos Finitos*, 1989.

[24] J. Torres. Time-marching solution of transonic duct flows. Master's thesis, University of London, 1980.

[25] Y. Yang, L. Wilson, M. Makela, and M. Marcheti. Accuracy of numerical methods for solving the advection-diffusion equation as applied to spore and insect dispersal. *Ecological Modeling*, 1-24(1998), 109.

[26] J. Zabadal, D. Beck, and G. Santiago. Soluções exatas para o problema de helmholtz em duas dimensões. In *IV Escola de Primavera de Transição e Turbulência*, 2004.

[27] J. Zabadal and V. Ferreira. Flow fluid simulation in tube banks. In *IX Congreso Nacional de Ingenieria Mecanica*, 1990.

[28] J. Zabadal, M. Vilhena, S. Bogado, and C. Poffal. Solving unsteady problems in water pollution using lie symmetries. *Ecological Modelling*, 186:271–279, 2005.

[29] J. Zabadal, M. Vilhena, C. Poffal, and S. Bogado. Simulation of two-dimensional viscous flows using lie algebra. In *Proceedings of XXV Iberian Latin American Congress on Computational Methods in Engineering*, 2004.