A Theoretical Analysis of Transport Characteristics of Nanoparticles in Porous Medium

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Abstract: In the current investigation, the transport of nanoparticles in porous medium is described in a general way. The main objective of this study is the resolution of the equation that governs the transport and the performance of the nanoparticles along their path through the porous media. It is essential to highlight the significant role of nanoparticles at a present time, using vital and multidisciplinary uses. Especially in the field of sanitary-engineering nanoparticles possess a very vital usage that allows reducing the concentration of different contaminants in water. Various characteristics associated with the properties of nanoparticles in relation to the porous media are presented in this study. Relying upon the concepts developed, a mathematical equation is proposed to analyze the transport and behavior of the transport of nanoparticles in porous media. The finite differences method is utilized, and a computational model is developed using MATLAB program. The theoretical outcomes verified that the results and graphs obtained are satisfactory and comply with what was expected.

Keywords: Nanoparticles, Porous Media, Sanitary-Engineering, Finite Differences Method

1. Introduction

Nanotechnology is an approach, representation, construction and request of assemblies, tools and schemes through the control of dimension and form at a nanometric scales (Ramsden, 2016). Although this science may sound relatively new, nanoparticles (NPs) have existed on the planet long time ago. Examples of this are smoke particles and viruses (Ramsden, 2018).

The NPs are utilized in a set of requests in material science, medicine and various industrial applications. They can also interact with each other and with the environment that surrounds them. Currently, we are at the very beginning steps about using NPs to analyse the movement of solutes in a porous medium, with potential implications for decontaminating water resources and evaluating ecosystem services (Hao *et al*., 2010).

A porous medium is a material composed of a solid matrix containing a system of holes (pores) that may or may not be interconnected (Figure 1). Porous medium possesses different geometries and sizes depending on the origin of their training. The geometry of a porous system describes the shapes and sizes of its pores as well as the roughness of the surface (Bear, 2013). A porous medium is distributed continuously and indirectly consisting of three well differentiated phases: solid, liquid and gaseous. The first, called matrix is formed by the minerals and organic particles in the soil united by more or less stable aggregates. The other two, composed of water and air with water vapor, occupy the hollow spaces, pores between the solid particles. Water is not pure but also contains dissolved salts and organic substances.

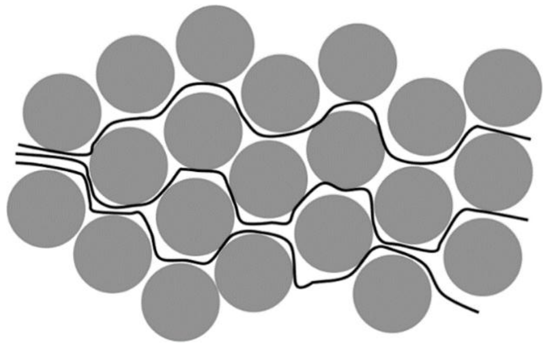

Figure 1: Geometry of the porous medium

Underground hydrology provides us with theoretical models that describe, on the one hand the movement of water in the aquifer, furthermore the movement of a certain solute in groundwater. In our case it will allow us to know the movement of the particles in groundwater (Kresic, 2006). The importance of this investigation is to know how the NPs move in the porous medium, often unknown, since different ways of using NPs have been studied to reduce the concentration of contaminants in drinking and waste water. The studies have been carried out mainly with inorganic NPs of Fe_2O_4, CeO_2 and TiO_2 through absorption processes and with NPs of elemental gold (Au) functionalized with organic chains (Mishra, 2016). On the other hand, it has also proceeded to anchor organic chains on the NPs with the aim that these are those that retain the contaminant. In this sense, experiments are currently being conducted with gold NPs functionalized with cyclodextrins to eliminate pesticides of various formulations. In all cases, special attention has been paid to determining the effect that NPs can cause in the environment where they are released (Nasrollahzadeh, Sajjadi, Maham, Sajadi, & Barzinjy, 2018). Accordingly, different toxicity tests standardized with NPs have been carried out (Kango *et al*., 2013).

The obtained results from different researchers show that the NPs possess a real potential to be utilized in the wastewater treatment (Qu, Alvarez, & Li, 2013). In some cases, we face with NPs with some environmental toxicity but with a high decontaminating potential, so one must find other ways to use the selective NPs, such as the immobilization of the NPs on porous supports. This can be achieved through circulating water, this would facilitate its application (Bystrzejewska-Piotrowska, Golimowski, & Urban, 2009).

The objective of this work is to make a compilation of the processes that govern the transportation of NPs in drenched porous media. It is also our aim to formulate these processes in the arrangement of differential-equations in partial derivatives of government, as well as to propose a method for numerical resolution, *i.e.* finite differences of the resulting transport equation.

2. Theory
2.1 Porosity

The ability of a soil to retain and let both water and air pass is related to its pore volume. The relationship between this and the whole dimensions of the soil is called *porosity* (n) and expressed as,

$$n = \frac{V_p}{V_t} \tag{1}$$

The porosity coincides with the water content of the saturated porous medium, however, it is not indicative of the amount of water it can transmit. The above expression can be expressed by,

$$n = \frac{\rho_m - \rho_a}{\rho_m} \tag{2}$$

where ρ_a is an apparent density, defined as the relationship between the mass of soil (excluding water and air) divided by the total volume (M/L^3). ρ_m is the real or particle density, which measures the relationship between the mass of the particles that make up the soil and the volume they occupy, that is, the total volume, excluding the volume occupied by the pores (M/L^3). The porosity depends on the composition, texture and structure of the soil. In general, it varies from 0.4 to 0.6 and may be higher in soils with an organic matter content (its irregular shape produces little compaction). An increase in the clay content favors the formation of soil aggregates and increases the porosity (Bronick & Lal, 2005).

2.2 Specific Area

The specific area of a solid, S_m, is well-defined by means of the interstitial area of the pore surface per unit mass and is one of the main parameters for evaluating the absorption capacity of soils. It varies from a few cm^2/g for rocks, reaches values between 600 and 1000 m^2/g for aerogels and for activated carbons approaches to 2000-3000 m^2/g (Dallas, Ding, Joriman, Zastera, & Weineck, 2004).

2.3 Tortuosity

The flow in the pores of the soil does not follow a straight path as shown in the Figure 2. Water moves around individual particles and pores of different sizes within the porous medium, resulting in a pattern much longer than a straight line. The tortuosity is defined and calculated as the relationship among the real length that a particle of fluid must travel to join two points in the central of the porous medium and the distance in a straight line between said points (Dullien, 2012) as,

$$\tau = \frac{l_o}{l} \tag{3}$$

Where τ is tortuosity, l_o is the straight-line length and l is the actual traveled length.

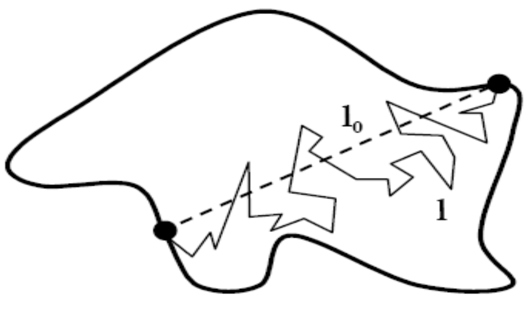

Figure 2: Representation of the tortuosity

2.4 Equation of Flow in Porous-medium

The equation of flow is the result of imposing the principle of mass conservation and assuming that the movement of water obeys Darcy's law (McDowell & Allen, 2015).

2.4.1 Darcy's Law

Darcy, designed a pragmatic method for the performance of movement over waterlogged soils (Darcy, 1856). He initiated that the amount of water ***q*** per second pouring over a cross sectional area of soil underneath hydraulic gradient ***i*** can be stated by the following equation (Wesley, 2009):

$$\vec{q} = K\vec{\imath}A \tag{4}$$

where, K is the hydraulic conductivity or permeability factor (length/time). While A is the cross-sectional-area of soil, it is perpendicular to the direction of flow and includes the area of the solids and the holes.

And the velocity of flow can be expressed as,

$$\vec{v} = \frac{\vec{q}}{A} = K\vec{\imath} \tag{5}$$

Darcy's law describes the dynamics of the movement of a non-compressible fluid in a porous medium. This law opened the way to the rational analysis of the flows of groundwater and other fluids flowing through porous media (Darcy, 1983).

This law was deduced empirically by Henri Darcy in the middle of the 19th century (Darcy, 1856). The laboratory experiment consisted of a vertical section A and length column L filled with a porous medium through which water was circulated (Figure 3).

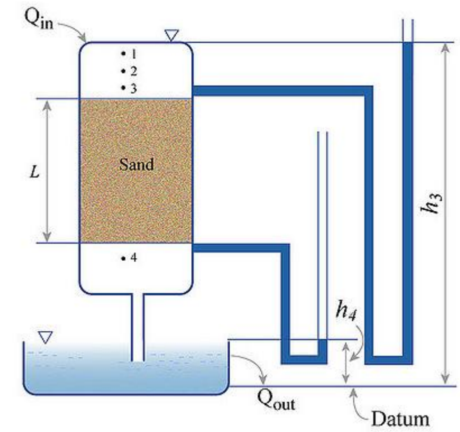

Figure 3: Darcy's experiment for hydraulic conductivity and porosity assessment (Domenico & Schwartz, 1998)

Darcy found a relation between the volume of water that crosses the column per unit of time, and the piezo-metric heights measured by a manometer at the ends of the column, h_3 and h_4. The resulting law can be written as:

$$Q = K.\frac{h_3 - h_4}{L}.A \tag{6}$$

where Q is flow (L^3/T), L is length of the sample in meters (L); h_3 is the height on the reference plane that reaches the water in a tube placed at the entrance of the filter layer and h_4 is the height reached by water in a tube placed at the outlet of the filter layer.

The law can be generalized to write it in vector notation.

$$\vec{q} = -K\vec{\nabla}h \tag{7}$$

where $\boldsymbol{q}$ is the Darcy velocity (length/time), defined as the quotient and ∇h is the hydraulic gradient (-). The negative sign is due to the fact that the flow vector has the opposite direction and sense that the gradient vector of piezo-metric heights (note that in this study vector variables are presented in bold).

Hydraulic conductivity is a measure of how easily the medium allows water to pass through it per unit area transverse to the flow direction. The value of this parameter is a function of the geological material. Sometimes it is preferable to work with the parameter permeability (T), which is the integral of K along the vertical of the aquifer.

The expression of Darcy's law is valid only if the soil is homogeneous (the properties do not depend on the position of the point from which it is measured) and isotropic (properties do not depend on the direction as measured). It should be noted that a solute moves at the same speed of water values, they are related by porosity which is not the same as the velocity of Darcy ($\boldsymbol{q}$).

$$\vec{v} = \frac{\vec{q}}{\Phi_{eff}} \tag{8}$$

where $\boldsymbol{v}$ is the linear velocity of water (length/time) and Φ_{eff} is effective porosity.

2.4.2 Permeability

Permeability is a property of the porous system that influences Darcy's law and allows fluids to flow. Normally, the size of the pores and their connectivity determine if the soil possess more or less permeability. The water can easily pour over a large porous soil through good connectivity among them. Minor pores using an equivalent amount of connectivity would require a low porousness, since water would pour over the soil further gently, as is the case with clay soils. The approximate values of permeability in a soil (expressed in m/day) are listed in Table 1.

Table 1: Values of permeability in a soil (m/day) (Whiffin, van Paassen, & Harkes, 2007)

Type of soil	Important	Gross sand	Arena fine	Silt	Clay
K (m/day)	>1000	10-1000	1-10	10^{-3}-1	$<10^{-3}$

3. The Transportation Equation of Nanoparticles

Once the one-dimensional transport equation of NPs in a porous medium has been obtained, it will be resolved with suitable boundary conditions. Once the method is presented, it will be solved numerically with a code written in MATLAB. In this section, the method of finite differences will be explained with a general formulation later apply to the NPs transport equation.

The method of finite differences consists of approximation of differential equations. These equations can be obtained, normally, from the truncation of Taylor series. The resulting set of equations constitutes a linear system, which can be solved numerically in a computer obtaining an approximate solution of the original problem.

The first step of the finite difference method is to select (sample) a set of discrete points (mesh of points) of the region, a temporal subdomain of observation *y*, and a temporal sampling interval Δt. The second step is to approximate the differential equation by means of an equation in incremental differences. The third step involves solving the equation independently in each point of the mesh and the selected temporal subdomain. The set of discrete points (x_i) can be constructed by selecting a constant spatial separation, Δx which is not restrictive, so that, $x_i = i\Delta x$ for the one-dimensional case as shown in Figure 4.

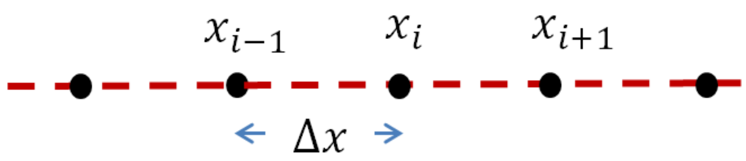

Figure 4: Point mesh in the method of finite differences (Mazumder, 2015)

Various approximations to the value of the derivative and of higher order derivatives can be used, through the development of Taylor series as,

$$\left.\frac{df}{dx}\right|_i = \frac{f_{i+1}-f_i}{\Delta x} + \theta(\Delta x) \tag{9}$$

Backward difference for the first derivative,

$$\left.\frac{df}{dx}\right|_i = \frac{f_i-f_{i-1}}{\Delta x} + \theta(\Delta x) \tag{10}$$

Centered difference for the first derivative,

$$\left.\frac{df}{dx}\right|_i = \frac{f_{i+1}-f_{i-1}}{2\Delta x} + \theta(\Delta x^2) \tag{11}$$

Forward difference for the second derivative,

$$\left.\frac{d^2f}{dx^2}\right|_i = \frac{f_{i+2}-2f_{i+1}+f_i}{\Delta x^2} + \theta(\Delta x) \tag{12}$$

Backward difference for the second derivative,

$$\left.\frac{d^2f}{dx^2}\right|_i = \frac{f_i-2f_{i-1}+f_{i-2}}{\Delta x^2} + \theta(\Delta x) \tag{13}$$

Centered difference for the second derivative,

$$\left.\frac{d^2f}{dx^2}\right|_i = \frac{f_{i+1}-2f_i+f_{i-1}}{\Delta x^2} + \theta(\Delta x^2) \tag{14}$$

It should be noted that there are approximations to derivatives of higher order although we will not use them in this work. Once the Taylor series are applied, there are different methods to solve the resulting equations. In this investigation the implicit method will be used as shown in Figure 5, hence only that method is explained,

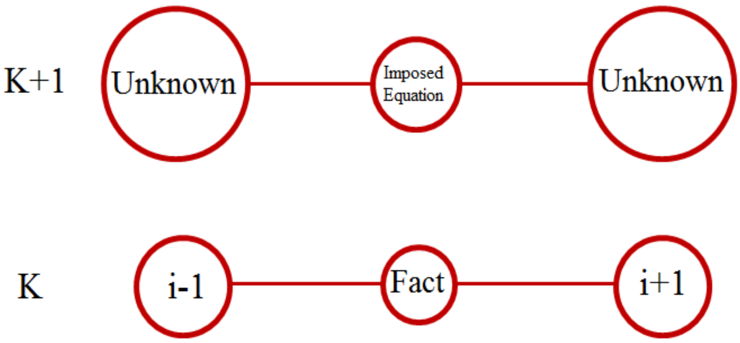

Figure 5: Representation of the implicit method (Chen, Huan, & Ma, 2006)

$$\frac{u_i^{K+1}-u_i^{K}}{\Delta t}=\frac{u_{i-1}^{i+1}-2u_i^{k+1}+u_{i+1}^{k+1}}{\Delta x^2} \tag{15}$$

Taking,

$$r=\frac{\Delta t}{\Delta x^2} \tag{16}$$

$$L\left(u_i^{k+1}\right)=u_{i-1}^{k+1}-2u_i^{k+1}+u_{i+1}^{k+1} \tag{17}$$

Obtaining,

$$u_i^{k+1}-rL\left(u_i^{k+1}\right)=u_i^{k} \tag{18}$$

In matrix form,

$$[A]\cdot\{U\}^{k+1}=[I]\cdot\{U\}^{k} \tag{19}$$

where,

$$[A]=\begin{bmatrix} (1-2r) & -r & & & & 0 \\ -r & (1-2r) & -r & & & \\ & -r & (1-2r) & -r & & \\ & & -r & (1-2r) & -r & \\ & & & -r & (1-2r) & -r \\ 0 & & & & -r & (1-2r) \end{bmatrix} \tag{20}$$

It can be seen that the matrix [A] is tri-diagonal and its length depends on the vector {U}.

Now we will apply the finite difference method to the NPs transport equation. It should be remembered that the equations described here,

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} - \frac{\rho_a}{n}\frac{\partial S}{\partial t} + R \tag{21}$$

$$\frac{\partial S}{\partial t} = \frac{n \cdot k_a}{\rho_a} \cdot C - k_b S \tag{22}$$

It is also important to know that the implicit method will be applied to each of the equations separately and later they will be put together in the form of matrices. Applying the implicit method to the first equation we obtain,

$$\left.\frac{\partial C_i}{\partial t}\right|_k = \frac{C_i^{k+1} - C_i^k}{\Delta t} = \frac{D}{\Delta x^2} \cdot \left(C_{i-1}^{k+1} - 2C_i^{k+1} + C_{i+1}^{k+1}\right) - v \cdot \frac{C_{i+1}^{k+1} - C_{i-1}^{k+1}}{2\Delta x} - \frac{\rho_a}{n} \cdot \frac{S_i^{k+1} - S_i^k}{\Delta t} \tag{23}$$

Grouping terms,

$$\left.\frac{\partial C_i}{\partial t}\right|_k = \left(1 + \frac{2D\Delta t}{\Delta x^2}\right) \cdot C_i^{k+1} + \left(-\frac{D\Delta t}{\Delta x^2} + \frac{v\Delta t}{2\Delta x}\right) \cdot C_{i+1}^{k+1} + \left(-\frac{D\Delta t}{\Delta x^2} - \frac{v\Delta t}{2\Delta x}\right) \cdot C_{i-1}^{k+1} + \frac{\rho_a}{n} \cdot S_i^{k+1} = C_i^k + \frac{\rho_a}{n} \cdot S_i^k \tag{24}$$

where,

$$A = \left(1 + \frac{2D\Delta t}{\Delta x^2}\right) \tag{25}$$

$$B = \left(-\frac{D\Delta t}{\Delta x^2} + \frac{v\Delta t}{2\Delta x}\right) \tag{26}$$

$$C = \left(-\frac{D\Delta t}{\Delta x^2} - \frac{v\Delta t}{2\Delta x}\right) \tag{27}$$

$$D = \frac{\rho_a}{n} \tag{28}$$

Finally, the equation presents the following aspect,

$$\left.\frac{\partial C_i}{\partial t}\right|_k = A \cdot C_i^{k+1} + B \cdot C_{i+1}^{k+1} + C \cdot C_{i-1}^{k+1} + D \cdot S_i^{k+1} = C_i^k + \frac{\rho_a}{n} \cdot S_i^k \tag{29}$$

On the other hand, applying the implicit method to the second equation, we obtain,

$$\left.\frac{\partial S_i}{\partial t}\right|_k = \frac{S_i^{k+1} - S_i^k}{\Delta t} = \frac{n \cdot k_a}{\rho_a} \cdot C_i^{k+1} - k_b \cdot S_i^{k+1} = (1 + \Delta t k_b) \cdot S_i^{k+1} - \left(\frac{n \cdot k_a}{\rho_a} \cdot \Delta t\right) \cdot C_i^{k+1} = S_i^k \tag{30}$$

where,

$$E = (1 + \Delta t k_b) \tag{31}$$

$$F = \left(\frac{n \cdot k_a}{\rho_a} \cdot \Delta t\right) \tag{32}$$

Therefore, one can get,

$$\left.\frac{\partial S_i}{\partial t}\right|_k = E \cdot S_i^{k+1} - F \cdot C_i^{k+1} = S_i^k \tag{33}$$

Finally, the resulting set of equations is expressed in matrix form,

$$\begin{pmatrix} \ddots & & \ddots & \\ & CAB & & D & \\ & & \ddots & & \ddots \\ \ddots & & \ddots & \\ & F & & E & \\ & & \ddots & & \ddots \end{pmatrix} \cdot \begin{pmatrix} C_i \\ \vdots \\ \vdots \\ S_i \\ \vdots \\ \vdots \end{pmatrix} = \begin{pmatrix} C_i^n + \frac{\rho_a}{n} \cdot S_i^n \\ \\ \\ \\ S_i^n \end{pmatrix} \tag{34}$$

Once the finite difference method is applied to the nanoparticle transport equation in a porous medium, it will be resolved using the MATLAB program. Therefore, the method must be programmed. It should be noted that initial conditions and boundary conditions must be applied to solve the equation (Vázquez, 2007). The conditions applied in our problem are the following:

The initial conditions,

$$C(x, t = 0) = C_i \tag{35}$$

$$\frac{\partial S}{\partial t} = 0 = \frac{n \cdot k_a}{\rho_a} \cdot C_i - k_b S_i \longrightarrow S_i = \frac{n \cdot k_a}{\rho_a \cdot k_b} \cdot C_i \tag{36}$$

The first initial condition indicates that there is an initial concentration at the first instant of the experiment. The second condition indicates the number of initial retained NPs.

The contour conditions:

Dirichlet boundary conditions (Moës, Béchet, & Tourbier, 2006),

$$C(x = 0, t) = C_o \tag{37}$$

Neumann boundary conditions (Alikakos & Rostamian, 1981),

$$\frac{\partial C(L,t)}{\partial x} = 0 \tag{38}$$

By operating on Neumann's condition, one can get,

$$\frac{C_n^{k+1} - C_n^k}{\Delta t} + q.\frac{0 - C_{n-\frac{1}{2}}}{\Delta x} - D \cdot \frac{0 - \frac{\partial C}{\partial x}\Big|_{n-\frac{1}{2}}}{\Delta x} = f_i \tag{39}$$

$$\frac{C_n^{k+1} - C_n^k}{\Delta t} + q \cdot \frac{-0.5 \cdot (C_{n-1}^{k+1} + C_n^{k+1})}{\Delta x} - D \cdot \frac{C_{n-1}^{k+1} - C_n^{k+1}}{\Delta x^2} = -\frac{q C_n^{k+1}}{\Delta x} \tag{40}$$

$$\frac{C_n^{k+1} - C_n^k}{\Delta t} + \left(-\frac{0.5q}{\Delta x} - \frac{D}{\Delta x^2}\right) C_{n-1}^{k+1} + \left(\frac{0.5q}{\Delta x} + \frac{D}{\Delta x^2}\right) C_n^{k+1} = 0 \tag{41}$$

where:

$$M_1 = -\frac{0.5q}{\Delta x} - \frac{D}{\Delta x^2} \tag{42}$$

$$M_2 = \frac{0.5q}{\Delta x} + \frac{D}{\Delta x^2} \tag{43}$$

Thus,

$$\Delta t\, M_1 C_{n-1}^{K+1} + (1 + M_2 \Delta t) C_n^{k+1} = C_n^k \tag{44}$$

The first Dirichlet boundary condition shows the input concentration at a time t at the beginning of the column. It is important that in order not to obtain oscillations and dispersion in the results, the values of the elements of the transport equation must comply:

Grid-Courant number,

$$C_u = \frac{v \cdot \Delta t}{\Delta x} < 1 \tag{45}$$

Grid-Peclet-number,

$$P_e = \frac{v \cdot \Delta x}{D} < 2 \tag{46}$$

4. Results and Discussion

When the finite difference method is applied to the nanoparticle transport equation in a porous medium, it will be resolved using the MATLAB program. It should be noted that initial conditions and boundary conditions must be applied to solve the equation. The conditions applied in this study are including two processes: in the first process concentration of NPs entered gradually, and then at half of the total time, the entered NPs decreased progressively. In the second process, the concentration of the entered NPs at the initial moment of time increased slowly. This followed by another step; *i.e.* stop entering NPs, then after at a quarter of the whole time NPs re-entered and finally at a half of the total time NPs concentration stop entering.

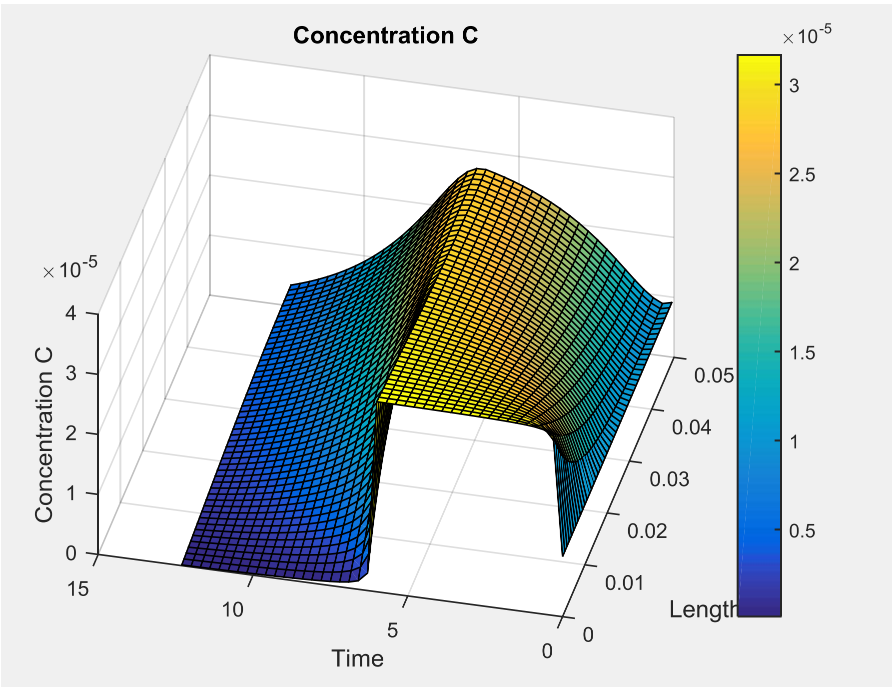

Figure 6: 3D graph of the evolution of the concentration of NPs in the first process

Figure 6 shows how the NPs flow enters at the beginning, halves the NPs concentration flow and halves the NPs concentration, obtaining an expected behaviour. There is also a different behaviour at the beginning with respect to the end of the period, where changes in concentration input are perceived more smoothly. In similar investigation Ben-Moshe *et al.* investigated experimentally the manners of four-types of untreated metal-oxide NPs, namely Fe_3O_4, TiO_2, CuO and ZnO in water-logged porous media. (Ben-Moshe, Dror, & Berkowitz, 2010).

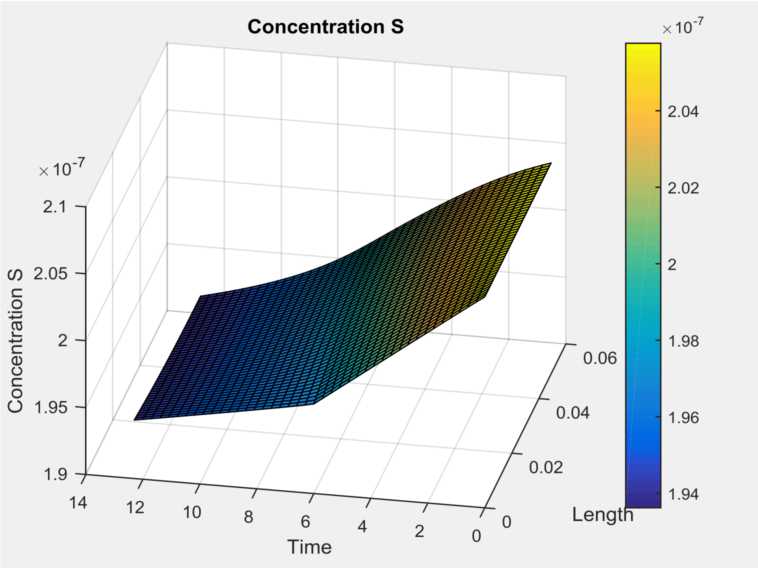

Figure 7: 3D graph of the evolution of the concentration of particles reserved in the first process

The evolution of the retained particles is observed, this can be seen in Figure 7. As it is logical in the initial moment there are more particles retained than in the final moment and the number decreases progressively. The mathematical model presented by Ju and Fan was capable to pretend effectively the transportation procedure of NPs in arbitrary porous media, and arithmetical outcomes agreed productively with investigational records (Ju & Fan, 2009). Their study depended on the hydrophilic and lipophilic poly silicon nanoparticle which is appropriate for increasing water instillation capability for small permeability artificial lake, and lipophilic and hydrophilic poly silicon nanoparticle can be utilized to increase oil reclamation.

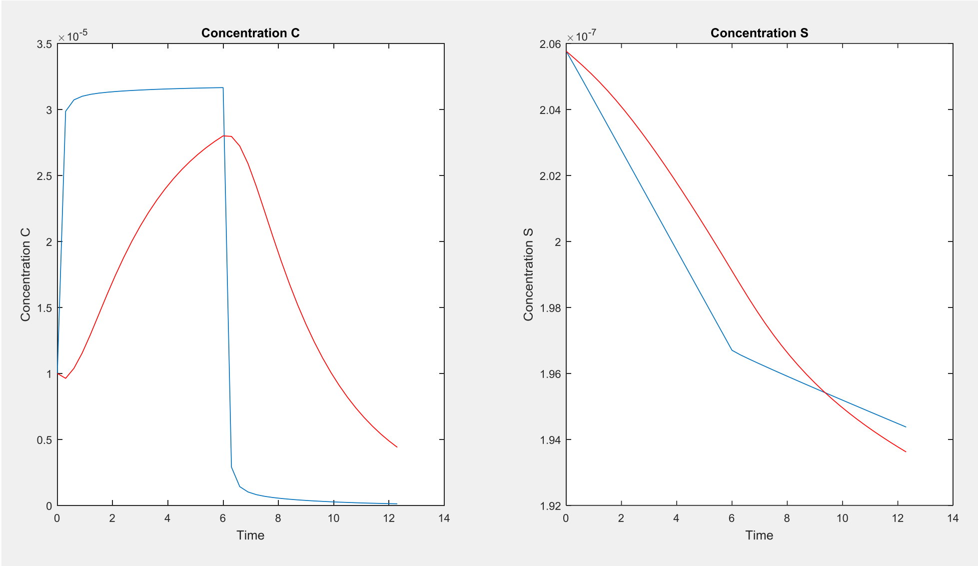

Figure 8: Cutting the 3D graphics at the beginning and end of the porous media in the first process

The authors have cut the 3D graphs of C and S at the beginning and at the end of the porous medium as shown in the Figure 8. The blue color shows the cut at the beginning and the red color at the end. In the graph of C, one can see a figure with two different curves. Since the end suffers from the change of concentration less abrupt and in a slower and progressive way. In the Figure 8, the retained particles S, one can observe how it behaves similar to the beginning and the end. Shen *et al.* designed a method to act out the 3D porous micro-structures of changing porosity rely upon negligible 2D microstructural statistics. They utilized a porous titanium material, which can be considered for bone implantations, to explain the process. Shen *et al.* stated that pore size and dissemination in the material at small porosity can be categorized by simple 2D mineralogy (Shen, Oppenheimer, Dunand, & Brinson, 2006).

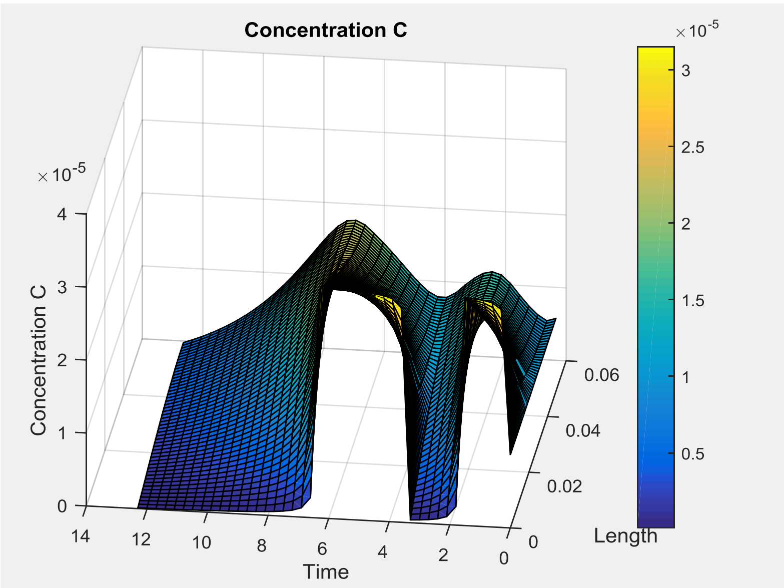

Figure 9: 3D graph of the evolution of nanoparticle concentration in the second process

One can see, in the Figure 9, how initially an initial concentration enters, later on to enter NPs concentration, then after 3s NPs re-enter and finally in half the time NPs stop entering. Davis *et al.* in analogous imitation outcomes indicated that the investigational statistics can be clarified by means of a technique where the originator NPs change to zeolite crystals over numerous in term diary conditions that can take part to aggregative growing (Davis *et al.*, 2006). Moreover, as stated by the anticipated method, the concentration of every single transitional type is considerably less than the original concentration of new particles (Davis *et al.*, 2006). Furthermore, the concentration of the transitional decreases considerably as the transitional growth near silicalite-1.

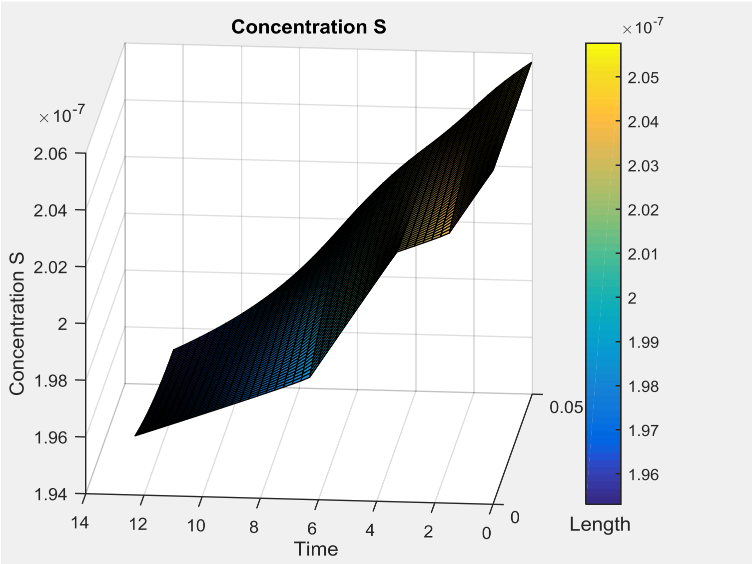

Figure 10: 3D graph of the evolution of the nanoparticle concentration retained in the second process

Figure 10, represents the second process, indicated that in the same way that in the first process the concentration of retained particles decreases progressively, since each time more NPs are coming out and there are fewer retained. Teng *et al.* (2006) stated that there are insufficient instances of the provision of porous metal NPs. Precisely, approaches for creating porous platinum nano structures have been established predominantly over the templating methods. Mesoporous platinum has been prepared by means of lyotropic liquid-crystal models (Teng *et al.*, 2006).

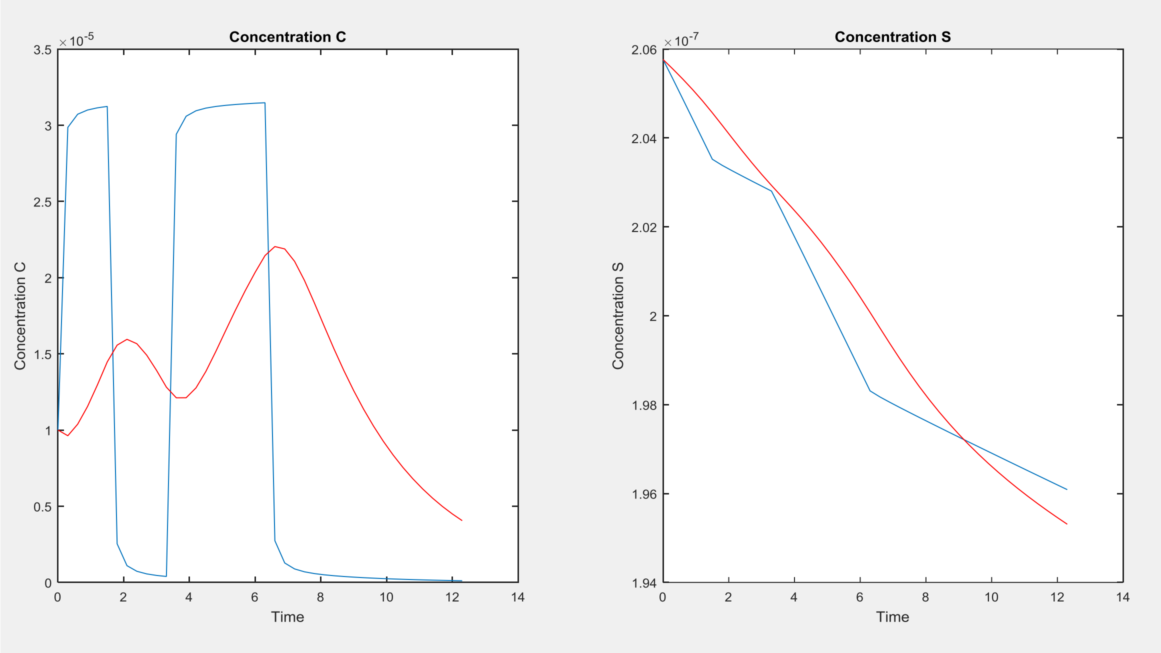

Figure 11: Cutting 3D graphics at the beginning and end of the porous media in the second process

One can clearly observe in Figure 11 the entrance process of beginning and end for NPs entrance. As in process 1, the graph in blue represents the beginning and in red the end. Doughty and Pruess (2004) used the injection and storage modelling of supercritical CO_2 in brine-bearing formations that can provide valuable insights into flow and transport behaviour. They also mentioned that under stated interactions between physical and numerical effects can happen. This requires the model development selections to be made with caution. Especially, grid determination and alignment effects can yield outcomes that mimic and mask physical procedures associated with floating flow in multi-phase varied systems (Doughty & Pruess, 2004).

5. Conclusions

NPs possess many applications at present and have a great possibility of progress in the field of sanitary-engineering as a mean to reduce the amount of contaminants in water and therefore to improve water quality. Therefore, it is important to emphasize the following aspects in the form of general conclusions for the work done and the program developed for the calculation of the transportation equation of NPs in porous media. At present, the sanitary nature of NPs has begun to be known and more researches should be done to obtain a better performance in its use. This effort is aimed to make a compilation of the processes that govern the transportation of NPs in drenched porous media. The authors formulated these processes in the arrangement of differential-equations in partial derivatives methods, in addition to proposing a method for numerical resolution, explicitly finite differences, of the resulting transport equation.

The toxic character of NPs must be taken into account, since in many occasions it can be harmful to humanoid health-condition and the atmosphere. This finite differences model is a suitable and simple model for the calculation of differential equations, specifically the transport equation of NPs in porous medium. There are more models for the calculation of differential equations, although it has been adopted to develop the method of finite differences for its easy understanding and management.

It is verified that the results and graphs obtained are satisfactory and comply with what was expected.

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