Spectral solution for the air stripping pollutants removal dynamic model with non linear steady state conditions

A. C. M. Castro[1], J. Matos[2], and A. Gavina[3]

[1] LEMA - Laboratório de Engenharia Matemática, ISEP, and CIGAR - Centro de Investigação em Geo-Ambiente e Recursos
`amc@isep.ipp.pt`

[2] LEMA, ISEP and CMUP - Centro de Matemática da Universidade do Porto
`jma@isep.ipp.pt`

[3] LEMA, Instituto Superior de Engenharia do Porto `alg@isep.ipp.pt`

Summary. This work deals with the numerical simulation of air stripping process for the pre-treatment of groundwater used in human consumption. The model established in steady state presents an exponential solution that is used, together with the Tau Method, to get a spectral approach of the solution of the system of partial differential equations associated to the model in transient state.

Key words: Tau Method; Partial Differential Equations; Air stripping; Volatile Organic Compounds.

1 Background

The air stripping process in packed columns is a physical process traditionally used in the groundwater volatile organic compounds (VOCs) removal[2, 3, 5, 8]. This operation, that is carried out without any chemical reaction, has as main characteristic the fact that operates with counter-current phases. Thus, through a pump group, the groundwater is caught from the soil to be introduced at the top of the column as drops, which constitutes a discontinuous phase, as far as the drops are able to flow through the packing material at the same time a compressor introduces, in counter-current from the base of the column, clean air as a continuous phase. In this air stripping operation, the packing material is used to to supply the area for contact between the gas and the liquid needed for the contaminant mass transfer. This type of technology operates under level values for pressure and temperature generally near the typical ones from the common environment, is ideal for pollutant concentration levels under $200 mg/l$ and offers a level of removal often higher than 90% [11, 17, 20, 26].

2 The Differential Model

Castro [4] presents a mathematical model that translates the space-time dynamics of the air stripping process in a packed column. In this model it is considered that exists only one space dimension, that the variation in time is limitless, that the mass transfer is based on the "Two Films Theory" [22, 21], that the air used in the VOCs removal is pure, that the flows are constant in all column. This model also considers that the system works under constant temperature and pressure values and in uniform conditions[6, 7].

Considering the following referential, see figure 1, in which the origin of the space is the base of the column, for the velocities u_L and u_G, corresponding VOC mass concentrations, x_{in} and y_{in}.

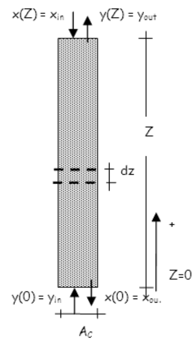

Fig. 1. The dynamic model referential

Considering that γ represents the volumetric relation of debits, K the global mass transfer coefficient, H the inverse of the dimensionless value for the Henry's constant for the VOC and ϵ the porosity of the packing material, the global dynamic system that translates the air stripping process is represented by the following system of equations [10, 1, 12, 15, 18, 27, 25]

$$\begin{cases} \frac{\epsilon}{1+\gamma}\frac{\partial x}{\partial t} + \frac{\epsilon\gamma}{1+\gamma}\frac{\partial y}{\partial t} = u_L\frac{\partial x}{\partial z} - u_G\frac{\partial y}{\partial z} \\ \frac{\epsilon}{1+\gamma}\frac{\partial x}{\partial t} = u_L\frac{\partial x}{\partial z} - K(x - Hy) \end{cases}, \ 0 < z < Z, \ t > 0 \quad (1)$$

2.1 The boundary conditions

In this model, the characterization of the dynamic state of the air stripping operation implies the consideration of Dirichlet boundary conditions that can be translated with the input data of the concentrations of the liquid and gaseous phases, at the column entrance, ie

$$\begin{cases} x(t, Z) = x_{in}(t) \\ y(t, 0) = 0 \end{cases}, \ t \geq 0 \quad (2)$$

This problem is exactly determined and can be solved when the values of the boundary conditions and the disturbances at the entrance are specified.

2.2 The steady state

The representation of the steady state can be achieved from the consideration, in the global model, that the time derivatives are all null, which implies that the VOC concentration gradients, in the gaseous phase and the liquid phase, can be given by

$$\begin{cases} \frac{\partial}{\partial z}x(0,z) = \frac{K}{u_L}\left[x(0,z) - Hy(0,z)\right] \\ \frac{\partial}{\partial z}y(0,z) = \frac{K}{u_G}\left[x(0,z) - Hy(0,z)\right] \end{cases}, \quad 0 < z < Z \tag{3}$$

The analytic solution for the steady state equations can be found deriving the first equation of (3) with respect to z

$$\frac{\partial^2}{\partial z^2}x(0,z) = \frac{K}{u_L}\left(\frac{\partial}{\partial z}x(0,z) - H\frac{\partial}{\partial z}y(0,z)\right) \tag{4}$$

and, since we know that $\frac{\partial}{\partial z}y(0,z) = \frac{u_L}{u_G}\frac{\partial}{\partial z}x(0,z)$, then the equation (4) can be written as a second-order linear homogeneous ordinary differential equation (ODE) with constant coefficients

$$\frac{\partial^2}{\partial z^2}x(0,z) - D\frac{\partial}{\partial z}x(0,z) = 0 \tag{5}$$

with $D = K\left(\frac{1}{u_L} - \frac{H}{u_G}\right) \neq 0$, in order to guarantee that the process occurs. The general solution for this equation is given by

$$x(0,z) = m_{11} + m_{12}e^{Dz} \tag{6}$$

In the same way, we have the general solution for $y(0,z)$

$$y(0,z) = m_{21} + m_{22}e^{Dz} \tag{7}$$

According to the boundary conditions, for $t = 0$, we have

$$\begin{cases} x(0,Z) = x_{in}(0) \\ y(0,0) = 0 \end{cases} \tag{8}$$

If we substitute (6) and (7) in (8) we have the solution for the system of differential equations in steady state

$$\begin{cases} x_S(z) \equiv x(0,z) = M(\frac{u_G}{u_L}e^{Dz} - H) \\ y_S(z) \equiv y(0,z) = M(e^{Dz} - 1) \end{cases}, \quad 0 < z < Z \tag{9}$$

with

$$M = X_0\left(\frac{u_G}{u_L}e^{DZ} - H\right)^{-1}$$

and $X_0 = x_{in}(0)$.

3 The transient state

Defining $A = \varepsilon/(1+\gamma)$, the equations (1) of the model in transient state can be written as

$$\begin{cases} A\frac{\partial x}{\partial t} = u_L \frac{\partial x}{\partial z} - K(x - Hy) \\ A\gamma \frac{\partial y}{\partial t} = -u_G \frac{\partial y}{\partial z} + K(x - Hy) \end{cases}, \tag{10}$$

with $x = x(t,z)$ and $y = y(t,z)$ for $0 < z < Z,\ t > 0$

In order to approximate the solution of (10), subject to initial conditions (2), the functions x and y can be represented by

$$\begin{cases} x(t,z) = t x_S(z) + x_T(t,z) \\ y(t,z) = t y_S(z) + y_T(t,z) \end{cases}, \tag{11}$$

where x_S and y_S are the solutions (9) for the steady state, and x_T and y_T are the initial solutions for the transient state. Replacing this expressions in (10) and using (3), we have for x_T and y_T the following differential equations

$$\begin{cases} A\frac{\partial x_T}{\partial t} - u_L \frac{\partial x_T}{\partial z} + K(x_T - Hy_T) = -A x_S \\ A\gamma \frac{\partial y_T}{\partial t} + u_G \frac{\partial y_T}{\partial z} - K(x_T - Hy_T) = -A\gamma y_S \end{cases}, \tag{12}$$

And, for the initial conditions,

$$\begin{cases} x_T(t,Z) = x_{in}(t) - tX_0 \\ y_T(t,0) = 0 \end{cases} \tag{13}$$

This representation allows to approach the solution for the system of differential equations, maintaining the exact form of the solutions for the steady state and reducing the error to the initial solutions of the transient state.

4 The Lanczos's Tau Method

Given the differential problem

$$\begin{cases} Dy = f \\ D_j y = f_j,\ j = 1:\nu \end{cases} \tag{14}$$

where D represents a linear differential operator with polynomial coefficients, f and f_j are polynomials and D_j represents the ν initial or boundary conditions associated to the problem, the Tau method [13, 14] can be formulated by solving the perturbed problem

$$\begin{cases} Dy_n = f + \tau_n \\ D_j y_n = f_j,\ j = 1:\nu \end{cases}$$

where τ_n is a perturbation term that allows the perturbed differential problem to have a unique polynomial solution y_n.

Following the implementation of the Tau method proposed in Matos *et al.*[16], based in Ortiz's operational approach [19] and in the formulation of the Tau method presented in [23, 24] we begin by chose m and n the degrees of the polynomial

$$\begin{cases} x_{m,n}(t,z) = \sum_{i,j=0}^{m,n} x_{i,j} t^i z^j \\ y_{m,n}(t,z) = \sum_{i,j=0}^{m,n} y_{i,j} t^i z^j \end{cases} \tag{15}$$

and we proceed by determining the coefficients $x_{i,j}$ and $y_{i,j}$ imposing that $x_{m,n}(t,z)$ and $y_{m,n}(t,z)$ satisfies the initial and the boundary conditions of the problem and satisfies the perturbed differential equation.

4.1 Initial conditions and differential equations

In the case of the initial conditions (13), with

$$x_{in}(t) = \sum_{i=0}^{m} X_i t^i$$

being a, at least approximated, polynomial representation of the liquid phase initial VOC concentration, in the top of the column $x_{in}(t) = x(t, Z)$ then

$$\begin{cases} \sum_{j=0}^{n} x_{0,j} Z^j = X_0, \\ \sum_{j=0}^{n} x_{1,j} Z^j = X_1 - X_0, \\ \sum_{j=0}^{n} x_{i,j} Z^j = X_i, \ i = 2:m \end{cases}$$

The initial condition for the gas phase initial VOC concentration, in the bottom of the column, is given by $y_{m,n}(t,0) = 0$. Then, we get

$$y_{i,0} = 0, \ i = 0:m$$

The determination of the $2(m+1)(n+1)$ unknowns $x_{i,j}$ e $y_{i,j}$ needs more $2(m+1)n$ equations that come from the differential equations imposed to $x_{m,n}$ and to $y_{m,n}$ as far as possible[23, 24], in the sense of the respective polynomial degrees.

In that case, the non polynomial character of the right hand side of the differential equations, introduced by the exponential solution of the steady state problem, introduces another approximation problem. To have a polynomial approximation of the steady state problem solution, we proceed by use the Taylor approximation of the exponential function

$$e^{Dz} \approx \sum_{j=0}^{n} \frac{D^j}{j!} z^j$$

to get

$$\begin{cases} x_S(z) \approx M(\frac{u_G}{u_L} - H) + M \frac{u_G}{u_L} \sum_{j=1}^{n} \frac{D^j}{j!} z^j \\ y_S(z) \approx M \sum_{j=1}^{n} \frac{D^j}{j!} z^j \end{cases}$$

Differentiating (15) we get

$$\begin{cases} \frac{\partial}{\partial t} x_{m,n}(t,z) = \sum_{i=0}^{m-1} \sum_{j=0}^{n} (i+1) x_{i+1,j} t^i z^j \\ \frac{\partial}{\partial z} x_{m,n}(t,z) = \sum_{i=0}^{m} \sum_{j=0}^{n-1} (j+1) x_{i,j+1} t^i z^j \end{cases} \tag{16}$$

for the partial derivatives of the polynomial $x_{m,n}(t,z)$ and analog expressions for the partial derivatives of $y_{m,n}(t,z)$. Introducing those formulas in equations (12) we get

$$A \sum_{i=0}^{m-1} \sum_{j=0}^{n} (i+1) x_{i+1,j} t^i z^j - u_L \sum_{i=0}^{m} \sum_{j=0}^{n-1} (j+1) x_{i,j+1} t^i z^j$$

$$+K \sum_{i=0}^{m} \sum_{j=0}^{n} (x_{i,j} - H y_{i,j}) t^i z^j = -AM \left(-H + \frac{u_G}{u_L} \sum_{j=0}^{n} \frac{D^j}{j!} z^j \right)$$

and

$$A\gamma \sum_{i=0}^{m-1} \sum_{j=0}^{n} (i+1) y_{i+1,j} t^i z^j + u_G \sum_{i=0}^{m} \sum_{j=0}^{n-1} (j+1) y_{i,j+1} t^i z^j$$

$$-K \sum_{i=0}^{m} \sum_{j=0}^{n} (x_{i,j} - H y_{i,j}) t^i z^j = -A\gamma M \sum_{j=1}^{n} \frac{D^j}{j!} z^j$$

and, identifying term by term the corresponding coefficients, this results in a algebraic over-determinated system of $2(m+1)(n+1)$ linear equations.

4.2 Algebraic equations

By applying the Tau method we choose suitable[9, 16] $2(m+1)n$ equations defining a regular linear system of algebraic equations whose unique solution $x_{i,j}$ and $x_{i,j}$ give us the polynomial approximation of the exact solution.

With $x_{in}(t) = X_0$ constant, the solution $x(t,z)$ and $y(t,z)$ of the problem coincides with $x(0,z)$ e $y(0,z)$, the solution of the steady state (9).

For the more general situation where $x_{in}(t)$ depends on t, we have supposed that $x_{in}(t) = \sum_{i=0}^{m} X_i t^i$ at least by approximation. That is, if the function $x_{in}(t)$ is not a $\leq m$ degree polynomial, it is replaced by a polynomial approximation.

In the following test we consider a periodic function for $x_{in}(t)$. In the case, we made

$$x_{in}(t) = 100(1 + \sin(t)/5) = 100(1 + \frac{1}{5} \sum_{i \geq 0} \frac{(-1)^i}{(2i+1)!} t^{2i+1})$$

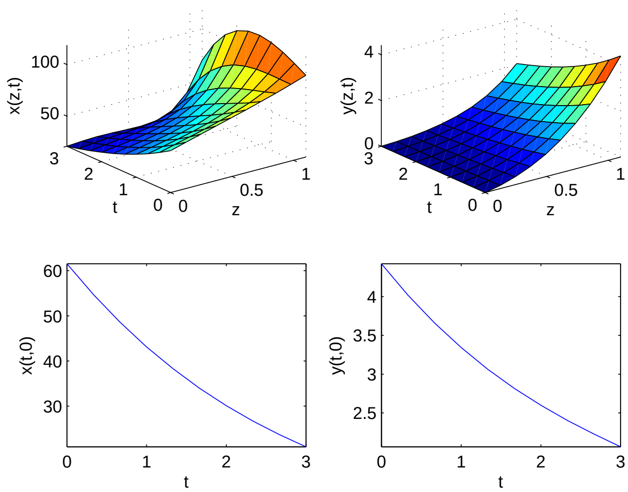

Fig. 2. Variation of the contaminant concentration in the water $x(t, z)$ and in the air $y(t, z)$ with $m = n = 3$

5 Conclusions and future work

The Tau method was tested for several polynomial degrees and for the case study presented in[4].

The numerical results that were found revealed to be coherent with the experimentally achieved data [4], which suggests that the model is consistent under a numerical, physical and mathematical approach and that the use of the Tau method allows an approach, with reasonable precision, to the exact solution of the model.

As the numerical results achieved show some increasing instability with the time, it can be suggested that the use of orthogonal polynomials will be able to allow the increment of the precision of the results in an larger time interval.

References

1. W. Ball and M.C. Kavanaugh. Mass transfer of volatile organic compounds in packed tower aeration. *Journal WPCF*, 56 (2):127–136, 1984.
2. E. Bouwer and M.C. Kavanaugh. Coping with groundwater contamination. *Journal WPCF*, 60 (8):1415–1427, 1988.
3. A . O. Bradley. Remove vocs from wastewater by air stripping. *Chemical Engineering Progress*, 60:89–93, 1992.
4. A. C. M. Castro. *Projecto e simulação dinâmica utilizando um sistema de parâmetros distribuidos*. PhD thesis, Faculdade de Engenharia da Universidade do Porto, Portugal, 2004.

5. W.V. Chang. Stripping of tce from water at low air/water ratios. *Environmental progress*, 14 (2):111–114, 1995.
6. I. A. Furzer. Liquid dispersion in packed columns i. *Chemical Engineering Science*, 39:70–76, 1984.
7. I. A. Furzer. Liquid dispersion in packed columns ii. *Chemical Engineering Science*, 39:77–80, 1984.
8. D. Hand. Design and evaluation of an air stripping tower for removing vocs from groundwater. *Journal AWWA*, pages 87–97, 1986.
9. M. Hosseini Ali Abadi and E.L. Ortiz. Numerical treatment of moving and free boundary value problems with the tau method. *Computers and Mathematics with Applications*, 35 (8):53–61, 1998.
10. E. James and W. Byers. Limitations and practical use of mass transfer model for predicting air stripper performance. *Environmental Progress*, 12 (1):61–66, 1993.
11. J. G. Kunesh. Recent developments in packed columns. *The Canadian Journal of Chemical Engineering*, 65:907–913, 1987.
12. P. Lamarche and R. Droste. Air stripping mass transfer correlations for volatile organics. *Journal AWWA*, pages 78–89, 1989.
13. C. Lanczos. Trigonometric interpolation of empirical and analytical functions. *J. Maths Phys*, 17:123–199, 1938.
14. C. Lanczos. *Applied Analysis*. Pitman, London, 1957.
15. M. Leva. Reconsider packed-tower pressure-drop correlations. *Chemical Engineering Progress*, January:65–72, 1992.
16. J. Matos, M. J. Rodrigues, and P. B. Vasconcelos. New implementation of the tau method for pdes. *J. Comput. Appl. Math.*, 164-165:555–567, 2004.
17. A. Mersmann and A. Deixler. Packed columns. *German Chemical Engineering*, pages 265–276, 1986.
18. K. Onda. Mass transfer coefficients between gas and liquid phases in packed columns. *Journal of Chemical Engineering of Japan*, 1:56–62, 1968.
19. E. L. Ortiz. The tau method. *SIAM J. Numer. Anal. Optim.*, 12:480–492, 1969.
20. R. W. Rousseau. Analyzing chemical absorbers and strippers. *The Chemical Engineering*, June:91–95, 1985.
21. J. L. Schnoor. *Environmental modelling - fate and transport of pollutants in water, air and soil*. John Wiley & Sons, INC., 1996.
22. J. D. Seader and E. J. Henley. *Separation process principles*. John Wiley & Sons, Inc., 1998.
23. M. R. Silva. Numerical treatment of differential equations with the tau method. *J. Comput. Appl. Math.*, 20:167–173, 1987.
24. M. R. Silva and M. J. Rodrigues. A simple alternative principle for rational τ-method approximation. In A. Cuyt, editor, *Nonlinear Numerical Methods and Rational Approximation*, pages 427–434. Reidel, Dordrecht, 1988.
25. V. Stanek. Transients of the hydrodynamics of counter-current packed-bed columns. *Chemical Engineering Science*, 45 (2):449–455, 1990.
26. W. Yang. Removal of trihalomethanes from water by air stripping. *Water Treatment*, June:267–282, 1991.
27. C. Yaws. Henrys law constants for organic compounds in water. *Chemical Engineering*, November:179–185, 1991.