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Numerical Methods for the Evaluation of Pollutant Dispersion Based on Advection-Diffusion Equation

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Several pollutant dispersion models have been developed to provide subsidies for environmental impact assessment and monitoring of natural resources such as air, soil and water. In this work, we solve the one-dimensional advection-diffusion equation using an adaptive-step algorithm for the analysis of pollutant dispersion and compare it with other recent work, obtaining very similar results for two solute dispersion scenarios, one along steady flow through inhomogeneous medium and another along uniform flow through homogeneous medium. Our method is characterized by low computational time and simplicity of the code, and may contribute as a numerical background for pollutant source management.

1. Introduction

Several factors may influence the accumulation or dispersion of pollutants, such as the emission source characteristics, the emission rate, meteorological factors and land use (Lora, 2002). The advection-diffusion equation Eq(1) may be used to estimate air pollutant concentration levels in a given location and is also applied in other areas, such as dispersion analysis in water surface, soil mechanics and petroleum engineering (Savovic and Djordjevich, 2012). In one space dimension, the advection-diffusion equation is written as:

$$\frac{\partial C(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[D(x,t)\frac{\partial C(x,t)}{\partial x} - u(x,t)C(x,t)\right] , \qquad (1)$$

where *C(x,t)* is the dispersing pollutant concentration at position x along the longitudinal direction at time t. *D* and *u* are constants, called dispersion coefficient and uniform flow velocity, respectively.

Various pollutant dispersion model have been developed, such as AERMOD (*"AMS/EPA Regulatory Model"*) and Industrial Source Complex (ISC), both developed by the US-EPA (*"United States - Environmental Protection Agency"*) for estimating the concentration of atmospheric pollutant being applicable to a wide variety of emission sources.

Savovic and Djordjevich (2012) employed the explicit finite difference method for solving one-dimensional advection-diffusion equation, using variable coefficients in semi-infinite media for three dispersion problems: solute dispersion along steady flow through inhomogeneous medium, temporally dependent solute dispersion along uniform flow through homogeneous medium and solute dispersion along temporally dependent unsteady flow through inhomogeneous medium. Considering the existence of a continuous point source for all the situations, the results obtained by the authors showed good agreement with analytical solutions discussed in the literature.

A similar study was developed by Singh et al. (2012), who derived an analytical solution for the space-time variation of contaminant concentration in one-dimensional uniform groundwater flow in a homogeneous semi-infinite porous formation subjected to time-dependent source contamination, using Laplace transform technique. Two cases of temporally dispersion along uniform flow are simulated, with an uniform source concentration and with mixed-type boundary conditions. The results were obtained for two expressions of temporally dependent dispersion, sinusoidally and exponentially increasing forms. The analytical solution

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purposed by the authors was validated using the same set of inputs adopted by Jaiswal et al. (2009), except for the decay rate coefficient.

Another analytical solution to the one-dimensional advection-diffusion equation was developed by Mazaheri et al. (2013), considering several point sources. Initially, a solution for linear pulse point source was obtained using Laplace transform technique. Based on this solution, the superposition principle was employed to extend the derived solution for several point sources through arbitrary time pattern. After performing four tests, constant pulse source, instantaneous spill, decaying point sources and several point sources with irregular patterns, the results showed that the purposed analytical solution can provide accurate estimation of the concentration.

Kaabeche and Belbaki (2013) solve the one-dimensional advection-diffusion equation for investigating the coupling effect of non-linearity adsorbed solute dispersion and chemical heterogeneity, using the Finite Volume Method to discretize the partial differential equation. Numerical results obtained by the authors showed that nonlinear interactive solute transport differ from that in the homogeneous one. It was observed that chemical heterogeneity cannot be ignored in predicting the breakpoint and that fixing the heterogeneity of the medium, the porous media length has also an effect. Appadu (2013) use three numerical methods to solve one-dimensional advection-diffusion equation, an explicit, an implicit, and a nonstandard finite difference scheme, with specified initial and boundary conditions, for which the exact solution is known using all these three schemes. The author observed that the explicit Lax-Wendroff scheme, in general, is the most efficient method followed by the nonstandard finite difference scheme. Another factor was verified, that the choice of space and time step sizes affected expressively the results.

A fairly used tool in dispersion analysis in Computational Fluid Dynamics (CFD), which solve the Navier-Stokes equation using different kinds of refinement depending of the goal. Velocity is divided in mean and fluctuation components, using turbulence model in order to close the equation systems. CFD model require solving continuity, momentum and energy equations. CFD software solve advection-diffusion equation using discrete approach, involving discretization in space and time (Lauret et al., 2014).

Modenesi et al. (2004) use CFD to analyse the dispersion of an effluent from REPLAN (PETROBRAS refining unit) on the Atibaia River in São Paulo, Brazil. The authors observed that the effluent is dispersed in a distance of 485 m after the releasing point, where concentration becomes constant. As main vantages of CFD, it was emphasized the speed while performing the simulation.

Gousseau et al. (2011) compare the convective and turbulent mass fluxes predicted by two approaches, solving the Reynold's-averaged Navier-Stokes (RANS) and Large-Eddy Simulation (LES), for two configurations of isolated buildings with distinctive features. It is shown that when the source is located outside of recirculation regions, both LES and RANS can provide accurate results. The authors conclude that the choice of the appropriate turbulence model depends on the configuration of the dispersion problem under study.

Dourado et al. (2012) evaluates the use of two CFD models (LES-Dynamic Smagorinsky and LES-Wale) and two regulatory dispersion models (AERMOD and CALPUFF) to assess odour impact, comparing the average concentration results obtained by each model with experimental wind tunnel data. Peak-to-mean concentration ratio (P/M) concentration ratio estimated by the regulatory models were underestimated when compared to CFD results and wind tunnel measurements. Results obtained by the authors indicated that CFD can provide good estimates of the concentration field, its fluctuation intensity and thus, the peak-to-mean concentration ratio, making it a viable tool for studying fluid flow characteristics for odour impact assessment.

This study aims to determine whether the use of a numerical method, employing an adaptive-step Runge-Kutta algorithm (Wolfram Research, 2012), to estimate pollutant concentration, is satisfactory compared to other existing models in the literature.

2. Theoretical background

In this work, we have solved the one-dimensional advection-diffusion equation Eq(1) using an adaptive-step algorithm. Even though there are analytical and statistical tools for estimating the concentration of pollutant, such as Gaussian methods (Lora, 2002), they cannot solve partial differential equations (PDE's) with non-linear terms. When the nonlinearities in the PDE's cannot be neglected, the use of numerical integration methods is essential for obtaining an accurate solution for differential equations (Potter, 2004).

Savovic and Djordjevic (2012) have solved the one-dimensional advection-diffusion equation with variable coefficients in semi-infinite media using explicit finite difference method for three dispersion problems with continuous point sources.

For the first scenario, characterized by a medium inhomogeneity that causes variation in the flow velocity, the concentration distribution as a function of time was obtained by solving Eq(2). The authors assume that dispersion parameter is proportional to square of the velocity:

$$\frac{\partial c(x,t)}{\partial t} = [(1+ax)(2aD_0 - u_0)]\frac{\partial c(x,t)}{\partial x} + D_0(1+ax)^2\frac{\partial^2 c(x,t)}{\partial x^2} - u_0 aC(x,t) \ , \tag{2}$$

where a accounts for the medium inhomogeneity (10^{-3} m^{-1}), u is the uniform flow velocity (10^3 m/y), D is the dispersion coefficient (10^6 m^2/ y), t is the time (y) and x is the distance (10^3 m).
For the second scenario, a temporally dependent solute dispersion along uniform flow through homogeneous medium, it was considered an uniform and steady longitudinal flow in a semi-infinite homogeneous and initially solute-free medium. The concentration for this scenario was obtained according to Eq(3),

$$\frac{\partial c(x,t)}{\partial t} = -u_0\frac{\partial c(x,t)}{\partial x} + D_0 Exp(mt)\frac{\partial^2 c(x,t)}{\partial x^2} \ , \tag{3}$$

where m is a coefficient having dimension reciprocal to time t, and is considered proportional to (u_0^2/d_0^2).
Savovic and Djordjevich (2012) also simulated a third scenario, solute dispersion along temporally dependent unsteady flow through inhomogeneous medium. As in the first scenario, it's assumed that the inhomogeneity causes a linear increase in velocity and that dispersion is proportional to square of velocity. The flow is supposed to vary with time hence dispersion is also supposed to vary temporally in the same proportion.

3. Results and discussion

3.1 Convergence

In a variable-step integration algorithm, the maximum allowed step size is a critical parameter. Using the same initial and boundary conditions adopted by Savovic and Djordjevich (2012), we performed convergence tests using different maximum step sizes in the equation solver for both scenarios when compared with that paper.
The results are displayed in Figure 1, where we show the ratio between *C(x,t)* and *C(0,t)* as a function of the distance to the source. The solution converges fast using a step of 0.1 year and 0.1 kilometre in both scenarios. To ensure the accuracy of results, we adopt the maximum step size of 0.001 for both parameters in our simulations.

3.2 Solute dispersion through an inhomogeneous medium

The solutions obtained with the numerical integration of Eq(2) are shown in Figures 2 and 3 where we show the ratio C/C_0 as a function of the distance to the source for several values of the time. Results obtained by our method are very similar to those obtained by Savovic and Djordjevich (2012). As already expected, ratio C/C_0 increases with time and starts decreases with distance, being less than 0.2 for distances larger than 2 kilometres from the source, considering time up to one year, when solute

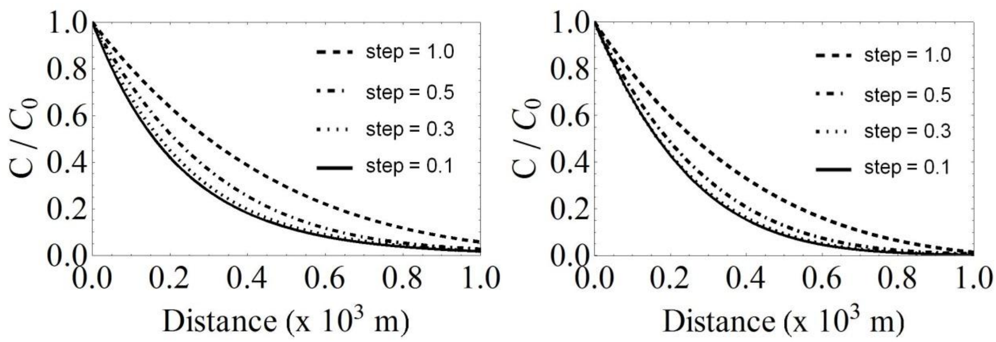

Figure 1: Convergence of the solution for solute dispersion through homogeneous medium (left) and for temporally dependent solute dispersion along uniform flow through homogeneous medium (right).The time was fixed to t = 0.1 y for some values of the maximum allowed step size

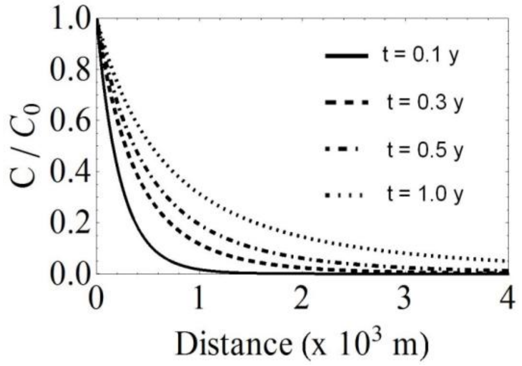

Figure 2: Ratio C/C_0 to distances up to 4 kilometres from the source considering time up to one y for solute dispersion through inhomogeneous medium

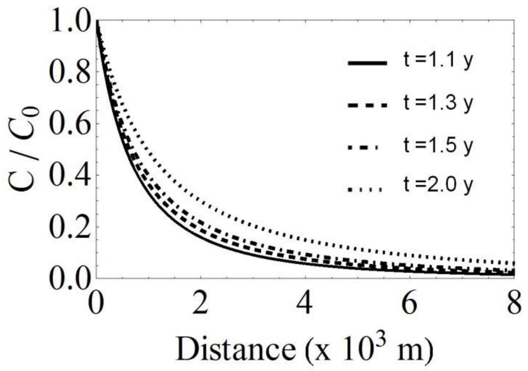

Figure 3: Ratio C/C_0 to distances up to 8 kilometres from the source considering time of one to two y for solute dispersion through inhomogeneous medium

dispersion occurs through an inhomogeneous medium (Figure 2).

We also have performed simulations considering time of one to two years. According to Figure 3, it was observed that ratio C/C_0 decreases more slowly than for time up to one year and that there is a minor difference in the ratio variation with *t* adopted. It is noticed that for distance of 8 kilometres, there is still influence of the source in the solute concentration.

3.3 Temporally dependent solute dispersion along uniform flow through homogeneous medium

As in the first scenario, the result of numerical integration of Eq(3) using our method have showed a good agreement with those obtained by Savovic and Djordjevich (2012). According to Figure 4, the ratio C/C_0 for a temporally dependent solute dispersion along uniform flow through homogeneous medium decreases faster than solute dispersion through an inhomogeneous medium. For time up to 1.0 y, the ratio C/C_0 is close to zero for distances larger than 3×10^3 m showing that solute is largely disperse, unlike the other scenario.

As observed for solute dispersion through inhomogeneous medium, the ratio C/C_0 decreases more slowly for time of 1 to 2 years than for shorter times and there is a minor difference in the ratio variation with *t* adopted in this range. However, for temporally dependent solute dispersion along uniform flow through homogeneous medium, for more than 4 kilometres from the source, the ratio C/C_0 is close to zero, indicating that solute is already largely dispersed in this scenario (Figure 5). It's noticeable that ratio C/C_0

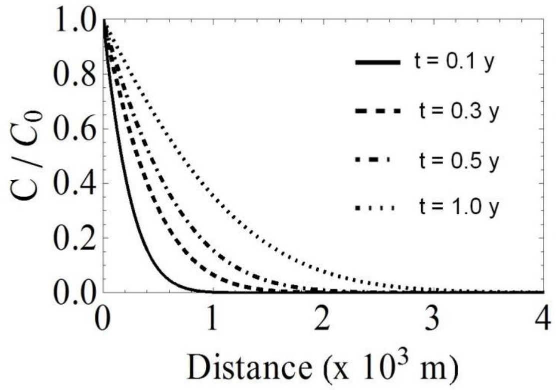

Figure 4: Ratio C/C_0 to distances up to 4 km from the source considering time up to one y for temporally dependent solute dispersion along uniform flow through homogeneous medium

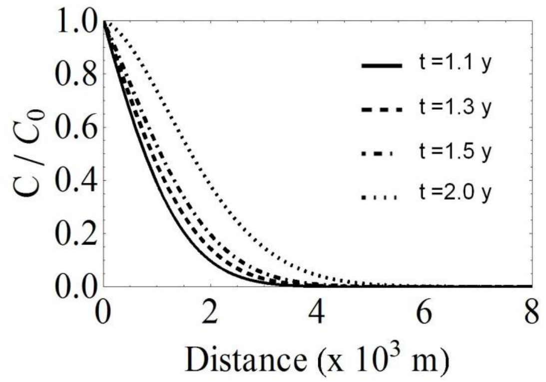

Figure 5: Ratio C/C_0 to distances up to 8 kilometres from the source considering time of one to two y for temporally dependent solute dispersion along uniform flow through homogeneous medium

in Figures 4 and 5 reaches zero with shorter distances than in Figures 2 and 3, indicating that medium homogeneity facilitate solute dispersion.

3.4 Method advantages

As presented in sections 3.1 and 3.2, the results were consistent and as method advantage, we appoint the fact of being simpler than methods adopted by other authors, such as explicit finite difference, Laplace transform technique and generalized integral transform technique, and the fact of being able to solve a wide variety of differential equation systems with initial and boundary conditions pre-established. Other factors may be considered, such as low computational time, rapid convergence and only a few lines of code.

4. Conclusion

We have used a variable-step numerical integration algorithm for solving the one-dimensional advection-diffusion equation with the same initial and boundary conditions adopted by Savovic and Djordjevich (2012), obtaining very similar results. We observed that the ratio C/C_0 decreases faster for temporally dependent solute dispersion along uniform flow through homogenous medium than for solute dispersion through inhomogeneous medium, and that for both scenarios, the ratio C/C_0 decreases more slowly with distance for time of one to two years than for shorter times.
The method used in this work estimates pollutant concentration as function of emission time and distance from the source with a simple code and low computational time, and may contribute as a numerical background for pollutant source management.
We have also made a detailed investigation on the behavior of the advection-diffusion equation as we change the parameters (a, D_0, u_0) independently. The results provide an interesting quantitative view of the one-dimensional problem and will be presented in a longer paper. In future works, we plan to extend our

method to the two and the three-dimensional cases, which will enable applications such as forecasting critical episodes of pollution and development of surveillance systems.

References

Appadu A.R., 2013, Numerical solution of the 1D advection-diffusion equation using standard and nonstandard finite difference schemes, Journal of Applied Mathematics, Article ID 734374, 14 pages.

Dourado H., Santos J., Reis Jr N., Melo A.M.V., 2012, The effects of atmospheric turbulence on peak-to-mean concentration ratio and its consequence on the odour impact assessment using dispersion models, Chemical Engineering Transactions, 30, 163-168, DOI: 10.3303/CET1230028.

Gousseau P., Blocken B., van Heijst G.J.F., 2011, CFD simulation of pollutant dispersion around isolated buildings: On the role of convective and turbulent mass fluxes in the prediction accuracy, Journal of Hazardous Materials, 194, 422-434.

Jaiswal D.K., Kumar A., Kumar N., Yadav R.R., 2009, Analytical solutions for temporally and spatially dependent solute dispersion of pulse type input concentration in one-dimensional semi-infinite media, Journal of Hydro-Environment Research, 2(4), 254-263.

Kaabeche K., Belbaki A., 2013, Coupling effect of non-linearity and chemical heterogeneity on reactive solute transport in a fixed bed, Chemical Engineering Transactions, 32, 1549-1554 DOI: 10.3303/CET1332259.

Lauret P., Heymes F., Aprin L., Johannet A., Dussere G., Lapebie E., Osmont A., 2014, Atmospheric turbulent dispersion modelling methods using machine learning tools, Chemical Engineering Transactions, 36, 517-522 DOI: 10.3303/CET1436087

Lora E.E.S., 2002, Prevention and Control of Pollution on the Energy, Industrial and Transport Sectors, 2nd Edition, Interciência, 862p (in Portuguese).

Potter M.C., Wiggert D.C., Hondzo M., Shih T.I.P., 2004, Fluid Mechanics, Cengage Learning, São Paulo, Brazil, 688 pages (in Portuguese).

Savovic S., Djordjevich A., 2012, Finite difference solution of the one-dimensional advection-diffusion equation with variable coefficients in semi-infinite media, International Journal of Heat and Mass Transfer, 55, 4291-4294.

Singh M.K., Ahamad S., Singh V.P., 2012, Analytical solution for one-dimensional solute dispersion with time-dependent source concentration along uniform groundwater flow in a homogeneous porous formation, Journal of Engineering Mechanics, 138(8), 1045-1056.

Mazaheri M., Samani J.M.V., Samani H.M.V., 2013, Analytical solution to one-dimensional advection-diffusion equation with several point sources through arbitrary time-dependent emission rate patterns, Journal of Agricultural Science and Technology, 15, 1231-1245.

Modenesi K., Furlan L.T., Tomaz E., Guirardello R., Núnez J.R., 2004, A CFD model for pollutant dispersion in rivers, Brazilian Journal of Chemical Engineering 21, 557-568.

Wolfram Research, Inc., 2012, Mathematica 9.0, Champaign, Illinois, USA.