Proceeding Series of the Brazilian Society of Applied and Computational Mathematics, Vol. 5, N. 1, 2017.

Trabalho apresentado no CNMAC, Gramado - RS, 2016.

Proceeding Series of the Brazilian Society of Computational and Applied Mathematics

Multidimensional Unsteady Solutions to the Convection-Diffusion-Reaction Equation with a Time Dependent Boundary Condition

Alcéstes G. de Oliveira Filho[1]
Norberto Mangiavacchi[2]
Department of Mechanical Engineering, Rio de Janeiro State University (UERJ)

Abstract. This paper provides analytical solutions to one, two and three-dimensional convection-diffusion equation with decay term, subjected to a time dependent and periodic boundary condition. These solutions are suitable benchmarks to asses the correctness of computational codes implemented for the problems of multidimensional reactive flows, which are of considerable interest to many fields of science and engineering. Tests are illustrated through computational codes and is remarked the feature of representing periodic oscillations in all dimensions considered.

Keywords. Analytical solutions, code validation, convection-diffusion equation, periodic boundary condition, reactive flows.

1 Introduction

Classical solutions of the Convection-Diffusion Equation (CDE), with or without the reaction term, have been catalogued for many initial and boundary conditions. Among them, it can be found in the works by van Genuchten and Alves [6], Logan and Zlotnik [4], Logan [3], Goltz and Dorroh [2], Ziskind et al. [7], Chen and Liu [1] and Pérez Guerrero et al [5], analytical solutions pertaining to time varying boundary conditions, which is of practical interest to many fields as hydrogeology, pollution dispersion and process industry.

However, it must be remarked that, in general, these works restrict their analysis to one-dimensional domain, while real cases demand 2D and 3D calculations. Multidimensional codes are then constructed in order to perform such calculations but their validation would require comparison with suitable benchmark solutions.

Although it is possible to approach validation by extracting 1D results from numerically calculated multidimensional profiles in order to compare them to preexisting analytical solutions, we think that a plain validation would be only attained if multidimensional solutions were available. So, in this paper, we seek these solutions for the linear equation:

$$\frac{\partial c}{\partial t} = a_0 c + a_1 \vec{n}.\nabla c + a_2.\nabla^2 c \tag{1}$$

[1]guanabarino@ime.eb.br
[2]norberto@uerj.br

which is a model equation for many physical problems. Typically, a_0 is the reaction rate, a_1 is the negative of the fluid velocity, $\vec{n}$ is a unit vector tangent to the velocity direction, and a_2 is the composed diffusion coefficient, while c is the dependent function, representing the chemical species concentrations.

In particular, we are interested in the validation of codes for the simulation of reacting pollutant transport where the input at the inlet boundary is a continuous periodic function of time, for example, in the case of liquid waste disposal operating on a periodic cycle, or any natural cyclic water-quality variations [1, 3, 4], employing a generalization of one of the 1D solutions proposed by Logan and Zlotnik [4].

2 Analytic Solution for the 1D Transient Problem

In the case of 1D problems, Eq.(1) reduces to:

$$\frac{\partial c}{\partial t} = a_0 c + a_1 \frac{\partial c}{\partial x} + a_2 \frac{\partial^2 c}{\partial x^2} \tag{2}$$

subjected to $c(x,\, t_0){=}\, g(x)$. For $t{>}t_0$, we have the following boundary conditions: $c(0{,}t){=}\, f(t)$ and, at the outflow, we assume continuous concentration, forcing an homogeneous Neumann exit, which is also referred to as Danckwerts condition in finite transport domains [2, 5, 7].

Assuming that $f(t)$ is time periodic and has a Fourier representation, we may consider that Eq.(2) admits a solution of the form [3, 4]:

$$c = e^{\hat{\alpha}x + \hat{\beta}t} \tag{3}$$

where $\hat{\alpha}$ and $\hat{\beta}$ are complex valued, thus $\hat{\alpha} = \alpha_R + i\alpha_I$ and $\hat{\beta} = \beta_R + i\beta_I$.

Then, substituting the above relations in Eq.(2), we obtain:

$$\hat{\beta} = a_0 + a_1\hat{\alpha} + a_2\hat{\alpha}^2 \tag{4}$$

Following, we may conclude that any solution given by Eq.(3) satisfying Eq.(4) is a solution of Eq.(2).

2.1 Periodic time and constant forcing

Taking the real and imaginary parts of Eq.(4) and considering that:

$$\hat{\alpha}^2 = (\alpha_R + i\alpha_I)^2 = \left(\alpha_R^2 - \alpha_I^2\right) + i\,(2\alpha_R\alpha_I) \tag{5}$$

we obtain the following relations:

$$\beta_R = a_0 + a_1\alpha_R + a_2\left(\alpha_R^2 - \alpha_I^2\right) \tag{6}$$

$$\beta_I = a_1\alpha_I + a_2\,(2\alpha_R\alpha_I) = \alpha_I\,(a_1 + 2a_2\alpha_R) \tag{7}$$

Solutions that do not decay in time, but are forced at a fixed value of x by a time periodic value, imply in $\beta_R = 0$. Then, inserting that condition into Eq.(6), we have:

DOI: 10.5540/03.2017.005.01.0411

$$a_0 + a_1\alpha_R + a_2\left(\alpha_R^2 - \alpha_I^2\right) = 0 \text{ and, therefore: } \alpha_I = \pm\sqrt{\alpha_R^2 + \frac{a_1}{a_2}\alpha_R + \frac{a_0}{a_2}} \tag{8}$$

which, after substitution in Eq.(7), implies in:

$$\beta_I = \pm\sqrt{\alpha_R^2 + \frac{a_1}{a_2}\alpha_R + \frac{a_0}{a_2}}\left(a_1 + 2a_2\alpha_R\right) \tag{9}$$

By noting that the concentration c cannot take negative values, in order to provide a physically consistent solution, we need to add a constant forcing such that this nonnegative restriction is satisfied. Also, for a constant in time forcing, we have $\beta_R = \beta_I = 0$ and, therefore, substituting this condition in Eq.(4), we obtain:

$$\hat{\alpha} = -\frac{a_1}{2a_2} \pm \sqrt{\frac{a_1^2}{4a_2^2} - \frac{a_0}{a_2}} \tag{10}$$

As expected, Eq.(2) has negative real solutions in case of $a_0 < 0$, thus producing a steady solution that decays in the x direction, representing the amplitude decay with the distance. So, given a_0, a_1, a_2, and an arbitrary α_R, we may construct a solution employing Eq.(3) and Eqs.(8) to (10).

2.2 Sample code test

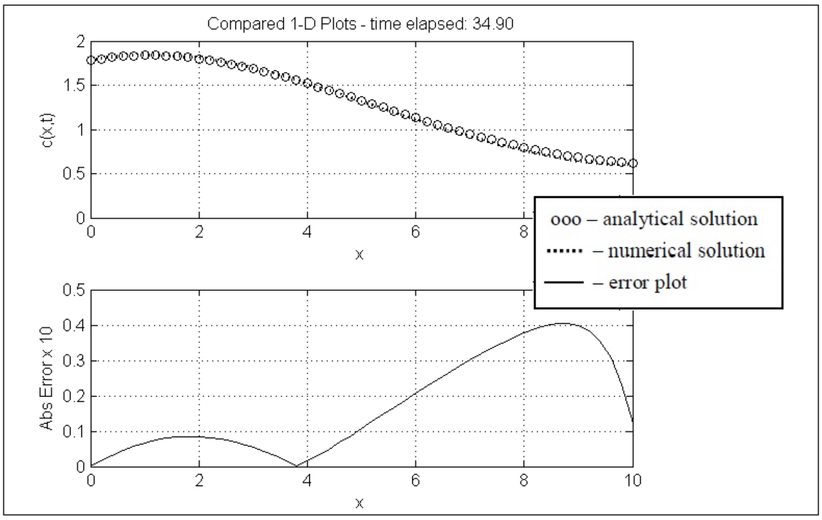


Figure 1: 1D Sample Code Graphics Output.

We show a test (Fig. 1) where a simple 1D explicit finite difference (FD) code that solves Eq.(2) is tested against the analytical solution given above. Entry parameters are: L (computational domain size) = 10; $\Delta x = 0.2$; $\Delta t = \Delta x^2/2$; $a_0 = -0.01$; $a_1 = -1.0$; $a_2 = 1.0$ and α_R is arbitrarily set as -0.1. The transient analytical and numerical solutions are plotted on the upper graph and the absolute error (amplified by 10) is plotted below.

3 Analytic Solutions for 2D and 3D Transient Problems

In the case of 2D and 3D problems, we may consider as ansatz, respectively:

$$c = e^{\hat{\alpha}_x x + \hat{\alpha}_y y + \hat{\beta} t} \quad \text{and} \quad c = e^{\hat{\alpha}_x x + \hat{\alpha}_y y + \hat{\alpha}_z z + \hat{\beta} t} \tag{11}$$

Once more, observing that $\hat{\alpha}_i$ and $\hat{\beta}$ are complex valued, we have:

$$\hat{\alpha_x} = \alpha_{xR} + i\alpha_{xI} \ , \ \hat{\alpha_y} = \alpha_{yR} + i\alpha_{yI} \ , \ \hat{\alpha_z} = \alpha_{zR} + i\alpha_{zI} \quad \text{and} \ \hat{\beta} = \beta_R + i\beta_I \tag{12}$$

By substituting these in each ansatz and in the correspondent forms of Eq.(1), we obtain, for two dimensions:

$$\hat{\beta} = a_0 + a_{1x}\hat{\alpha}_x + a_{1y}\hat{\alpha}_y + a_2\left(\hat{\alpha}_x^2 + \hat{\alpha}_y^2\right) \tag{13}$$

and for three dimensions:

$$\hat{\beta} = a_0 + a_{1x}\hat{\alpha}_x + a_{1y}\hat{\alpha}_y + a_{1z}\hat{\alpha}_z + a_2\left(\hat{\alpha}_x^2 + \hat{\alpha}_y^2 + \hat{\alpha}_z^2\right) \tag{14}$$

In the same way as before, any solution given by Eq.(11), satisfying Eqs.(13) and (14) are, for each case, solutions of Eq.(1).

3.1 Periodic and time constant forcing

Taking the real and imaginary parts of Eq.(14) and considering accordingly the relation of Eq.(5), we obtain for the most generic case of three dimensions:

$$\beta_R = a_0 + a_{1x}\alpha_{xR} + a_{1y}\alpha_{yR} + a_{1z}\alpha_{zR} + a_2\left(\alpha_{xR}^2 + \alpha_{yR}^2 + \alpha_{zR}^2 - \alpha_{xI}^2 - \alpha_{yI}^2 - \alpha_{zI}^2\right) \tag{15}$$

and:

$$\beta_I = a_{1x}\alpha_{xI} + a_{1y}\alpha_{yI} + a_{1z}\alpha_{zI} + 2a_2\left(\alpha_{xR}\alpha_{xI} + \alpha_{yR}\alpha_{yI} + \alpha_{zR}\alpha_{zI}\right) \tag{16}$$

We also consider periodicity in y and z directions, hence β_R, α_{yR} and α_{zR} are set to zero, in order to obtain bounded solutions, while α_{yI} and α_{zI} are both arbitrarily prescribed constants, in order to properly represent oscillations in these coordinates.

So, inserting these conditions in Eq.(15), we have:

$$a_0 + a_{1x}\alpha_{xR} + a_2\left(\alpha_{xR}^2 - \alpha_{xI}^2 - \alpha_{yI}^2 - \alpha_{zI}^2\right) = 0 \tag{17}$$

and:

$$a_{xI} = \pm\sqrt{\alpha_{xR}^2 - \alpha_{yI}^2 - \alpha_{zI}^2 + \frac{a_{1x}}{a_2}\alpha_{xR} + \frac{a_0}{a_2}} \tag{18}$$

which, upon substitution in Eq.(16), yields:

$$\beta_I = \pm\sqrt{\alpha_{xR}^2 - \alpha_{yI}^2 - \alpha_{zI}^2 + \frac{a_{1x}}{a_2}\alpha_{xR} + \frac{a_0}{a_2}}\,(a_{1x} + 2a_2\alpha_{xR}) + a_{1y}\alpha_{yI} + a_{1z}\alpha_{zI} \tag{19}$$

and the solution can be expressed as:

$$c = e^{(\alpha_{xR} + i\alpha_{xI})x + i\alpha_{yI}y + i\alpha_{zI}z + i\beta_I t} \tag{20}$$

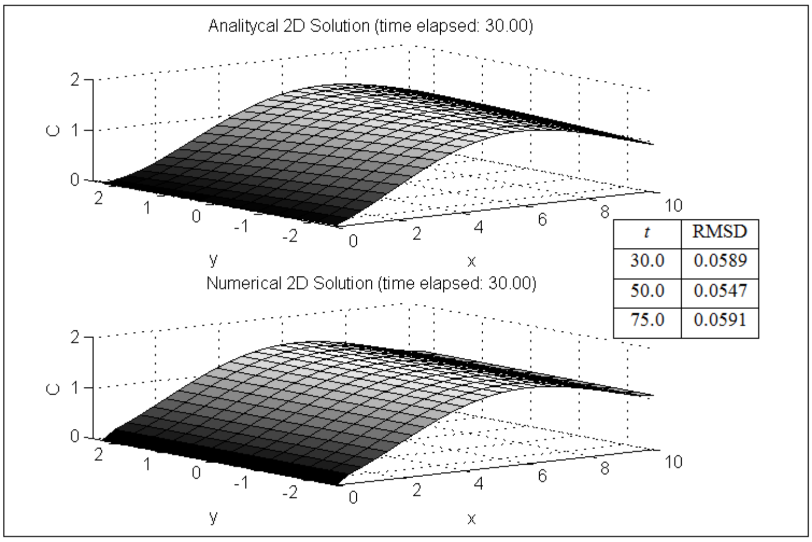
DOI: 10.5540/03.2017.005.01.0411

Also, to assure the nonnegative restriction for the concentration profile, we must have also $\beta_I = 0$ and this supplies the constant forcing:

$$c_0 = e^{(\alpha_{xR}+i\alpha_{xI})x+i\alpha_{yI}y+i\alpha_{zI}z} \tag{21}$$

For the 2D case, we can proceed analogously, considering that there is not the z component and, as a consequence, periodicity in the z direction. Thus, given a_0, a_1, a_2 and arbitraries α_{xR}, α_{yI} and α_{zI}, according to the case, we may construct a 2D or 3D solution, employing Eqs.(18) to (21).

3.2 Sample code test



t	RMSD
30.0	0.0589
50.0	0.0547
75.0	0.0591

Figure 2: 2D Sample Code Graphics Output (1250 elements mesh).

A 2D code employing a simple Galerkin formulation through finite elements method (FEM) is employed for test and the outcome for a given elapsed time is shown by Fig. 2. The entry parameters are L = 10; W = 5; $\Delta x = 0.4$; $\Delta y = 0.4$; $\Delta t = 0.1$; $a_0 = -0.01$; $a_{1x} = -2.0$; $a_{1y} = -0.2$; $a_2 = 1.0$; α_{xR} and α_{yI} are arbitrarily set as -0.1. The error is evaluated through Root Mean Square Deviation (RMSD), which is also shown in Fig. 2, or:

$$\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{m}\left(C_i - C_i^a\right)^2}{m}} \tag{22}$$

where C_i^a is the analytical solution at node i for a given total number of nodes m.

We further observe that for 2D, Eq.(21) assumes the form:

$$c_0 = e^{\hat{\alpha}_x x+i\alpha_{yI}y} \tag{23}$$

DOI: 10.5540/03.2017.005.01.0411

where α_{yI} is arbitrarily prescribed and:

$$\hat{\alpha}_x = -\frac{a_1}{2a_2} \pm \sqrt{\frac{a_{1x}^2}{4a_2^2} - \left(\frac{a_0 + a_{1y} i\alpha_{yI} - a_2\alpha_{yI}^2}{a_2}\right)} \tag{24}$$

4 Supplementary Remarks

In the absence of diffusion and reaction, $a_0 = a_2 = 0$. Considering that, with time periodic forcing at $x = 0$, the boundary condition does not decay in time, $\beta_R = 0$ and, therefore, Eqs.(6) and (7) reduce to:

$$\beta_R = \alpha_R = 0 \text{ and } \beta_I = a_1\alpha_I \tag{25}$$

and Eq.(8) reduces to the pure convection solution:

$$c = e^{i(\alpha_I x + a_1\alpha_I t)} \tag{26}$$

The phase velocity v is then obtained by considering the movement of a constant phase point:

$$\alpha_I x + a_1\alpha_I t = const. \tag{27}$$

thus:

$$\frac{\partial}{\partial t}\left(\alpha_I x + a_1\alpha_I t\right) = 0 \text{ and } v = \frac{dx}{dt} = -a_1 \tag{28}$$

the phase velocity v is, therefore, the same as the convection velocity u.

In the case of nonzero diffusion and reaction, the phase velocity is given by:

$$\alpha_I x + \beta_I t = const. \text{ and } v = \frac{dx}{dt} = -\frac{\beta_I}{\alpha_I} = -\left(a_1 + 2a_2\alpha_R\right) = u - 2D\alpha_R \tag{29}$$

Considering that α_R will be negative for a solution decaying in the x direction, and $a_2 = D$ will be positive, the phase velocity in the case of nonzero diffusion will be increased, representing the periodic concentration amplitude decrease due to larger spreading of the solute mass, to solute convective transport, or to higher solute consumption, depending on the case [1].

The frequency is:

$$f = 2\pi\omega = -2\pi\beta_I \tag{30}$$

and from Eqs.(28) and (29), we have that the wavelength of the travelling waves is:

$$\lambda = \frac{v}{f} = \frac{1}{2\pi\alpha_I} \tag{31}$$

It must also be highlighted that the periodicity of the solution not only depends on the input temporal frequency, but also on the physical parameters a_0 (reaction rate), a_1 (convection velocity) and a_2 (diffusion coefficient) [4], as pointed out by Eq.(4).

These remarks can easily be extended to 2D and 3D, following the same steps as above.

DOI: 10.5540/03.2017.005.01.0411

5 Conclusion

Analytical solutions for the 1D, 2D and 3D CDE with reaction term, subjected to time-periodic inlet boundary problem have been presented. These solutions are suitable to be used as benchmark for codes validation as illustrated by the applications to a 1D FD code and to a 2D FEM code.

Since the considered CDE is linear, these solutions can be combined to find solutions for any arbitrary time, y and z periodic boundary conditions and, as a consequence, for many cases of oscillatory behavior in the three considered dimensions, which do not seem to have yet appeared in the literature.

Acknowledgments

The authors wish to thank the Fundação de Amparo à Pesquisa do Rio de Janeiro (FAPERJ) for its support to this research under the program number E-26/111.079/2013.

References

[1] J. S. Chen and C. W. Liu, Generalized analytical solutions for advection-dispersion equation in finite spatial domain with arbitrary time-dependent inlet boundary condition. *Hydrol. Earth Syst. Sci.*, 15:2471-2479, 2011. DOI:10.5194/hess-15-2471-2011.

[2] W. J. Goltz and J. R. Dorroh, The convection-diffusion equation for a finite domain with time varying boundaries. *Appl. Math. Lett.*, 14:983-988, 2001. DOI:10.1016/S0893-9659(01)00076-3.

[3] J. D. Logan, Solute transport in porous media with scale-dependent dispersion and periodic boundary conditions. *J. Hydr.*,volume 184, 3:261-276, 1996. DOI: 10.1016/0022-1694(95)02976-1.

[4] J. D. Logan and V. Zlotnik, The convection-diffusion equation with periodic boundary conditions. *Appl. Math. Lett.*, volume 8, 3:55-61, 1995. DOI: 10.1016/0893-9659(95)00030-T.

[5] J. S. Pérez Guerrero, E. M. Pontedero, M. Th. van Genuchten and T. H. Skaggs, Analytical solutions of the one-dimensional advection-dispersion solute transport equation subject to time-dependent boundary conditions. *Chem. Eng. J.*, 221:487-491, 2013. DOI 10.1016/j.cej.2013.01.095.

[6] M. Th. van Genuchten and W. J. Alves. *Analytical solutions of the one-dimensional convective-dispersive solute transport equation.* US Department of Agriculture Technical Bulletin, number 1661, Washington, 1982.

[7] G. Ziskind, H. Shmueli and V. Gitis, An analytical solution of the convection-dispersion-reaction equation for a finite region with a pulse boundary condition. *Chem. Eng. J.*, 167:403-408, 2011. DOI: 10.1016/j.cej.2010.11.047.

