NUMERICAL AND ANALYTICAL STUDY OF THE INORGANIC IONS DIFFUSION IN THE INTERIOR OF SOIL PARTICLE

Adriana de Souza Forster Araújo, adriana@metal.eeimvr.uff.br
José Adilson de Castro, adilson@metal.eeimvr.uff.br
Universidade Federal Fluminense – Av. dos Trabalhadores, nº 420, Vila Snata Cecília, Volta Redonda - RJ

Alexandre José da Silva, ajs@metal.eeimvr.uff.br
Universidade Federal Fluminense – Av. dos Trabalhadores, nº 420, Vila Snata Cecília, Volta Redonda - RJ

Abstract. *The processes that involve soil contamination by inorganic ions are usually controlled by diffusion and sorption of ions within the soil particles. In the present work, a study of the diffusion of inorganic ions in spherical coordinates was carried out on the basis of analytical and numerical solutions for typical situations of diffusion in the ground interior. The boundary conditions of prescribed values and kinetic of first order at the interface of the particles were analyzed. The analytical solutions obtained for the two cases were carried out using a FORTRAN computer code. Both cases were found to produce good sets of results. In the first case it was propose to solve particularities of the equation, such as when $r = 0$ or the diffusion is very slow, considering that the ions from the center of the sphere do not reach the surface. In the second case, it was considered a convection surface, or either, the inner ion concentration is consumed by a constant mass transfer rate, which depends on a mass transfer coefficient β.*

Keywords*: Diffusion, spherical coordinates, inorganic ions*

1. INTRODUCTION

The phenomena such as sorption or adsorption, diffusion and convection are directly related with inorganic contaminants that reach the ground and subsoil. Such processes are originated from the interaction between the ground liquid and solid phases. In the systems modeling that involves contaminants and soil it is necessary that the mass transfer phenomena be quantified (Perry *et al.* 1995). Thus, a risk evaluation or a decontamination alternatives definition becomes possible.

Field studies (Goodall and Quigley, 1977; Crooks and Quigley, 1984; Quigley *et al.*, 1987; Johnson *et al.*, 1989), evidenced the molecular diffusion as preponderant mechanism in the transport of the contaminants found in solutions that migrate in fine ground with low permeability. Then, the study of this transport mechanism has been addressed by several authors (Cheung, 1989; Mitchell, 1994; Shackelford, 1994; Quigley, 1994; Shackelford and Redmond,1995; Jessberger and Onnich, 1993; Jessberger *et al*, 1995; Boscov *et al*, 1999; Leite and Paraguassu, 2002).

Ions with significant concentration in the leachate of landfill are chloride, sodium, calcium, potassium, magnesium, iron and ammonium (Christensen *et al.*, 2001). Previous works based on numerical and experimental analysis indicated that calcium ions behave in different way and model based on diffusion was not capable of reproduce experimental data.

Nowadays with the actual necessity to deal with ground and the underground water contamination problems, the study of the contamination problems by chemical products becomes important. These studies involve the determination of the physical parameters of these composites as well as its dynamics when dissolved in the underground water.

This research was focused on studying the diffusive transport process of an ion inside a soil particle. Therefore, the calcium ion was selected since it presented divergent results when compared with simulated models and experimental tests. The mass flow was analyzed from the center to the surface of the soil particle. Due to a spherical shape approaching of the soil particle, the studies were considered under spherical coordinates. It has been expected that the phenomenological models are able to accurately foresee the behavior of this lecheate in these environments.

The diffusive transport in spherical coordinates was evaluated considering two different boundary conditional cases.

In the first case a fix ion concentration condition in the surface and prescribed derivation in the center of the soil particle were considered. However, in order to solve a single problem of the diffusion equation in spherical coordinates, a hollow sphere of internal radius (*a*) and external radius (*b*) was considered (Lü and Bülow, 2000). In this case the analytical solution shows a superposition of the linear solution over the non linear solution.

In the second case, it was considered prescribed derivation conditions in the center and in the surface of a spherical particle. However, the convection condition was applied in the surface, or either, the ion concentration inside the particle is consumed through a constant mass transfer rate. This rate depends on a mass transfer coefficient β.

This paper was focused in a diffusive transport modeling of the calcium contaminant inside a soil particle considering different boundary conditions with the aim to better understand these phenomena.

2. METODOLOGY

2.1. Analytical solution for the diffusion equation in spherical coordinates

Due to the uniform shape of the soil particles, the diffusion process analysis under spherical coordinates is limited in three conditions: unidimensional, constant diffusion coefficient and isothermal conditions.

The diffusion process is evaluated through the concentration changes in time of the chemical specimen. This can be seen in the Eq. (1) bellow which represents the spherical coordinates diffusion equation in three dimensions (Bird, 2004):

$$\frac{1}{D}\frac{\partial C}{\partial t} = \nabla.(\nabla C) \tag{1}$$

Where D is the diffusion coefficient.

After solving the gradient divergent or the concentration Laplacian, and considering that there is a symmetry related the angles θ and ϕ:

$$\frac{\partial}{\partial \theta} \equiv \frac{\partial}{\partial \phi} = 0 \tag{2}$$

In this way, the diffusion equation in radial direction is:

$$\nabla^2 C = \frac{\partial C}{\partial t} = D\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial C}{\partial r}\right] \tag{3}$$

In order to solve the diffusion equation in radial direction, Eq. (3), it was necessary to change a variable (Crank, 1979), or either, in order to solve such equation by the variable separation method, it considers:

$$u = C \times r \tag{4}$$

From this change, the Eq. (3) shall be written as follows:

$$\frac{\partial u}{\partial t} = D\,\frac{\partial^2 u}{\partial r^2} \tag{5}$$

2.2. Boundary and initial conditions

In order to determine the Ca^{2+} ion in a spherical soil particle, it is necessary to solve the Eq. (3). However, each result depends on the physical conditions in the sphere limits. If the problem depends on the time, an initial condition will be required: the initial concentration value of the ion inner the sphere. There are many boundary conditions alternatives which can be simply expressed as mathematical equations.

In this paper, the diffusive phenomenon was evaluated in spherical coordinates from two different boundary conditions.

Case 1:

It was analyzed the diffusive process in hollow particles based on analytical solutions of the basic diffusion equation (Lü and Bülow, 2000).

This solution proposes to solve particularities of the equation, such as when r = 0 or the diffusion is very slow, considering that the ions from the center of the sphere do not reach the surface.

From the diffusion equation in the radial direction with constant coefficient (Eq. 3) it was considered a hollow sphere with inner and outer radius, *a* and *b*, respectively. The hollow sphere is initially at uniform concentration, C_0, and the outer surface concentration is maintained at constant concentration, C_1. If the boundary condition at the inner surface, r = a, is the type of the inner surface is not permeable to any species, the initial and boundary conditions would be:

Boundary conditions

$$\left.\frac{\partial C}{\partial r}\right|_{r=a} = 0 \tag{6}$$

$$C\big|_{r=b} = C_1 \tag{7}$$

Initial condition

$$C\big|_{t=0} = C_0 \tag{8}$$

In order to solve the Eq. (3), the parameters radius (r), time (t) and concentration (C) were considered non-dimensional:

$$x = \frac{r-a}{b-a} \qquad \tau = \frac{Dt}{(b-a)^2} \qquad u = \frac{(C-C_0)r}{(C_1-C_0)b}$$

Therefore, the Eq. (3) becomes:

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial x^2} \tag{9}$$

And the new boundary and initial conditions are:

Boundary conditions

$$\left.\left(\frac{\partial u}{\partial x} - hu\right)\right|_{x=o} = 0 \tag{10}$$

$$u\big|_{x=1} = 1 \tag{11}$$

Initial condition

$$u\big|_{\tau=0} = 0 \tag{12}$$

Case 2:

In the second case, it was considered a convection surface, or either, the inner ion concentration is consumed by a constant mass transfer rate, which depends on a mass transfer coefficient β. In this case, it was not necessary to consider a hollow sphere due to the set of initial and boundary conditions.

From the Eq. (5), $\frac{\partial u}{\partial t} = D\,\frac{\partial^2 u}{\partial r^2}$, the following boundary and initial conditions were set:

Boundary conditions

$$\left.\frac{\partial u}{\partial r}\right|_{r=0} = 0 \tag{13}$$

$$\left.\frac{\partial u}{\partial r}\right|_{r=a} = -\frac{\beta}{D}\left(u - u_\infty\right) \tag{14}$$

Initial condition

$$u\big|_{t=0} = u_0 \tag{15}$$

The parameters *r, t, u* and β were considered non-dimensional.

$$x=\frac{r}{a} \qquad \tau=\frac{Dt}{a^2} \qquad \theta=\frac{(u-u_\infty)}{(u_0-u_\infty)} \qquad Sh=\frac{\beta\cdot a}{D}$$

Where *Sh* is the non-dimensional Sherwood number $\left[\frac{m/s\cdot m}{m^2/s}\right]$.

Thus, the Eq. (5) becomes:

$$\frac{\partial\theta}{\partial\tau}=\frac{\partial^2\theta}{\partial x^2} \tag{16}$$

And the new boundary and initial conditions are:

Boundary conditions

$$\left.\frac{\partial\theta}{\partial x}\right|_{x=0}=0 \tag{17}$$

$$\left.\frac{\partial\theta}{\partial x}+Sh\theta\right|_{x=1}=0 \tag{18}$$

Initial condition

$$\left.\theta\right|_{\tau=0}=1 \tag{19}$$

2.3. Solution method to the studied cases:

The method to solve both cases is the variables separation method (Boyce, 1988).

Case 1:

Suposing that the solution for $u\,(x,\ \tau)$ is:

$$u(x,\tau)=\rho(x)\times\mu(\tau) \tag{20}$$

By solving the Eq. (20) through variables separation method, the following result can be found:

$$\mathrm{u}(\mathrm{x},\tau)=\mathrm{f}(\mathrm{x})+\left[\sum_{\mathrm{n}=1}^{\infty}\mathrm{A_n}\cos(\lambda_\mathrm{n}\mathrm{x})+\mathrm{B_n}\mathrm{sen}(\lambda_\mathrm{n}\mathrm{x})\right]\exp\left(-\lambda_\mathrm{n}^2\tau\right) \tag{21}$$

It can be noted as from Eq. (21) the superposition of the linear to the non-linear solutions.

Since sin and cosine are periodical functions, there is a conjunct of possible λ_n to be determined by boundary conditions. Therefore, the most common solution is the sum (superposition) of the solutions.

Then, *f(x)* is a linear function of *x*. Since the concentration of diffusing species anywhere inside the hollow sphere after infinite time ($\tau \to \infty$) approaches the value, C_1, the limits of *u* as $\tau \to \infty$ at the inner and outer surfaces, are u $(0,\infty)$ = $\frac{a}{b}=\frac{1}{h+1}$ and u $(1,\infty) = 1$, respectively. Considering the fact that the second term in Eq. (21) becomes zero as $\tau \to \infty$, the linear term, *f(x)*, in the general solution expression Eq. (20) should be:

$$f(x)=\frac{hx+1}{h+1} \tag{22}$$

By applying the proposed boundary and initial conditions, the terms A_n, B_n and λ_n are determined (refer to the appendix) and the solution to the Eq. (20) should be written as follows:

$$u(x,\tau)=\frac{hx+1}{h+1}-\sum_{n=1}^{\infty}\frac{\alpha_n}{\varsigma_n}\left[sen(\lambda_n x)+\frac{\lambda_n}{h}\times\cos(\lambda_n x)\right]\times\exp\left(-\lambda_n^2\tau\right) \tag{23}$$

In which λ_n (n = 1, 2, 3, ..., ∞) are the positive roots of the transcendental equation, where λ_n are the roots of the equation that presents an infinite number of parameters values and α_n and ζ_n are calculated as from the analytical equations (refer to the appendix).

Case 2:

Also the case 2 was solved as from the variable separation method. Base don Eq. (16), it was supposed that the solution for θ (x, τ) is:

$$\theta(x,\tau)=\rho(x)\times\mu(\tau) \qquad 24$$

The solution 24 should be written in agreement Eq. (25):

$$\theta(x,\tau)=\left[\sum_{n=1}^{\infty}A_n\cos(\lambda_n x)+B_n sen(\lambda_n x)\right]\exp\left(-\lambda_n^2\tau\right) \qquad 25$$

By applying the proposed boundary and initial conditions, the terms A_n, B_n and λ_n are determined (refer to the appendix) and the solution to the Eq. (25) should be written as follows:

$$\theta(x,\tau)=\left[\sum_{n=1}^{\infty}\left(\frac{\left(\frac{1}{\lambda_n}\right)\times sen(\lambda_n)}{\frac{1}{2}+\frac{1}{4\cdot\lambda_n}\times sen2\cdot\lambda_n}\right)\times\cos(\lambda_n x)\right]\times\exp\left(-\lambda_n^2\tau\right) \qquad 26$$

In which λ_n (n = 1, 2, 3, ..., ∞) are the positive roots of the transcendental equation, where λ_n are the roots of the equation that presents an infinite number of parameters values (refer to the appendix).

3. RESULTS AND DISCUSSIONS

Based in the solution of the Eqs. (23) and (26), it were analyzed the diffusion cases inner a soil particle, considering two different boundary conditions. In the first one, in which the particle presents an inner and an outer radius the concentration in the surface is continuous and in its center the concentration rate (∂C/∂x) vary as a time function. In the second case, the particle presents only a radius *a* and the concentration rates vary as in the center as in the sphere surface.

The analytical solutions were implemented in a Fortran program and the graphical results were analyzed by considering the applied boundary conditions.

The considered data in both cases are specified in the table bellow:

Table 1: Considered data for simulation in cases 1 and 2.

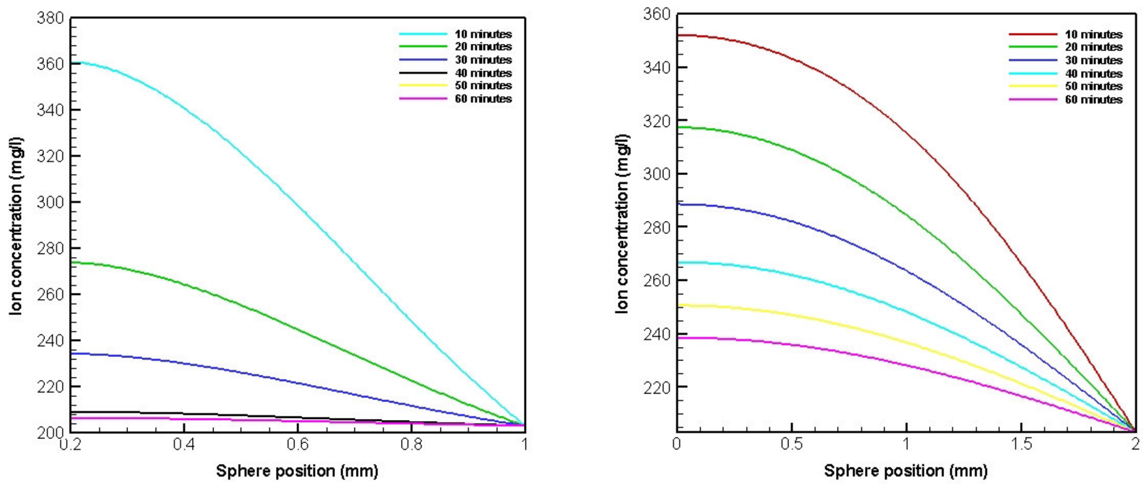
Case	The number of terms ∑	D (m^2/ano)	C_0 (mg/l)	C_1 (mg/l)	Ray *a* (mm)	Ray *b* (mm)	Time (minutes)	β (m/s)
1	200	0.025	* 365	* 203	0.2	1	20	3E-03
2	200	0.025	* 365	* 203	2	---	60	3E-03
								3E-06

(*) Values taken from experimental method (Ritter and Gatto, 2003).

Ritter and Gatto (2003) realized molecular diffusion and balance in lot (sorption) experimental tests with ions contained in a landfill leached. The results about calcium ion are presented in table 1. The numbers shows the calcium ion concentration extracted of the interstitial solution in the soil.

Figure 1 presents the concentration profile in the hollow sphere. For the calcium concentration analyses in different points into the sphere on the time, it can be noticed that the calcium amount reduces in an exponential way until it reaches a concentration value equal to C_0 (203 mg/l), confirming with this, the boundary condition on the surface (radius b). It can be also noticed that after 60 minutes the chemical specimen concentration stabilizes.

The graphic 1b represents the concentration profile diffusive behavior to the boundary conditions applied in the case 2. The Ca^{2+} ion concentration is consumed as a function of a constant mass transfer rate. The final concentration values do not converge as suggested in the picture 1b. In fact, such values are very close but not identical, confirming in this way the boundary condition in the surface.



(a) case 1 (b) case 2

Figure 1: Diffusion profile for cases 1 and 2.

The graphic 2 presents the same diffusion profile as the second case, however with different values of β. The red line represents $\beta = 3.10^{-3}$ m/s and the green line represents $\beta = 3.10^{-6}$ m/s. It can be noted that the lower β, the lower is the diffusion, it means, the diffusive process runs slowly.

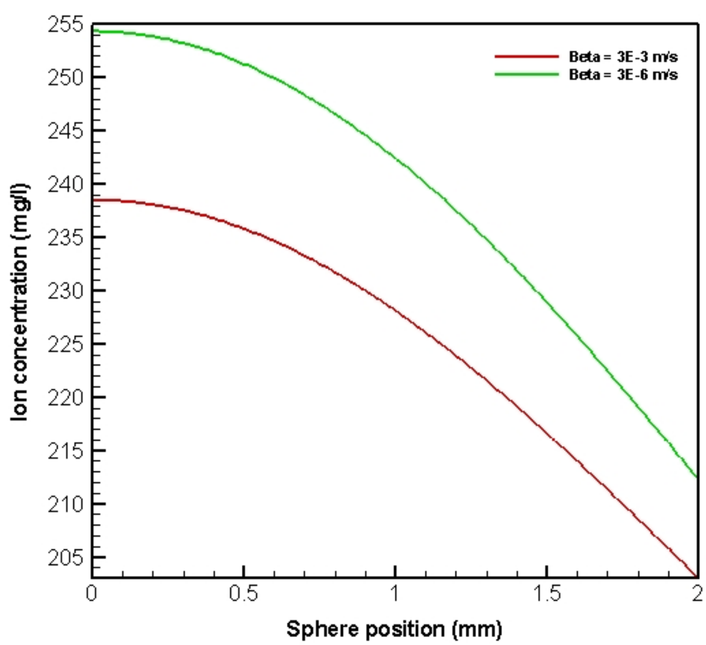


Figure 2: Diffusion profile for different β.

4. CONCLUSION

To the analytical solution for both cases proposed in this paper, it was obtained a calcium concentration profile for a period of time converging to the expected results. That is, the obtained concentration profile is coherent to the applied boundary conditions.

The hollow spheres analysis results in a simplified solution to profile the equation singularity when the sphere radius is zero or even so when considering such a very slow diffusion that the ions which are concentrated in the sphere center do not reach its surface.

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7. RESPONSIBILITY NOTICE

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APPENDIX: Solution of the Equation for the Diffusion in Hollow Sphere

In case one, the general solution to Eq. (9) becomes:

$$u(x,\tau)=\frac{hx+1}{h+1}+\left[\sum_{n=1}^{\infty}A_n\cos(\lambda_n x)+B_n\,\mathrm{sen}(\lambda_n x)\right]\exp\left(-\lambda_n^2\tau\right) \tag{A1}$$

Where A_n, B_n and λ_n are determined by the initial and boundary conditions.

From the boundary condition at x = 0, we have

$$\left.\left(\frac{\partial u}{\partial x} - hu\right)\right|_{x=o} = \sum_{n=1}^{\infty}(B_n\lambda_n - hA_n)\exp\left(-\lambda_n{}^2\tau\right) = 0 \qquad \text{(A2)}$$

Which can be satisfied by

$$B_n\lambda_n - hA_n = 0 \qquad \text{(A3)}$$

A_n can be expresses by

$$A_n = \frac{B_n\lambda_n}{h} \qquad \text{(A4)}$$

From the boundary condition at x = 1, we have:

$$\sum_{n=1}^{\infty}(A_n\cos\lambda_n + B_n sen\lambda_n)\exp\left(-\lambda_n{}^2\tau\right) = 0 \qquad \text{(A5)}$$

Or:

$$A_n\cos\lambda_n + B_n sen\lambda_n = 0 \qquad \text{(A6)}$$

Replacing Eq. (A4) into Eq. (A6) gives:

$$\tan\lambda_n = -\frac{\lambda_n}{h} \qquad \text{(A7)}$$

The Eq. (A7) is a transcendental equation, where λ_n are roots of the equation that possesses an infinite number of values of parameters (refer to figure 3).

Applying the initial condition (Eq. 12) to Eq. (A1) results in:

$$\frac{hx+1}{h+1} + \sum_{n=1}^{\infty}B_n\left[sen(\lambda_n x) + \frac{\lambda_n}{h}\cos(\lambda_n x)\right] = 0 \qquad \text{(A8)}$$

Or:

$$-f(x) = \sum_{n=1}^{\infty}B_n F_n(x) \qquad \text{(A9)}$$

Where:

$$F_n(x) = sen(\lambda_n x) + \frac{\lambda_n}{h}\cos(\lambda_n x) \qquad \text{(A10)}$$

In order to find B_n coefficient into Eq. (A9), we need to prove that this equation has the orthogonally propriety. This boundary problem is called a Sturm-Liouville probelm (Kreyzig, 1989). Then, as the Eq. (A11):

$$-\int_0^1 f(x)\times F_n(x) = B_n\int_0^1 F_n^2 \qquad \text{(A11)}$$

Solving the left side of Eq. (A11), results:

$$\int_0^1 f(x)\times F_n(x)=\frac{1}{h+1}\times\left[sen\lambda_n\left(1+\frac{h}{\lambda_n^2}+\frac{1}{h}\right)-\frac{h}{\lambda_n}\times\cos\lambda_n\right]=\alpha_n \tag{A12}$$

And solving the right side:

$$\int_0^1 F_n^2=\frac{1}{h^2}\times\left[\lambda_n^2+h^2+\left(\frac{\lambda_n^2+h^2}{2\times\lambda_n}\right)\times sen(2\cdot\lambda_n)+2\times h\times sen^2\lambda_n\right]=\varsigma_n \tag{A13}$$

With this, it is possible to determine the coefficient B_n:

$$B_n=-\frac{\alpha_n}{\varsigma_n} \tag{A14}$$

Replacing B_n value founs in Eq. (A14) into Eq. (A4) we have:

$$A_n=-\frac{\alpha_n\times\lambda_n}{\varsigma_n\times h} \tag{A15}$$

Therefore, the solution to Eq. (9) can be written as:

$$u(x,\tau)=\frac{hx+1}{h+1}-\sum_{n=1}^{\infty}\frac{\alpha_n}{\varsigma_n}\left[sen(\lambda_n x)+\frac{\lambda_n}{h}\times\cos(\lambda_n x)\right]\times\exp\left(-\lambda_n^2\tau\right) \tag{A16}$$

In a case two, the general solution to Eq. (16) is:

$$\theta(x,\tau)=\left[\sum_{n=1}^{\infty}A_n\cos(\lambda_n x)+B_n sen(\lambda_n x)\right]\exp\left(-\lambda_n^2\tau\right) \tag{A17}$$

Where A_n, B_n and λ_n are to determined by the initial and boundary conditions.
From the boundary condition at x = 0, we have:

$$\left.\frac{\partial\theta}{\partial x}\right|_{x=0}=[-A\lambda\cdot\mathrm{sen}(\lambda x)+B\cdot\cos(\lambda x)]\cdot\exp\left(-\lambda^2\tau\right)=0 \tag{A18}$$

Which can be satisfied by

$$B=0 \tag{A19}$$

From the boundary condition at x = 1, we have:

$$[A\lambda\times\mathrm{sen}(\lambda_n)]=Sh\times A\times\cos(\lambda_n) \tag{A20}$$

Thus, Eq. (A20) becomes:

$$\tan\lambda_n=\frac{Sh}{\lambda_n} \tag{A20}$$

Where the Eq. (A20) is a transcendental equation, where λ_n are roots of the equation that possesses an infinite number of values of parameters (refer to figure 3).

Applying the initial condition (Eq. 19) to Eq. (A17) results in:

$$A_n\cos(\lambda_n x)=1 \tag{A21}$$

Again, we need to prove that this equation has the orthogonally propriety. Both sides of this equation are multiplied by *cos* $\lambda_n x\ dx$ and integrate enter the 0 to 1 limits. Than we have that:

$$A_n \int_0^1 \cos(\lambda_n x)\cdot\cos(\lambda_n x)dx = \int_0^1 \cos(\lambda_n x)dx \tag{A22}$$

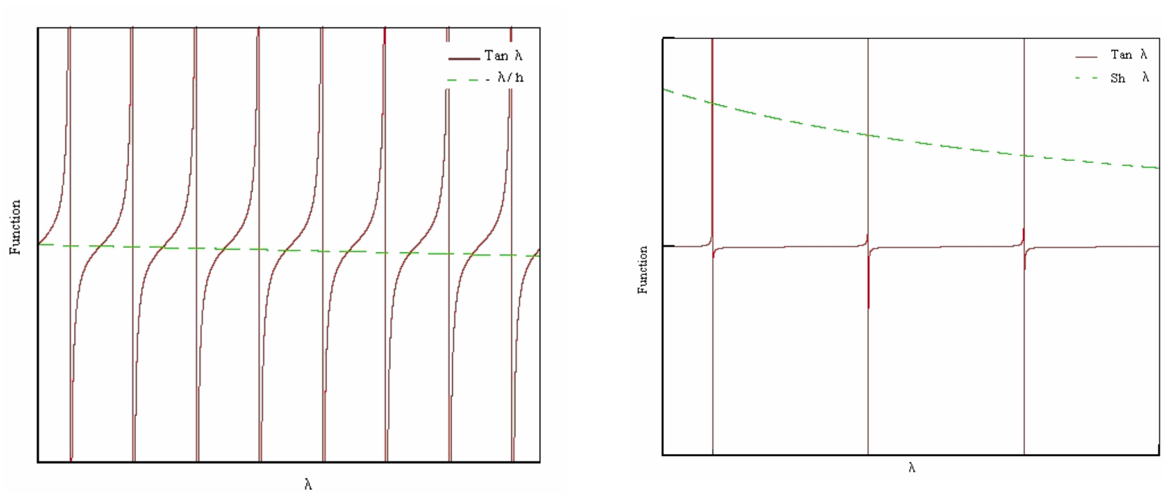
And

$$A_n = \frac{\left(\frac{1}{\lambda_n}\right)\cdot \mathrm{sen}(\lambda_n)}{\frac{1}{2}+\frac{1}{4\cdot\lambda_n}\cdot \mathrm{sen}2\cdot\lambda_n} \tag{A23}$$

Therefore, the solution to Eq. (16) can be written as:

$$\theta(x,\tau)=\left[\sum_{n=1}^{\infty}\left(\frac{\left(\frac{1}{\lambda_n}\right)\cdot \mathrm{sen}(\lambda_n)}{\frac{1}{2}+\frac{1}{4\cdot\lambda_n}\cdot \mathrm{sen}2\cdot\lambda_n}\right)\cdot\cos(\lambda_n x)\right]\cdot\exp\left(-\lambda_n^2\tau\right) \tag{A24}$$

The figure bellow represents the transcendental equation for cases 1 (figure a) and 2 (figure b).



a) case 1 b) case 2

Figure 3 – Solution to the transcendental equation for λ .