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Application of Fractional Calculus in Mechanics : Contaminant Diffusion Problem with Two Different Layers

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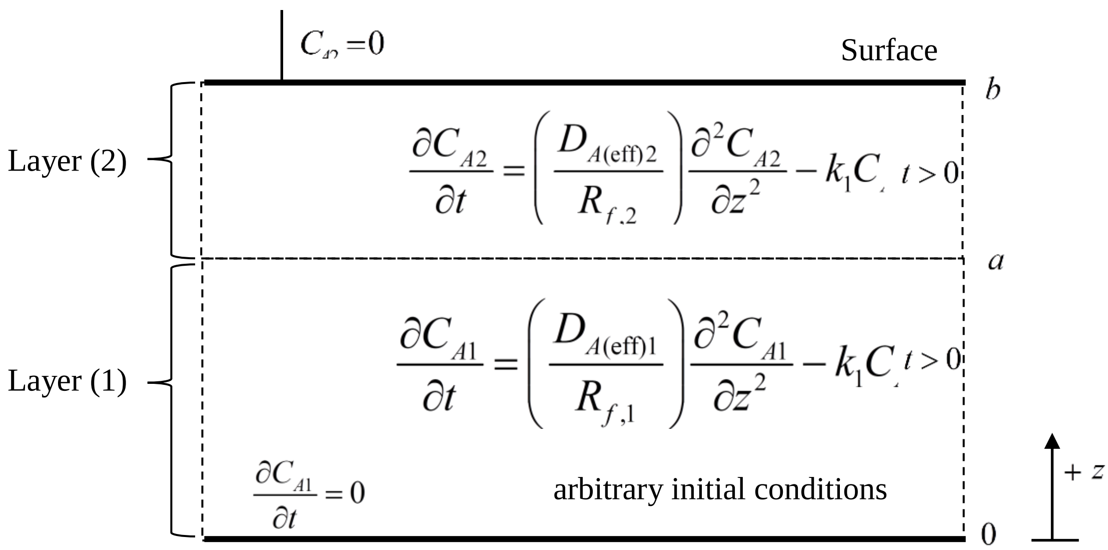
Abstract : *This work proposes an approximate solution of a system of differential equations governing contaminant transport in a porous medium by fractional integration. This methodology is described by transforming the classical diffusion equation into a fractional differential equation. In this case, four parameters appear, two of which are for each equation. For the first equation, , α_1 and β_1 and the second α_2 and β_2 such that*
$0 < \alpha_1 \leq 1$, $1 < 2\beta_1 \leq 2$, $0 < \alpha_2 \leq 1$ *and* $1 < 2\beta_2 \leq 2$. *We searched for the parameter values α_1 and α_2 by setting $\beta_1 = 1$ and $\beta_2 = 1$. The comparison of the results obtained by the numerical method with those of the analytical solution is finally presented and analyzed.*

I. Introduction

Nowadays, the fractional approach appears. The works on fractional approaches are very vast and concern many different fields, in particular porous medium. The motivation of this work is the transport of contaminant in porous medium with two layers of different characteristics. The general diffusion equation of contaminant transport in each layer is known under the formulas of equations (1) and (2) [1] :



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Where :

$C_{Ai}(z,t)$: Mobile phase species *Ai* concentration at altitude z and at time *t*;

$D_{A(eff)i}$: effective diffusion coefficient of species *A*

$R_{f,i}$: Retardation factor

k_1 : first-order reaction rate constant

Initial conditions :
$C_{A1}(z,t=0) = C_{A0}(z),\ \ C_{A2}(z,t=0) = C_{A0}(z)$

Boundary conditions

$\left.\frac{\partial CA1}{\partial z}\right|_{z=0}$=0, $C_{A1}(z,t)|_{z=a}$=$C_{A2}(z,t)|_{z=a}$, $C_{A2}(z,t)|_{z=b}$=0

$$D_{A(eff)1}\left.\frac{\partial CA1}{\partial z}\right|_{z=a} = D_{A(eff)2}\left.\frac{\partial CA2}{\partial z}\right|_{z=a}$$

To find the analytical solutions of equations (1) and (2), there are several methods: either the separation of variables method, or the Laplace transform, etc.

For a=0.070 m, b=0.100 m, $k_1 = 10^{-5}s^{-1}, D_{A(eff)1} = 10^{-7}m^2/s, D_{A(eff)2} = 5X10^{-7}m^2/s,\ R_{f,1} = 1000$ and $R_{f,2} = 600$ [1]

Here is the analytical curve obtained, see figure 1

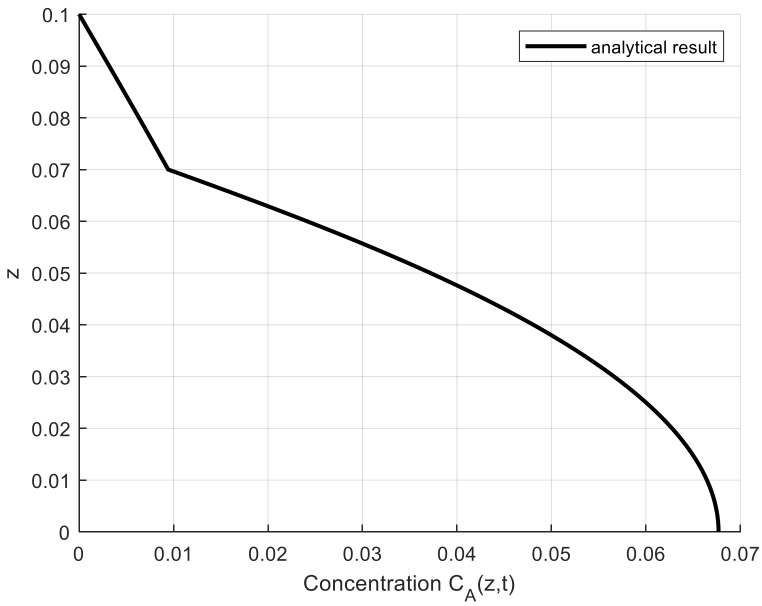
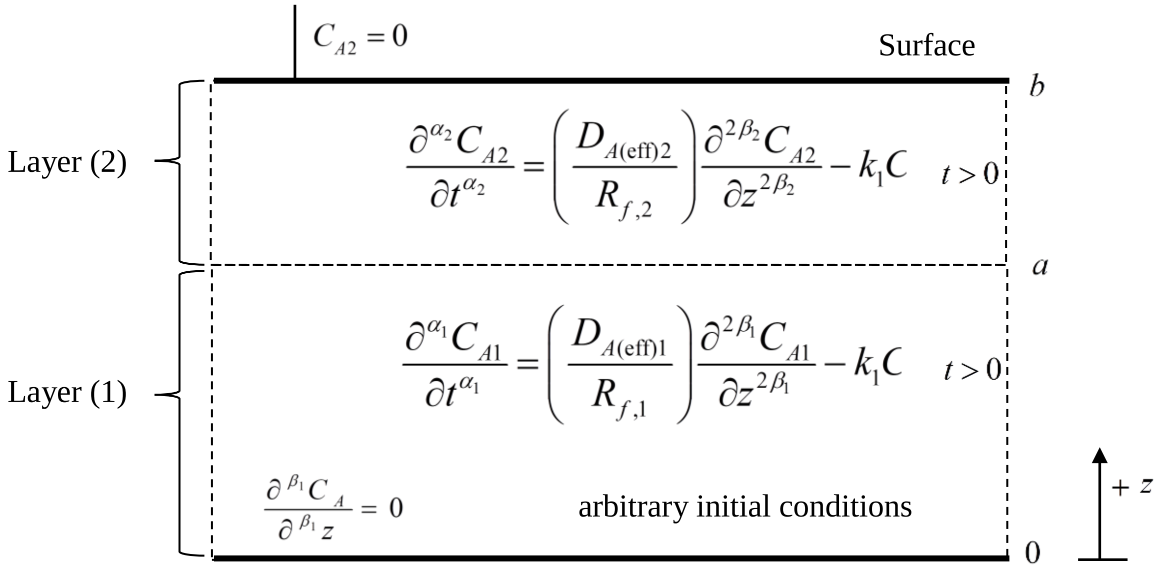


Figure 1: Analytical curve obtained



If we write equations (1) and (2) in fractional differential equations [2] we have :

Where $0 < \alpha_1 \leq 1$, $1 < 2\beta_1 \leq 2$, $0 < \alpha_2 \leq 1$ and $1 < 2\beta_2 \leq 2$

Both α_1 and α_2 are called the exponents of the anomalous scattering. They are used to characterize the type of scattering. The β_1 and β_2 are the stability coefficients.

If $0 < \alpha_i < 1$, we have under-diffusion and $\alpha_i > 1$ a super-diffusion.

The objective of this work is to determine the parameters $\alpha_{1,}\ \alpha_2$ of equations (3) and (4) using the Laplace transform of the fractional derivative for $\beta_1 = 1$ and $\beta_2 = 1$. Finally, comparing the results obtained with the analytical solutions of equations (1) and (2)

II. Methodology

1.1 Calculate of α_2

Take equation (3) for $\beta_2 = 1$, i.e., the second fractional layer equation, we have the following differential equation :

$$\frac{\partial^{\alpha_2} C_{A2}}{\partial t^{\alpha_2}} = \left(\frac{D_{A(\text{eff})}}{R_{f,2}}\right)\frac{\partial^2 C_{A2}}{\partial z^2} - k_1 C_{A2} \qquad (5)$$

For the fractional time derivative, we use the Laplace transform of the fractional time derivative in the

Riemann-Liouville sense :

$$L_p\left(\frac{\partial^{\alpha_2} C_{A2}(z,t)}{\partial t^{\alpha_2}}\right) = p^{\alpha_2} C_{A2}(z,p) - \sum_{k=0}^{n-1} p^k \left[D^{\alpha_2-k-1} C_{A2}(z,t=0)\right] \quad [3,4] \qquad (6)$$

Since $0 < \alpha_2 \leq 1$, we therefore have $n = 1$. The initial condition $C_{A2}(z,t=0) = C_{Ao}$ is a constant regardless of the value of z.

For Riemann-Liouville, the derivative of order α of a constant number is not zero [3,4].

$D^{\alpha_2}C_{Ao}=\frac{C_{Ao}}{\Gamma(1-\alpha_2)}t^{-\alpha_2}$ then we have : $D^{\alpha_2-1}C_{Ao}=\frac{C_{Ao}}{\Gamma(2-\alpha_2)}t^{1-\alpha_2}$ (7)

Where $\Gamma(1-\alpha_2)$ is the gamma of $(1-\alpha_2)$.

We obtain the following relationship:

$$L_p\left(\frac{\partial^{\alpha_2}C_{A2}(z,t)}{\partial t^{\alpha_2}}\right)=p^{\alpha_2}C_{A2}(z,p)-\frac{C_{Ao}}{\Gamma(2-\alpha_2)}t^{1-\alpha_2} \quad (8)$$

For the second member, of the equation

$$L_p\left(\frac{D_{A(eff)2}}{R_{f,2}}\frac{\partial^2 C_{A2}}{\partial z^2}-k_1C_{A2}\right)=\frac{D_{A(eff)2}}{R_{f,2}}\frac{d^2}{z^2}C_{A2}(z,p)-C_{A2}(z,p) \quad (9)$$

Since (8) and (9) are equal, we obtain a new fractional differential equation :

$$\frac{D_{A(eff)2}}{R_{f,2}}\frac{d^2}{z^2}C_{A2}(z,p)-k_1C_{A2}(z,p) = p^{\alpha_2}C_{A2}(z,p)-\frac{C_{Ao}}{\Gamma(2-\alpha_2)}t^{1-\alpha_2}. \quad (10)$$

Equation (10) can be written as :

$$\frac{D_{A(eff)2}}{R_{f,2}}\frac{d^2}{z^2}C_{A2}(z,p)-(k_1+p^{\alpha_2})C_{A2}(z,p) = -\frac{C_{Ao}}{\Gamma(2-\alpha_2)}t^{1-\alpha_2}. \quad (11)$$

(11) is a second order differential equation whose unknown is $C_{A2}(z,p)$.

Solving equation (11) and taking into account the condition for $z=b$, $C_{A2}(z=b,t)=0$, and posing $a_2=\frac{D_{A(eff)2}}{R_{f,2}}$, the solution of equation (11) is :

$$C_{A2}(z,p)=A(p)exp\left(-\sqrt{\frac{k_1+P^{\alpha_2}}{a_2}}\ z\right)+B(p)exp\left(\sqrt{\frac{k_1+P^{\alpha_2}}{a_2}}\ z\right)+\frac{C_{Ao}}{(k_1+P^{\alpha_2})\Gamma(2-\alpha_2)}t^{1-\alpha_2} \quad (12)$$

Now we will look for the expressions of $A(p)$ and $B(p)$.

$C_{A2}(z,p)=\int_0^{+\infty}C_{A2}(z,t)e^{-pt}\,dt$ and if $z=b$, we have: $C_{A2}(b,t)=0$.

$$A(p)exp\left(-\sqrt{\frac{k_1+P^{\alpha_2}}{a_2}}\ b\right)+B(p)exp\left(\sqrt{\frac{k_1+P^{\alpha_2}}{a_2}}\ b\right)+\frac{C_{Ao}}{(k_1+P^{\alpha_2})\Gamma(2-\alpha_2)}t^{1-\alpha_2}=0 \quad (13)$$

Moreover, if we calculate $\lim_{z\to\infty}C_{A2}(z,t)$ to make physical sense, necessarily we have $B(p)=0$, so we can determine $A(p)$:

$$A(p)=-\frac{C_{Ao}}{(k_1+P^{\alpha_2})\Gamma(2-\alpha_2)}t^{1-\alpha_2}\ exp\left(\sqrt{\frac{k_1+P^{\alpha_2}}{a_2}}\ b\right) \quad (14)$$

Finally, we obtain the fractional Laplace transform :

$$C_{A2}(z,p)=\frac{C_{Ao}\,t^{1-\alpha_2}}{(k_1+P^{\alpha_2})\Gamma(2-\alpha_2)}\left[1-exp\left(\sqrt{\frac{k_1+P^{\alpha_2}}{a_2}}\ (b-z)\right)\right] \quad (15)$$

For $\alpha_2\neq 1$, β_2=1, we will use the numerical method of Harald Stehfest published in 1970 [6,7] because there is a big problem to get the fractional analytical solution.

Let $F(p)$ be the Laplace transform of the function $f(t)$. The inverse transform of $F(p)$ is defined by :

$$f(t)=\frac{\ln(2)}{t}\sum_{j=1}^{N}V_j\,F\left(\frac{j\ln(2)}{t}\right) \quad (16)$$

For $N = 20$, (double precision) the values of V_j are presented in the following table.

Table 1: Successive values of V_j for 1≤ $j \leq 20$

j	V_j	j	V_j
1	-5.511463844797178*10^-6	11	-2.870209211471027*10^11
2	1.523864638447922*10^-1	12	6.829920102815115*10^11
3	-1.174654761904762*10^2	13	-1.2190823300543374*10^12
4	1.734244933862434*10^4	14	1.637573800842013*10^12
5	-9.228069289021164*10^5	15	-1.647177486836117*10^12
6	2.377408778710318*10^7	16	1.221924554444226*10^12
7	-3.494211661953704*10^8	17	-6.488065588175326*10^11
8	3.241369852231879*10^9	18	2.333166532137059*10^11
9	-2.027694830723779*10^10	19	-5.091380070546738*10^10
10	8.946482982379724*10^10	20	5. 091380070546738*10^9

Using the method of Harald Stehfest, we obtained the fractional analytical solution :

$$C_{A2}(z,t) = \frac{\ln(2)}{t} \sum_{j=1}^{N} V_j \, C_{A2}\left(z, \frac{j\ln(2)}{t}\right) \quad (17)$$

$$C_{A2}\left(z, \frac{j\ln(2)}{t}\right) = \frac{C_{Ao}\, t^{1-\alpha_2}}{\left(k_1 + \left(\frac{j\ln(2)}{t}\right)^{\alpha_2}\right)\Gamma(2-\alpha_2)} \left[1 - exp\left(\sqrt{\frac{k_1 + \left(\frac{j\ln(2)}{t}\right)^{\alpha_2}}{\alpha_2}}\ (b-z)\right)\right] \quad (18)$$

$$C_{A2}(z,t) = \sum_{j=1}^{N} \ln(2)\, V_j \frac{C_{Ao}\, t^{-\alpha_2}}{\left(k_1 + \left(\frac{j\ln(2)}{t}\right)^{\alpha_2}\right)\Gamma(2-\alpha_2)} \left[1 - exp\left(\sqrt{\frac{k_1 + \left(\frac{j\ln(2)}{t}\right)^{\alpha_2}}{\alpha_2}}\ (b-z)\right)\right] \quad (19)$$

Equation (19) is a fractional analytical solution because it is a function of α_2 and gamma.

Known $C_{A2}(z,t) = 0$ for $z \geq b$, so for z tends to $+\infty$, $C_{A2}(z,t) = 0$ means that

$$\sum_{j=1}^{N} \ln(2)\, V_j \frac{C_{Ao}\, t^{-\alpha_2}}{\left(k_1 + \left(\frac{j\ln(2)}{t}\right)^{\alpha_2}\right)\Gamma(2-\alpha_2)} = 0 \quad (20)$$

Knowing that the $C_{Ao}t^{-\alpha_2}$, $\ln(2)$ and $\Gamma(2-\alpha_2)$ are independent of j, so we can take them out of the sum and we have equation (21)

$$\sum_{j=1}^{N} \frac{V_j}{\left(k_1 + \left(\frac{j\ln(2)}{t}\right)^{\alpha_2}\right)} = 0 \quad (21)$$

Since $k_1 + \left(\frac{j\ln(2)}{t}\right)^{\alpha_2} = k_1\left(1 + \frac{1}{k_1}\left(\frac{j\ln(2)}{t}\right)^{\alpha_2}\right)$, equation (21) can be written as

$$\sum_{j=1}^{N} \frac{V_j}{\left(1 + \frac{1}{k_1}\left(\frac{j\ln(2)}{t}\right)^{\alpha_2}\right)} = 0 \ \text{ with } k_1 \text{ not zero} \quad (22)$$

When t is large enough, $\left(\frac{j\ln(2)}{t}\right)^{\alpha_2}$ is close to zero, we can do a limited expansion of order 1 in the neighborhood of zero, so we have :

$$\frac{1}{1+\frac{1}{k_1}\left(\frac{jln(2)}{t}\right)^{\alpha_2}} \approx 1-\frac{1}{k_1}\left(\frac{jln(2)}{t}\right)^{\alpha_2} \quad (23)$$

Equation (22) becomes :

$$\sum_{j=1}^{N} V_j - \sum_{j=1}^{N} V_j \frac{1}{k_1}\left(\frac{jln(2)}{t}\right)^{\alpha_2} = 0 \quad (24)$$

Equation (24) is an equation for finding the value of the parameter α_2 for fixed t.

III. Results and discussions

Let's put $f(\alpha) = \sum_{j=1}^{N} V_j - \sum_{j=1}^{N} V_j \frac{1}{k_1}\left(\frac{jln(2)}{t}\right)^{\alpha}$, we will plot the curve of the function $f(\alpha)$ for $\alpha \in]0,1]$ to find the real α_2

3.1 Calculate of α_2 for $\beta_2 = 1$

We can find some approximate solutions, in particular $\alpha = 0.60$ shown in Figure 2

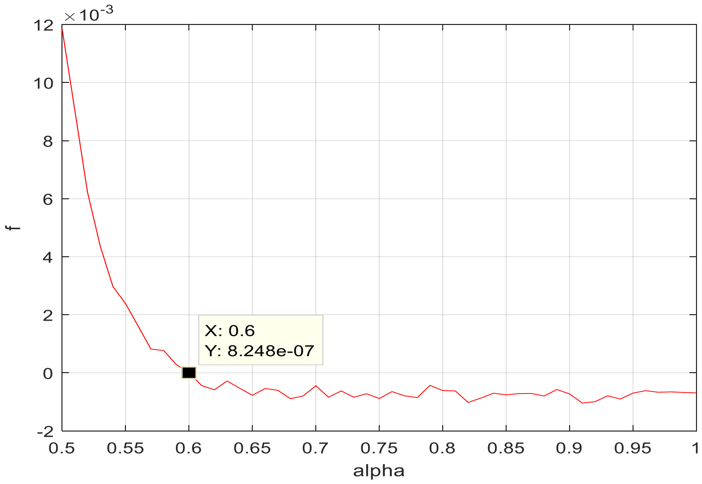


Figure 2

α	0.59	0.60	0.61
$f(\alpha)$	0.0002831	0.0000008248	-0.0004398

After solving graphically the equation $(\alpha) = 0$, we find the value of $\alpha_2 = 0.60$.

3.2 Finding the value of the parameter α_1

Consider equation (4) for $\beta_1 = 1$, i.e. the equation for the first layer :

$$\frac{\partial^{\alpha_1} C_{A1}}{\partial t^{\alpha_1}} = \left(\frac{D_{A(\text{eff})1}}{R_{f,1}}\right)\frac{\partial^2 C_{A1}}{\partial z^2} - k_1 C_{A1} \quad (25)$$

The objective is to calculate the parameter α_1 knowing $\alpha_2 = 0.60$

Given the conditions $C_{A1}(z,t)|_{z=a} = C_{A2}(z,t)|_{z=a}$ and $C_{A2}(z,t=0) = C_{A1}(z,t=0) = C_{A0}(z)$, we can conclude that : $\alpha_1 = \alpha_2$.
We will plot the curve obtained by fractional calculation for $\alpha_1 = \alpha_2 = 0.60$
And $\beta_1 = \beta_2 = 1$ (see the following figure).

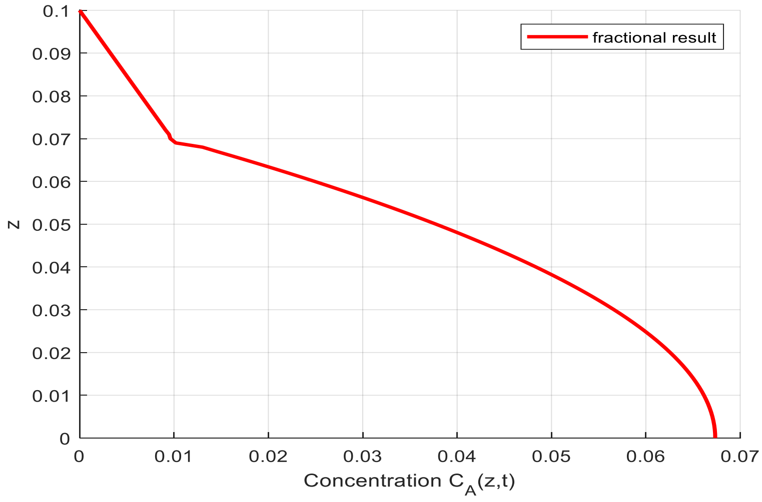


Figure 3 : curve obtained numerically by the fractional model.

IV. Comparison of the two analytical and numerical curves obtained

The following data is used:

a=0.07, b=0.1, $k_1 = 10^{-5}$, $D_{A(eff)1} = 10^{-7}$, $D_{A(eff)2} = 5 \times 10^{-7}$, $R_{f,1} = 1000$ and $R_{f,2} = 600$ [1]

1.2 For $\alpha_1 = \alpha_2 = 0.6$ and $\beta_1 = \beta_2 = 1$

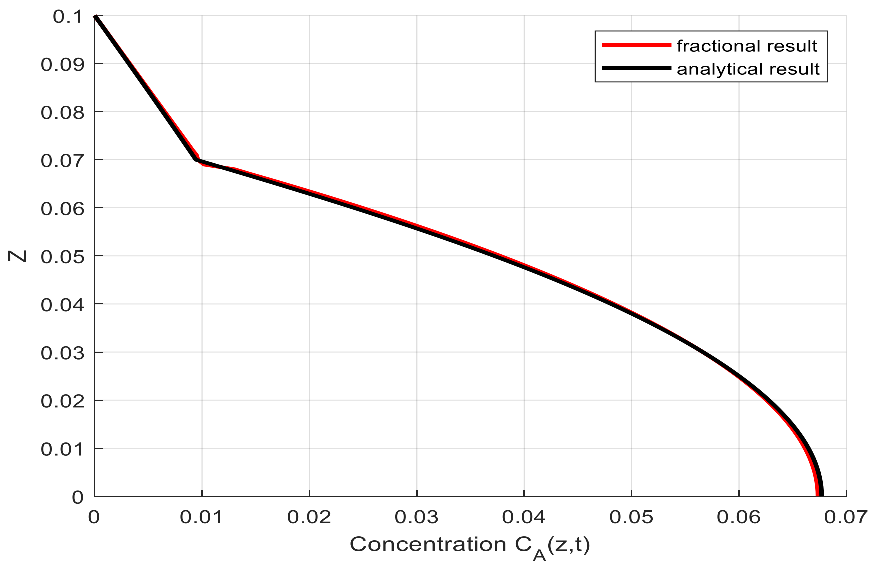


Figure 4 : *Comparison of the variation obtained analytically and that obtained numerically for* $\alpha_1 = \alpha_2 = 0.6$ *and* $\beta_1 = \beta_2 = 1$

Both curves represent the diffusion of contaminant in a medium with two layers of different characteristics. The black curve is found by the analytical resolution and the red curve by the numerical resolution. We notice that the two curves overlap, with a maximum error equal to 7.64e-04.

4.2 For $\alpha_1 = \alpha_2 = 0.59 < 0.6$,

Both curves have the same shape. But if si $\alpha_1 = \alpha_2 < 0.6$; the values of the concentrations found by the analytical method are higher than those of numerical.

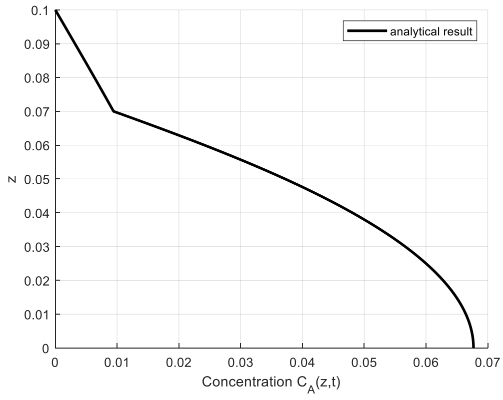


Figure 5-a : Result by analytical method

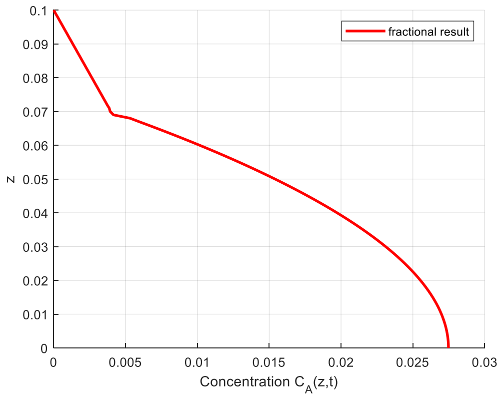


Figure 5-b: Result by fractional method

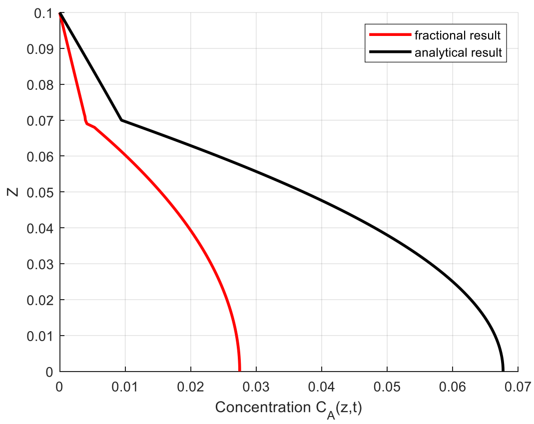
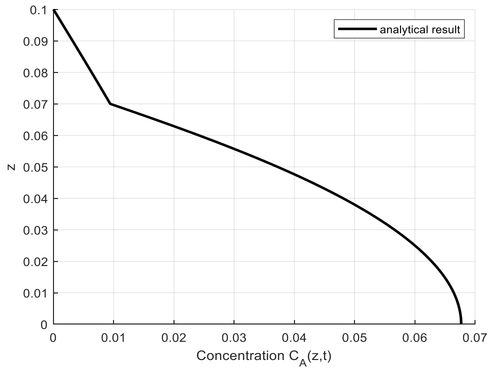


Figure 5-c : Comparison of analytical and fractional methods $\alpha_1 = \alpha_2 < 0.6$

4.3 For $\alpha_1 = \alpha_2 = 0.61 > 0.6$,

Both curves have the same shape. But if $\alpha_1 = \alpha_2 > 0.6$; the values of concentrations found by the numerical method are higher than those of analytical :



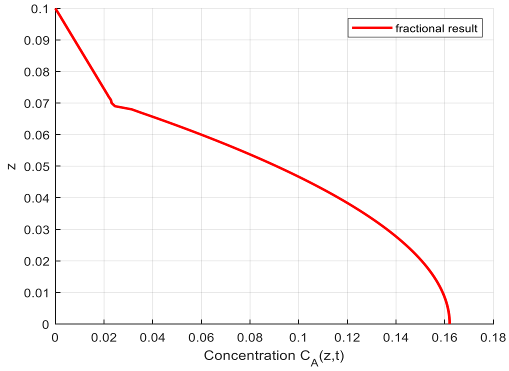


Figure 6-a : Result by analytical method

Figure 6-b: Result by fractional method

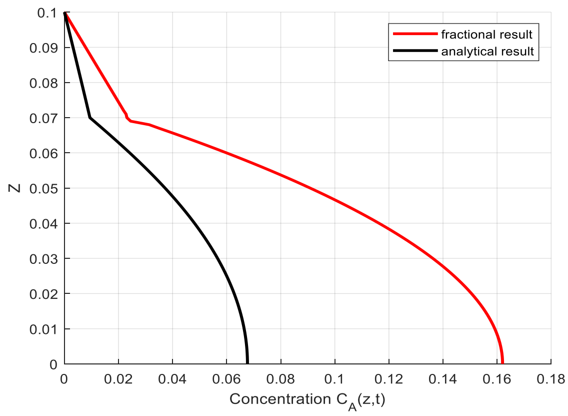


Figure 6-c : Comparison of analytical and fractional methods $\alpha_1 = \alpha_2 > 0.6$

V. Case where $\alpha_1 \neq \alpha_2$

Take for example $\alpha_1 = 0.59 \ and \ \alpha_2 = 0.61$

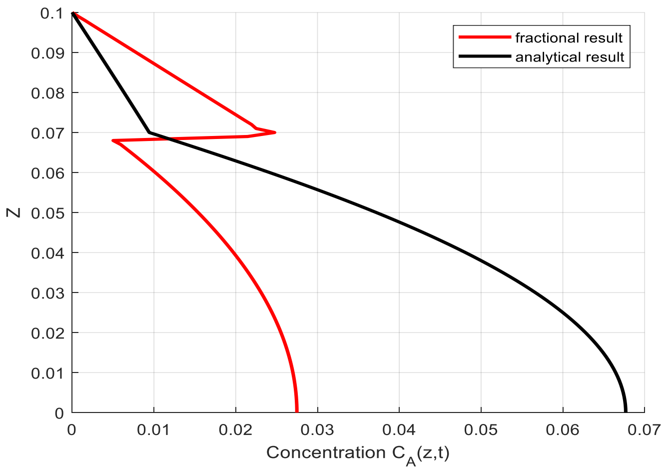


Figure 7 : Comparison of analytical and fractional methods for $0.59 = \alpha_1 \neq \alpha_2 = 0.61$

For figure 7 $\alpha_1 \neq \alpha_2$, this is impossible because according to the assumption, we should have : $C_{A1}(z,t)|_{z=a=0.07}$=$C_{A2}(z,t)|_{z=a=0.07}$ and $C_{A2}(z,t=0) = C_{A1}(z,t=0) = C_{A0}(z)$. We notice that at the point a=0.07, the difference of the two curves is obvious. Hence $\alpha_1 = \alpha_2$

VI. Conclusion

This paper has focused on the numerical solution of the contaminant diffusion equation in a medium with two layers of different characteristics using fractional approaches. In these approaches, we used the Grunwald - Letnikov scheme for the fractional time derivative. We used the results of the method of Harald Stehfest. The obtained results showed that for $\alpha_1 = \alpha_2 = 0.6$ and $\beta_1 = \beta_2 = 1$, the solution approximated by the fractional model is very close to the analytical solution. In perspective, we can consider the numerical solution of contaminant diffusion in a medium with three layers of different characteristics using the fractional approaches.

VII. Reference

1. Bruce Choy Danny D.Reibble « *Diffusion Models of Enviromental transport* », LEWIS PUBLISHERS, Boca Raton London New York Washington, D.C, 2000
2. M. GARG and P. MANOHAR, "*Analytical solution of Space-time fractional Fokker Planck Equation by Generalized differential transform Method*" Le MATEMATICHE,17(2011)91-101.
3. S. H. RAKOTONASY, « *Modèle fractionnaire pour la sous-diffusion : version stochastique* » Thèse de doctorat, Université d'Avignon et des Pays de Vaucluse, (2012).
4. A. MOHAMED-SALAH, « *Les systèmes Chaotiques à dérivées fractionnaire* », Mémoire de maitrise, Université Mentour-Constantine, Algérie, (2009).
5. A. OGATA. and R.B. BANKS, "*A Solution of the Differential Equation of Longitudinal Dispersion in porous medium*", US Geological Survey Professional Papers, (34) (1961), A1-A7.
6. H. STEHFEST « *Algorithm 368: Numerical inversion of Laplace transform*", Communications of the ACM-CACM,13(1) (1970)47-49.
7. Y. JANNOT, « *Transferts Thermique* », Supports de cours $\mathbf{2}^{\text{è}\boldsymbol{me}}$ année, Ecole de mine Nancy, (2012).
8. E. M. Lamy « Ecoulement *et transfert colloïdal dans des matrices hétérogènes stratifiées : Application à des milieux poreux modèles* ' Thèse de doctorat, Université centrale de Nantes (2008).
9. J. LIOUVILLE « *Intégration des équations différentielle à indices fractionnaire* », Journal de l'école polytechnique, 15(25) (1836)58-84.
10. AMBEONDAHY « *Modèles Fractionnaires Appliqués au Transport de Colloïdes en Milieux Poreux* » Thèse de doctorat, Université d'Antananarivo Madagascar (2016).