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Closed Form Solutions to Water Pollution Problems Using Auto-BäcklundTransformations

Vinicius G. Ribeiro¹, Jorge Zabadal², Fábio Teixeira³, Guilherme Lacerda⁴, Sidnei Silveira⁵, André Da Silveira⁶

¹(Departmentof Computer Science, Centro Universitário Ritter dos Reis, Porto Alegre, Brasil)

² (DepartmentofMechanicalEngineering, Universidade Federal do Rio Grande do Sul, Brazil)

³ (Department of Design and Graphic Expression, Universidade Federal do Rio Grande do Sul, Brazil)

⁴(Department of Computer Science, Centro Universitário Ritter dos Reis, Porto Alegre, Brasil)

⁵(Department of Computer Science, Universidade Federal de Santa Maria, CESNORS, Frederico Westphalen, Brasil)

⁶(Department of Computer Science, Centro Universitário Ritter dos Reis, Porto Alegre, Brasil)

ABSTRACT

Air pollution can be very harmful to human health, especially in urban areas of large cities and in the vicinity of chemical industries. In order to prevent and minimize environmental impacts from these industries, it is necessary to use mathematical models, which can simulate scenarios associated with dispersion of pollutants. This work presents a new analytical method for solving pollutant dispersion problems. The method uses two first-order differential restrictions from which are found auto-Bäcklund transformations for the two-dimensional advection-diffusion equation at steady state. The main characteristic of the formulation is the reduced time required to obtain analytical solutions.

Keywords-Dispersion of pollutants, Exact solutions, Mathematical modeling, Project to prevent contingencies

I. INTRODUCTION

In order to estimate the environmental impacts caused by the emission of gaseous effluents from a chemical industry, it is necessary to simulate several alternatives associated with the level and type of effluent treatment to be implemented in the production process. This evaluation must be done by simulating the situations corresponding to these alternatives, so as to minimize the environmental impact without ignoring the costs related to each one. The minimization of environmental impacts aims to limit the concentration of the pollutants released within values set by the environmental legislation.

The simulations are performed from mathematical modeling that provide through maps or tables, the distribution of the concentrations for the substances of interest over the space surrounding the discharge point. The models represent boundary value problems based on the advection-diffusion equation, which governs the dispersion of atmospheric pollutants. The demand for the simulation of several situations to select the best alternative makes necessary to use methods of resolution possessing the following characteristics:

- reduced processing time
- possibility to simulate discharges in sub domains with variable spatial resolution
- flexibility in relation to the region topography and conditions of contour to be prescribed.

The choice of the best alternative for treating gaseous effluents from an industrial unit potentially polluter of the atmosphere, which minimizes the environmental impact and meets the current environmental legislation, by the selection of several possibilities of treatment, requires the use of a typically steady model, once it is sought the simulation of situations at steady state.

Another important application in environmental engineering concerns the accidental release of gaseous effluents, as consequence of serious accidents during the production process. In this situation, an instantaneous dump leads to a typically transient problem, whose resolution should be obtained with methods that allow evaluating spatial and temporal distribution of toxic pollutants. In this case, the reduced processing time, more than a desired characteristic, is a criterion of viability, because the decision aiming the adoption of measures minimize environmental impact should be to performed timely. These measures, such as warnings to the population, or the immediate evacuation of residences and industrial or commercial installations, are based on situations that reflect the progress of the pollution cloud.

However most methods employed in the resolution of problems of atmospheric pollution uses the Gaussian plume model. This model considers that when pollutants are released by an emitting source are carried away by the wind – whose speed is considered constant and uniform –which determines the main direction of the gaseous flow trajectory in the atmosphere [1, 2].

In this model some significant hypotheses are considered which considerably detail the space of solutions of the advection-diffusion equation in its original form:

- i. The components of the velocity vector are considered constant and uniform, i.e., they do not vary in space and time.
- ii. The diffusive model is considered linear, disregarding an important effect of anomalous diffusion.
- iii. The environment is considered infinite, so that, at first, only conditions of contour of second species can be applied near the ground.

In the proposed study is presented a model of pollutant propagation which constitutes a factored form of the advection-diffusion equation, composed of two first-order partial differential equations. This model enables to consider not only the non-linearity comes from the dependence of the diffusivity coefficient on the concentration, but also all the possible anisotropic terms eventually considered when performing successive integrations over the master equation.

II. THEORETICAL BACKGROUND

The main advantage of employing this factored form is because no future implementations or alteration are needed in the corresponding resolution method, in opposition to what occurs with the original forms of second order advectiondiffusion equation. This implies directly in four advantages from the operational point of view:

- i. the generation of a very compact source code, whose depuration steps become relatively simple.
- ii. the high performance of the resolution method based on symbolic processing.
- iii. the analytical character of the solution eases the physical interpretation of the phenomena in the simulated conditions and allows performing several sensitivity tests in relation to thermodynamic variables, such as temperature and pressure, without involving great computational effort.
- iv. once the temperature and pressure can explicitly appear on the solution, at first there is no need to split the domain into regions characteristics of the boundary atmospheric layer.

The air quality determined from its monitoring and performed through periodical measurements of some parameters at certain sites of the area of interest can be useful in evaluating the level of atmospheric pollution. However, these measurements allow a static and fragmented view of the phenomenon of atmospheric pollutant dispersion. As a result of the cost involved in the collection, environmental data is scarce and usually consists of time series measured at a critical region, such as the central area of some cities. However to evaluate the dispersion of gaseous pollutants in a larger area, the cost increases significantly, preventing the achievement of a spatial and temporal mesh with satisfactory resolution to assess the dynamics of pollutant dispersion. Thus, a combined perspective, spatial and temporal, of the pollutant dispersion should be made using a model that enables, from the simulation of the dispersion dynamics, the spatial and temporal interpolation.

Models are indispensable tools for studying a system, because allow to integrate spatially dispersed formations, to interpolate information for regions in which there are no measurements, to assist the interpretation of measurements made in punctual stations, to provide understanding for the dynamics and to predict situations simulating future scenarios. In the evaluation of the air quality, the system consists in the region of interest, delimited by its contour, and the possibly existing pollution sources. Mathematical models are used to represent the flow and dispersion of gaseous pollutants in a region, based on principles of conservation expressed in terms of differential equations and appropriate conditions of contour.

Other possibility is that representing the phenomenon of interest using a physical model, which generally consists in reproducing, on a reduced scale, the system object of study. Although used until the mid-1970s, with the marked increase in the processing power and storage capacity of computers physical models were gradually replaced by mathematical models. These are composed of differential equations which govern the phenomena of interest, subject to conditions of contour and an initial condition. The solution is obtained with the employment of numerical methods and, in some more recent cases, analytical methods.

In the evaluation of air quality, in a region of interest, in which can be estimated a field of speeds corresponding to the wind regime in this region, it is employed the advection-diffusion equation to evaluate the atmospheric dispersion of gaseous pollutants. The resolution of this equation, whose formulation involves diffusion associated with concentration gradient of the environment, and the advection, associated with the transport caused by winds, provides a function that translates the spatial and temporal distribution for the concentration of gaseous pollutants in the region of interest.

The advection-diffusion equation can be solved with the use of numerical, analytical and

hybrid methods [3], but still there are no analytical solutions known for various problems of great interest in environmental engineering.

The main numerical methods used to solve the advection-diffusion equation are: finite differences, finite elements, finite volumes and spectral methods. It is presented a summarized description for the characteristics of these methods, focused on their advantages and limitations for the application in solving the problem proposed.

The method of finite differences presents the inconvenience to require a great computational effort in the treatment of transient multidimensional problems. This is due to the need of discretization into fine mesh in interfaces or regions where presumably occur large gradients of concentration, temperature or pressure. The use of meshes with variable density [4] or the employment of curvilinear coordinates which adapt to the geometry of the contour [5,6,7] are resources used to reduce the processing time of these methods.

The use of formulations in finite elements is versatile to represent complex geometries, once possesses automatic generators of triangular and hexagonal meshes, it allows the variation in size of the elements composing the mesh and the conditions of contour can be easily implemented [8,9,10]. However, for the two-dimensional problems there are the productions of algebraic systems of order excessively high.

In order to combine the versatility of the computational numerical methods and performance of analytical formulations, it can be used exact solutions valid in very extensive sub domains. These solutions contain a sufficient number of arbitrary constants to preserve the spatial resolution for the respective maps of concentration and speed, without producing source codes whose processing time becomes excessively high. This occurs because the algebraic systems resulting from the imposition of the solution continuity in the interfaces among sub domains and from the application of the conditions of contour possess relatively low order and, eventually, can also possess high uncoupling degree.

These solutions are obtained through hybrid formulations that, in opposition to the traditional methods of analytical solution, seek for particular solutions instead of general ones. These solutions would be very restrictive to describe a large number of scenarios, but proved to be very easy and quick to apply when using symbolic computing programs. Such programs, developed over recent decades, enabled the use of analytical tools in problems, which would be computationally expensive when processed by conventional numerical methods [11]. These analytical tools, extremely useful to solve nonlinear partial differential equations, come from methods emerged in the late nineteenth century, based on the application of symmetries and mappings [12, 13, 14], as well as switching relationships [15, 16, 17, 18].

Thus, it became possible the application of this class of methods in real cases, so-called of engineering, as a result of the fact that some particular solutions for the advection-diffusion equation have the capacity to describe the flow in regions much larger than the usual scale for the elements of a numerical mesh. We can thus see them as particular models of sub mesh in a space discretization, which could be considered very rough to any other method. The widest solution, although never general, of the flow requires the resolution of a system of equations that imposes the solution continuity and of its derivatives in the interfaces of the many space sub domains described by each local analytical solution.

The achievement of particular solutions for sub domains applies perfectly to cases where the equations that describe the physical problem do not allow the easy achievement of a solution comprehensive enough for the entire domain, or even when their achievement means a very great computational effort when compared with the required for problems in fine mesh. There are, however, partial differential equations whose factored forms, obtained through reduction of order, produce solutions containing not only arbitrary constants, but also arbitrary functions of one or more variables [19,20]. These solutions are especially advantageous from the computational point of view, because possess, in general, very compact expressions. Such expressions facilitate the application of conditions of contour and transit through points - which establish the solution continuity in the interfaces – due to the fact that they do not produce a system of high order algebraic equations, as occurs when arbitrary elements are constants.

METHODOLOGY AND RESULTS OBTAINED

The transport and dispersion of pollutants in the atmosphere are provided by the advectiondiffusion equation, as follows:

$$\mathbf{u}.\frac{\partial \mathbf{C}}{\partial \mathbf{x}} + \mathbf{v}.\frac{\partial \mathbf{C}}{\partial \mathbf{y}} = \mathbf{D}.\left(\frac{\partial^2 \mathbf{C}}{\partial \mathbf{x}^2} + \frac{\partial^2 \mathbf{C}}{\partial \mathbf{x} \mathbf{y}^2}\right)$$
(1)

where C(x,y) is the function that represents the concentration of the desired pollutant, D is the diffusion coefficient of the pollutant in the atmosphere, u and v are the components for the speed vector in the directions x and y, respectively. The figure below illustrates the orientation of the system of axes used in the proposed formulation:

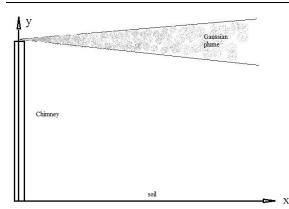


Fig. 1 system of axes used in the formulation of the proposed model

This equation can thus be factored into:

$$u.C = D.\frac{\partial C}{\partial x} + \frac{\partial a}{\partial y}$$
(2)

and

$$v.C = D.\frac{\partial C}{\partial y} - \frac{\partial a}{\partial x}$$
(3)

where a(x,y) is an arbitrary function.

The application of the divergent operator on the system represented by the equations (2) and (3), i.e., the sum of the expressions resulting from the partial derivation of these equations, in relation to x and y, respectively, results in:

$$u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + C \cdot \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) = D\left(\frac{\partial^2 C}{\partial x^2} + v\frac{\partial^2 C}{\partial y^2}\right)$$
(4)

which consists of the advection-diffusion equation plus the term represented by the product of the concentration by the velocity divergent, in which it is annulled for the incompressible flow, which constitutes a reasonable approximation for the flows whose order of the velocity module is much lower than the speed sound in air.

The system resolution requires the verification for the compatibility condition, which is made by imposing the equality of the concentration cross-derivatives, which is obtained by the partial derivation of (2) and (3) in relation to y and x, respectively:

$$D.\frac{\partial^2 C}{\partial x \partial y} = C.\frac{\partial u}{\partial y} + u.\frac{\partial C}{\partial y} - \frac{\partial^2 a}{\partial y^2}$$
(5)

and

$$D \cdot \frac{\partial^2 C}{\partial x \partial y} = C \cdot \frac{\partial v}{\partial x} + v \cdot \frac{\partial C}{\partial x} + \frac{\partial^2 a}{\partial x^2} \qquad (6).$$

By equaling equations (5) and (6), it is obtained:

$$C\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right) + v \cdot \frac{\partial C}{\partial x} - u \cdot \frac{\partial C}{\partial y} = -\left(\frac{\partial^2 a}{\partial x^2} + \frac{\partial^2 a}{\partial y^2}\right)$$
(7)

The expressions for the partial derivatives of C, in relation to x and y, obtained from the equations (2) and (3), are respectively:

$$\frac{\partial C}{\partial x} = \frac{\left(u.C - \frac{\partial a}{\partial y}\right)}{D} \tag{8}$$

and

$$\frac{\partial C}{\partial y} = \frac{\left(v.C + \frac{\partial a}{\partial x}\right)}{D}$$
(9).

Finally, by introducing the expressions obtained for the partial derivatives of C(x,y) in the equation (7), it is obtained:

$$D.C\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right) + u.\frac{\partial a}{\partial x} + v.\frac{\partial a}{\partial y} = D\left(\frac{\partial^2 a}{\partial x^2} + \frac{\partial^2 a}{\partial y^2}\right)$$
(10).

In this equation, the term inserted into the bracket that multiplies the concentration (C) is the vorticity. This can be disregarded when adopted the hypothesis of potential flow, which constitutes a good approximation to the geographical scale. It is important to observe that the small vortices, produced by locking and responsible for the high values of vorticity close to solid interfaces, do not significantly affect the dispersion of pollutant. This local effect of mixing can be introduced by employing models of turbulence to refine the local field of velocities. Thus, the equation (5.10) takes the following form:

$$u \cdot \frac{\partial a}{\partial x} + v \cdot \frac{\partial a}{\partial y} = D \cdot \left(\frac{\partial^2 a}{\partial x^2} + \frac{\partial^2 a}{\partial y^2} \right)$$
(11).

This means that it is possible to construct a symbolic iterative method in which is obtained a sequence of exact solutions for the advection-diffusion equation, following a recursive process defined by:

$$u.C_{i+1} = D.\frac{\partial C_{i+1}}{\partial x} - \frac{\partial C}{\partial y}$$
(12)

and

$$v \cdot C_{i+1} = D \cdot \frac{\partial C_{i+1}}{\partial y} - \frac{\partial C}{\partial x}$$
(13).

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In other words, once the functions C(x,y) and a(x,y) are solutions of the same differential equation, each solution found can be replaced in the

terms of the source
$$-\frac{\partial a}{\partial x}$$
 and $\frac{\partial a}{\partial y}$, which

appear in the system formed by the equations(2) and (3).

The great operational advantage of the proposed formulation lies in the following fact: in the first iteration, corresponding to i = 0, it is not necessary to know previously an exact solution for the advection-diffusion equation; simply use the own trivial solution to start the process.

This makes the formulation proposed more advantageous than the use of Lie symmetries in three fundamental aspects:

- i. dispenses the deduction and resolution of determinant equations, used to obtain the generator coefficients for the respective groups of symmetry [12];
- ii. does not require the use of rules for the manipulation of exponentials of operators [13] in order to obtain the symmetries in explicit form, i.e., expressed in terms of changes in variables; and
- iii. does not require the previous knowledge of any exact solution for the target equation as already mentioned.

Once (12) and (13) allow obtaining a sequence of exact solutions for the advectiondiffusion equation in Cartesian coordinates, the following question arises out: if the local relief of the soil is uneven, how to proceed to maintain the discretization in thick mesh? Is it not be necessary to refine the mesh together at the solid interface? The equations (12) and (13) can be easily adjusted to a generalized curvilinear orthogonal coordinate system, in which the new coordinates represent the current function (ψ) and the potential function velocity (ϕ) for the potential flow.

By using the curvilinear coordinates adjusted to the geometry of the domain, it is possible to replace the spatial derivatives of concentration by the expressions:

$$\frac{\partial C}{\partial x} = \frac{\partial C}{\partial \phi} \cdot \frac{\partial \phi}{\partial x} + \frac{\partial C}{\partial \psi} \cdot \frac{\partial \psi}{\partial x} = u \cdot \frac{\partial C}{\partial \phi} - v \cdot \frac{\partial C}{\partial \psi}$$

$$\frac{\partial C}{\partial y} = \frac{\partial C}{\partial \phi} \cdot \frac{\partial \phi}{\partial y} + \frac{\partial C}{\partial \psi} \cdot \frac{\partial \psi}{\partial y} = v \cdot \frac{\partial C}{\partial \phi} + u \cdot \frac{\partial C}{\partial \psi}$$
(15).

By redefining the partial derivatives of concentration in the equation (12) and (13), it is obtained:

$$u \cdot C_{i+1} = D \cdot \left(u \cdot \frac{\partial C_{i+1}}{\partial \psi} - v \cdot \frac{\partial C_{i+1}}{\partial \phi} \right) + v \cdot \frac{\partial C_i}{\partial \phi} + u \cdot \frac{\partial C_i}{\partial \psi}$$
(16)

$$v.C_{i+1} = D.\left(v.\frac{\partial C_{i+1}}{\partial \psi} - u.\frac{\partial C_{i+1}}{\partial \phi}\right) + u.\frac{\partial C_{i}}{\partial \psi} - v.\frac{\partial C_{i}}{\partial \phi}$$
(17).

Although the formulation proposed has been designed to solve the advection-diffusion equation in the two-dimensional form at steady state, the achievement of three-dimensional and transient solutions with these expressions constitutes a relatively simple task. Indeed, there is extensive literature about symmetries permitted by the advection-diffusion equations. Symmetries are changes of variable that transform exact solutions of a differential equation into new solutions, also exact, from the same equation. These new solutions present larger number of arbitrary elements and dependency in relation to variables not considered in a previous analysis. Importantly, the use of symmetries had not yet been widely applied to engineering problems yet, precisely due to the need of previous knowledge of exact solutions, which are functions of at least two independent variables. The achievement of these solutions is the decisive step for the viability of the use of symmetries in the resolution of problems of this nature.

III. CONCLUSION

The formulation proposed can be extended to problems of nonlinear diffusion in which the coefficient D directly depends on the spatial variables and indirectly on the temperature and concentration. This generalization produces terms that represent the anomalous diffusion occurring in regions of high gradient and low laplacian of concentration, and has origin in the definition of the diffusivity coefficient in micro scale, through the master equation of the statistical thermodynamics [21], an integral form of the equation of transport. Approximations of the master equation obtained via integration by parts produce the Fick's Law, and its extensions.

Depending on the number of terms considered in this recursive definition, it can be produced terms related to isotropic and anisotropic diffusion. This occurs because the advection-diffusion equation, twodimensional and stationary, in its vector form can be expressed as follows:

 $\vec{V} \cdot \nabla C = \nabla (D \cdot \nabla C) = D \cdot \nabla^2 + \nabla C \cdot \nabla D$ (18).

In the equation above, the term ∇C . ∇D corresponds to the anomalous diffusion, constituted by the scalar product for the concentration and the diffusion gradient. The diffusion gradient, in turn, as already mentioned directly depends on spatial variables and indirectly on temperature and concentration, as shown below. By using the chain rule to redefine the diffusivity gradient, it is obtained:

$$\nabla D = \frac{\partial D}{\partial T} \nabla T + \frac{\partial D}{\partial C} \cdot \nabla C$$
(19).

By replacing the equation (19) in the stationary twodimensional advection-diffusion equation:

$$u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = D\frac{\partial D}{\partial T}.(\nabla T.\nabla C) - \frac{\partial D}{\partial C}(\nabla C.\nabla C) + D\nabla^2 C$$
(20)

Although the resulting equation is nonlinear of second order, its factored form remains unchanged, so that the formulation proposed remains valid for the achievement of exact solutions.

In the equation (19), the partial derivatives $\frac{\partial D}{\partial C}$ and $\frac{\partial D}{\partial T}$ can be obtained through the definition of the diffusion coefficient in micro scale:

$$D = \frac{l^2}{\tau} \tag{21}$$

where 1 is the mean free path of the gas molecules, and τ is the average period elapsed between two successive collisions. It is noticed that 1 essentially depends on the concentration, while the quotient $\frac{l}{\tau}$, which represents the mean free velocity of the gas molecules, is a function of temperature. Thus, it can be used models from the kinetic theory of gases in order to express the diffusion coefficient as function of temperature and pressure, or temperature and concentration.

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