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ANALYSIS OF PARTICULATE MATTER DEPOSITION BY CONVECTIVE DIFFUSION IN TUBULAR FILTERS BASED ON GRAETZ PROBLEM

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Abstract. *The physical quantities found in transport phenomena, as well as the different physical mechanisms that involve these phenomena, have several applications discussed in several aspects, mainly in the areas of science and engineering. One of these applications is the analysis related to the rate of deposition of particles in a substrate and, in this view, several processes are listed, such as the deposition of particulate matter (PM). In this context, this work seeks to understand and interpret how the phenomenon of PM deposition behaves using a particular case and whose uniqueness promotes the interpretation of the phenomenon of PM deposition in a more limited scenario and that simplifies external variants. In the approach adopted here, particle deposition is analyzed in detail in a symmetrical circular tube with a fully developed laminar flow, which, in this way, can be interpreted as a PM tubular filter. The adoption of this approach will allow an analysis of the deposition analytically, based on the Graetz problem. The results show that the tests address what is expected from the physical problem in relation to the deposition of particles in cases of variation in the average speed and in the diameter of the particles. Particles of the same size tend to deposit more at low speeds, while larger particles have more significant advective effects than diffusive effects and, therefore, deposit less at the same average speed.*

Keywords: *Graetz Problem, Deposition Rate, Particulate Material*

1. INTRODUCTION

In natural flows, there is the presence of several scalars, chemical species, which are transported by different physical mechanisms. The transport of a scalar quantity within a flow is an area of study with many applications, and the substance transported in the flow may or may not affect such flow.

A widely discussed phenomenon in this context is the movement of particles suspended and transported by a fluid given a certain gradient. In the atmosphere, for example, the dispersion of pollutants, as comments Rodakoviski (2019) is influenced by heat flows and the amount of movement. These phenomena, which are of great interest, are due to their likely impact on health, the environment, and other processes that can be influenced by the dispersion of these pollutants.

In general, the study of the movement of suspended particles is not a simple task. Its complexity is anchored to the multidisciplinary nature of the problem, the diversity of applicable scales, and a number of other factors. This makes it necessary in general to apply the use of computational fluid dynamics simulations. The use of this computational tool is possible given the current availability of more sophisticated computers, but it still has high computational needs, and their use is still restricted (Oke *et al.*, 2017).

One of these applications is the analysis related to the rate of deposition of particles in a fluid and on this optics, a range of processes is listed, such as the deposition of particulate matter (PM). This deposition can occur after its emission in the atmosphere, which can cause damage to the environment, public health, and the conformity of systems or in the emission sources themselves, generally anthropogenic, such as chimneys. The related analyzes in this sense, generally have the idea of controlling and mitigating future impacts, so that they comply with the relevant legislation and/or can foster the analysis of the efficiency of the processes.

Oke *et al.* (2017) claim that without removal, air pollutants would accumulate in the atmosphere and concentrations would continually increase. The authors also point out that the removal of these, like the PM, can be done by four processes: gravitational settlement; dry deposition; wet deposition, and chemical and / or decay reactions.

This work seeks to understand and interpret how the phenomenon of PM deposition behaves using a particular case, in a more simplified way than the assessment of such deposition in the field. In the approach adopted here, the deposition of PM is analyzed in detail in a symmetrical circular tube with laminar flow fully developed through an analysis of deposition, in analytical format.

Analytically, the deposition of particles on the tube wall is treated based on an adaptation of the Graetz problem credited to the German physicist Leo Graetz. Graetz (1882) in his publication he talks about thermal conductivity and analyzes the heat exchange in a tube with a constant speed profile. The transfer of heat between a fluid and the wall of a tube can be generalized for several applications and its solution has been frequently researched in different approaches among studies of thermophoresis and other areas.

It is important to highlight that Ghiaasiaan (2011) also states that the development of concentration profiles in the mass transfer version for the Graetz problem would be similar. Thus, the study presented here is in line with the necessary reasoning to talk about an expression that represents the deposition of particles.

In the approach adopted here, the deposition of PM in the tube can be interpreted as a tubular filter that has the premise of removing particles from the flow, thus being retained/deposited on the wall of the tube, that is, it functions as a "non-porous filter" or "tubular membrane". In this context, a very important principle is applied for the adoption of the modeling described throughout this study, the adsorption principle (Seinfeld and Pandis, 2016).

According to Fernandes (2003) adsorption is a physical phenomenon in which one substance attaches itself to the surface of another, usually a solid medium, adsorbents (solids with microporous particles that retain particles without chemical reaction). Thus, the interactions between the tube wall and the particles start from the consideration that the particles when they find the wall are removed from the process if it is considered that its walls are formed by materials with adsorbent capacity.

This study aims to estimate the deposition of PM in a tube analytically based on the Graetz problem. To achieve this goal, the mathematical modeling of the dispersion problem is performed first. Their interpretations are discussed both from the adopted modeling and the results of the deposition of PM in a tube with a permanent and fully developed flow.

The interest of this study is to show that this approach, in addition to being in line with the physics of the proposed problem, can contribute in the future to field analysis as the PM data are more available and thus encourage the estimation of the concentration profile close to the surface and consequently estimate deposition. In this sense, with the expansion of the monitoring networks of the PM concentration in a location, such information will enhance the future determination of *Hotspot's* of greater attention, helping to take action regarding the effects of the deposition of these particles in the identified areas.

In short, the aim of this study is to propose PM deposition estimates in a tube with the analysis of the analytical solution of the Graetz problem.

2. METHODOLOGY

The methodology applied in this work consists of a qualitative and quantitative evaluation of the mathematical modeling and numerical simulation of the study problem and which seeks to understand the deposition of PM in a tube. The analytical and numerical methods can be understood as a group of theoretical methods for solving problems and here they are based on the thermophoresis theory which is extended to mass transfer by similarity. The laws of similarity between transport phenomena and different scales are powerful tools in engineering and therefore useful for the design of devices.

In this sense, the modeling adopted here is derived from the basic mechanics of fluids and simplifying assumptions for the study problem. For this, the phenomenon of interest is analyzed in such a way that it is possible to be treated similarly to the extended Graetz Problem and described by Flagan and Seinfeld (2012).

Although the mathematics involved is advanced and the methods are already disseminated in the literature, the results presented here, in addition to serving as a basis for review and the models obtained are useful for improving those of the analyzes already presented in the literature, given the greater availability tools that increase the accuracy of the analysis. Modeling involves a series of methods that include the delimitation of the general equation of the problem using Cartesian coordinates, separation of variables, dimensionless analysis, Sturm-Liouville problem, and the Kummer functions.

Finally, a discussion between the analytical results is analyzed to verify the potential of the modeling and the results obtained in the analyzed configurations and its interpretation of the tube as a PM filter medium.

2.1 Mathematical Modeling

The analytical modeling presented in this section for obtaining the general solution is based on the advection-diffusion equation, Eq. (1), which is the governing equation of the transport phenomenon that governs the study problem. In it, C represents the concentration of the particles, given in μg/m^3, for an incompressible fluid and described in Cartesian coordinates (x, y, z). In addition the velocity values are given by $\mathbf{U} = (u, v, w)$ and being $\mathcal{D}_{\mathcal{X}}$, $\mathcal{D}_{\mathcal{Y}}$, $\mathcal{D}_{\mathcal{Z}}$ are diffusion coefficients in each direction:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}\left(\mathcal{D}_{\mathcal{X}}\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mathcal{D}_{\mathcal{Y}}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mathcal{D}_{\mathcal{Z}}\frac{\partial C}{\partial z}\right) + S \tag{1}$$

For this work, a model similar to the Graetz problem will be adopted. For simplicity, it will be considered the case laminar in which $\mathbf{U} = (0, 0, w)$, that is, the case in which the speed is significant to only the z axis and has the same component equal to w. In addition, the diffusion coefficients in each direction by isotropy will be considered constant, so

$\mathcal{D}_{\mathcal{X}} = \mathcal{D}_{\mathcal{Y}} = \mathcal{D}_{\mathcal{Z}} = \mathcal{D}$. The term source will be considered null, that is, without source or sink. In this mode, a Eq. (1) can be simplified to a Eq. (2).

$$\frac{\partial C}{\partial t} + w\frac{\partial C}{\partial z} = \mathcal{D}\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) \tag{2}$$

As the tube has axial symmetry, it is convenient for this modeling to use a new coordinate system, called cylindrical coordinates and, the parabolic velocity profile w was obtained by the Poiseuille Equation where $\overline{U}$ is the average speed of the fluid and R is the radius of the tube, Eq. (3), already in cylindrical coordinates. The schematic representation of the problem is shown in the Fig. 1.

$$\frac{\partial C}{\partial t} + 2\overline{U}\left(1 - \frac{r^2}{R^2}\right)\frac{\partial C}{\partial z} = \mathcal{D}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C}{\partial \theta^2} + \frac{\partial^2 C}{\partial z^2}\right] \tag{3}$$

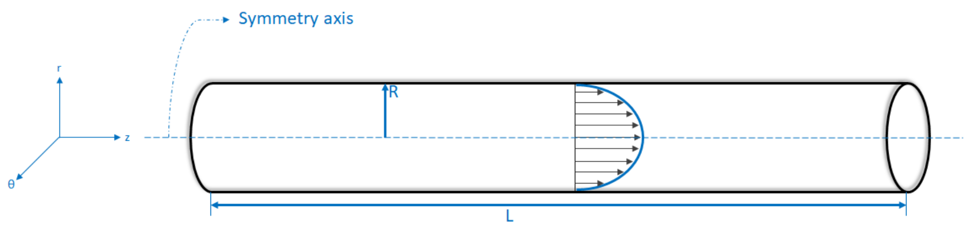


Figure 1. Schematic representation of the problem

Furthermore, considering the fully developed flow, with the independent variables limited to the problem domain: $0 < r < R$ and $0 < z < L$, where L is the length of the pipe, and $L >> R$ then the diffusion term in the direction of θ becomes very small in relation to an axial diffusion. This causes the Eq. (3) to be reduced to the Eq. (5) in the admensional format, applying dimensionless relations expressed by Eq. (4). Thus $\tilde{C}$ is now given as a function of only two variables, therefore $\tilde{C}(\tilde{Y}, \tilde{Z})$, which represent respectively the radial direction, and the axial direction in their admensional formats, where C_p is the concentration on the wall and C_0 the concentration at the entrance.

$$\tilde{C} = \frac{C - C_p}{C_0 - C_p} \quad \tilde{Y} = \frac{r}{R} \quad \tilde{Z} = \frac{z}{R\mathrm{Pe}} \tag{4}$$

Thus the equation is rewritten by the Eq. (5) and the boundary/initial conditions are expressed by the conditions Eq. (6), where (Pe) is the Peclet number. Adopting values for R, $\mathbf{U}$, $\mathcal{D}$ so that Pe $>> 100$ for the flow the term $\frac{1}{\mathrm{Pe}^2} << 1$ can be neglected.

$$(1 - \tilde{Y}^2)\frac{\partial \tilde{C}}{\partial \tilde{Z}} = \frac{1}{\tilde{Y}}\frac{\partial}{\partial \tilde{Y}}\left(\tilde{Y}\frac{\partial \tilde{C}}{\partial \tilde{Y}}\right) + \frac{1}{\mathrm{Pe}^2}\frac{\partial^2 \tilde{C}}{\partial \tilde{Z}^2} \tag{5}$$

Inlet: $\tilde{C}(\tilde{Y}, 0) = 1$
Wall: $\tilde{C}(1, \tilde{Z}) = 0$ (6)
Centerline: $\tilde{C}(0, \tilde{Z})$ is finite or $\frac{\partial \tilde{C}}{\partial \tilde{Y}} = 0$ em $\tilde{Y} = 0$

By associating the separation of variables, the Sturm-Liouville problems, and the Kummer Functions, it is possible to obtain the general solution given by the Eq. (7), and the self-functions represented by Eq. (8), obtained by applying the Kummer function. (Abramowitz and Stegun, 1965; Seinfeld and Pandis, 2016)

$$\tilde{C}(\tilde{Z}, \tilde{Y}) = \sum_{n=0}^{\infty} A_n Gz_n(\tilde{Y}) e^{\left(-\lambda_n^2 \tilde{Z}\right)} \quad \text{where} \quad A_n = \frac{\int_0^1 Gz_n(\tilde{Y})\tilde{Y}\left(1 - \tilde{Y}^2\right) \mathrm{d}\tilde{Y}}{\int_0^1 [Gz_n(\tilde{Y})]^2 \tilde{Y}\left(1 - \tilde{Y}^2\right) \mathrm{d}\tilde{Y}} \tag{7}$$

$$Gz_n(\tilde{Y}) = \mathrm{e}^{-\lambda_n \tilde{Y}^2/2} M\left(\frac{2 - \lambda_n}{4}, 1, \lambda_n \tilde{Y}^2\right) = \mathrm{e}^{-\lambda_n \tilde{Y}^2/2}\left(1 + \sum_{i=1}^{\infty} \frac{4i - 2 - \lambda_n}{4^i i! i!} \lambda_n^i \tilde{Y}^{2i}\right) \tag{8}$$

3. RESULTS AND DISCUSSION

The analyzes in this section of the concentrations in the tube and the deposition on the wall are treated, as already described above, analogously to the Graetz problem. They are described in a cylindrical tube with boundary conditions on the wall and on the central line (axis of symmetry) given by Dirichlet conditions, that is, with prescribed concentrations.

For a fully developed parabolic flow with a "non-porous" wall, the radial velocity is zero, where for a long tube, the axial changes are small and the axial diffusion is neglected compared to the radial one. In this sense, the general solution of the ordinary differential equation identified as a Sturm-Liouville problem and obtained using the separation of variables and series expansion is part of the general solution and must be analyzed and compared with information in the literature.

The values found in the Tab. 1 were obtained by interactive *Script's*. Standardized in the analyzes here, the use of five decimal places, the adoption of this standard was based on all tests here, as well as, in the analyzed literature, the use of more houses was not considered significant. Similar values have been found in the literature (Brown, 1960; Ghiaasiaan, 2011; Bhatti and Shah, 1987) for the first 11 λ_n, that is, the first eigenvalues of the general solution. This table also presents the values of A_n, which as expected and observed, such values only depend on the value of λ_n and are obtained by the equation defined in the chapter of mathematical modeling, applying finite-difference centered to the derivative.

Table 1. Eigenvalues and constants of the Graetz Problem

n	λ_n	A_n
0	2.70436	1.47644
1	6.67903	−0.80612
2	10.67338	0.58876
3	14.67108	−0.47585
4	18.66987	0.40502
5	22.66914	−0.35576
6	26.66866	0.31917
7	30.66832	−0.29074
8	34.66807	0.26789
9	38.66788	−0.24906
10	42.66773	0.23323

Physically, the problem takes into account that the concentration limit layer grows downstream of the flow road section and in this process, the transverse profile of concentration varies along with the axial positions, z. This interpretation leads to the definition of the mean flow concentration, which is a weighted average of the fluid concentration in the flow section.

The question now is whether to get the deposition rate. This estimate is based on the average concentration in the pipe section. This can be understood as the average concentration of particles at a distance below the tube, that is, the fraction of particles that survive diffusional deposition on the wall. In rectangular coordinates, this contraction can be obtained by Eq. (9), where A is the area of the cross-section (Bejan and Kraus, 2003). In dimensionless variables it is possible to rewrite the average concentration for Eq. (10). Then $\overline{\tilde{C}(\tilde{Z}=1)}$ is the average concentration to be estimated and based on it the deposition rate is obtained.

$$\overline{C(z)} = \frac{1}{\overline{U}A}\int_A wC\mathrm{d}A = \frac{\int_0^R C(r,z)2\pi rw dr}{\pi R^2 \overline{U}} \tag{9}$$

$$\overline{\tilde{C}(\tilde{Z})} = 4\int_0^1 \tilde{C}(\tilde{Z},\tilde{Y})\tilde{Y}(1-\tilde{Y}^2)\mathrm{d}\tilde{Y} \tag{10}$$

For the following results, a group of fixed variables were used, whose values are: $R = 0.002$ [m], $L = 1$ [m], where L is the length of the tube, the value of density $\rho = 1.2$ [kg/m^3] (Bejan and Kraus (2003)). The value of $D = 7.05 \times 10^{-10}$ [m^2/s] was obtained considering $D_p = 0.1$ [µm] (Flagan and Seinfeld, 2012). Cases 01 - 05 and were modified obtained by changing the velocity values in a regressive manner, decreasing the number of Reynolds Re for the five cases, thus maintaining the flow condition in laminar regime. The speed values were:

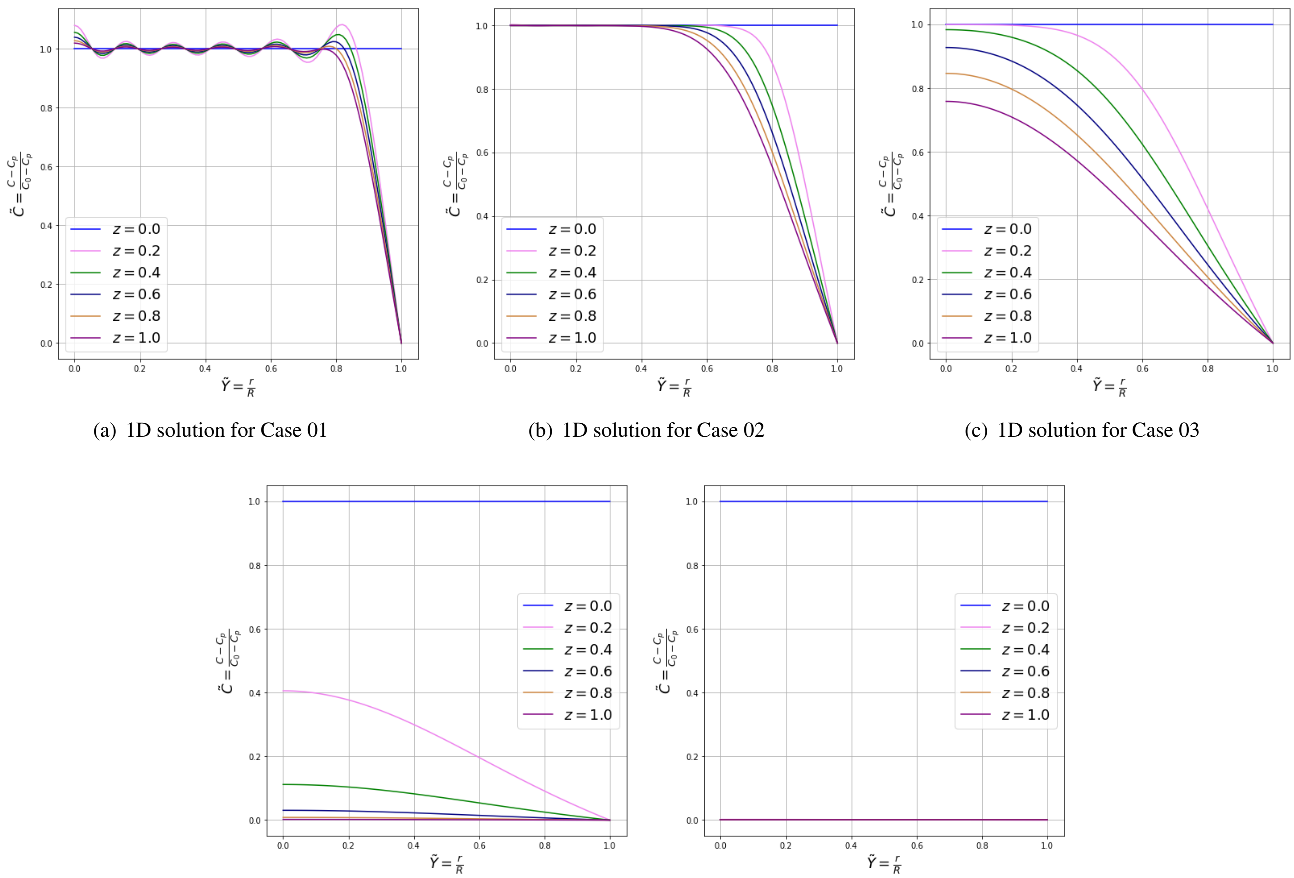
- (Case 01): $U = 0.1$ [m/s];
- (Case 02): $U = 0.01$ [m/s];
- (Case 03): $U = 0.001$ [m/s];

- (Case 04): $U = 0.0001$ [m/s];
- (Case 05): $U = 0.00002$ [m/s].

In addition, these values also meet the premises of the problem, such as the number of Peclet (Pe). All values obtained are described in the Tab. 2. For all cases the value of Schmidt's number, $\mathrm{Sc} = 2.126 \times 10^4$, since it depends on values that were fixed in all cases. Where the Gz represents the Graetz number that characterizes the laminar flow in a tube. Cases are tracked in the U speed range between 0.1 and 0.00002, since values greater than 0.1 have numbers from Re outside the laminar flow ranges and less than 0.0002 would have deposition of 100% of the particles on the wall.

Table 2. Results of dimensionless numbers

$Cases$	U [m/s]	Pe	Re	Gz	$\overline{\tilde{C}(\tilde{Z})}$ [%]	Deposition [%]
01	0.1	5.668×10^5	2.667×10^1	2.267×10^3	97.5	2.5
02	0.01	5.668×10^4	2.667×10^0	2.267×10^2	89.5	10.5
03	0.001	5.668×10^3	2.667×10^{-1}	2.267×10^1	58.6	41.4
04	0.0001	5.668×10^2	2.667×10^{-2}	2.267×10^0	2.4	97.6
05	0.00002	1.134×10^2	5.333×10^{-3}	4.535×10^{-1}	0	100



(a) 1D solution for Case 01 (b) 1D solution for Case 02 (c) 1D solution for Case 03

(d) 1D solution for Case 04 (e) 1D solution for Case 05

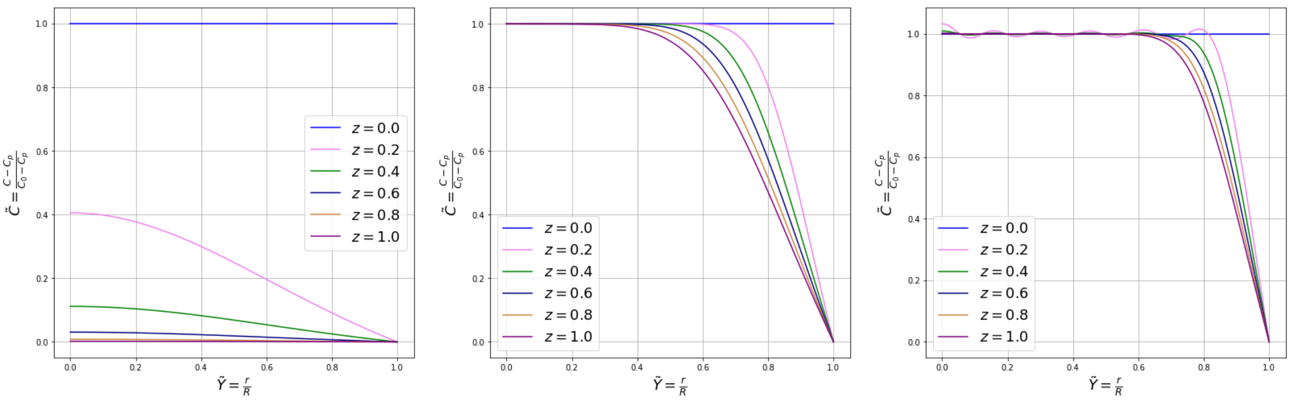
Figure 2. 1D concentration profiles for cases from 01 to 05

The analysis of Fig. 2 which are the profiles of concentrations along $\tilde{Y}$ in some points of the axial direction for each case associated with the values in Tab. 2 and allows us to conclude that the deposition increases as the mean velocity decreased.

Another test was done with different values of D_p, in this case the value of the diffusion coefficient was changed due to the particle diameter, being $D = 1.08 \times 10^{-11}$ [m^2/s] considering $D_p = 2.5$ [µm] e $D = 2.46 \times 10^{-12}$ [m^2/s] considering $D_p = 10$ [µm], named (Case 06) and (Case 07) respectively, in both cases were tested with U equal to Case 04 to observe the interference in deposition given the increase in particle Fig. 3 associated with the values in Tab. 3.

Table 3. Results of dimensionless numbers - Different D_p

$Cases$	D_p	Sc	Pe	Re	Gz	$\overline{\tilde{C}(\tilde{Z})}$ [%]	Deposition [%]
04	0.1	2.126×10^4	5.668×10^2	2.667×10^{-2}	2.267×10^0	2.4	97.6
06	2.5	1.383×10^6	3.668×10^4	2.667×10^{-2}	1.475×10^2	86.3	13.7
07	10	6.082×10^6	1.622×10^5	2.667×10^{-2}	6.488×10^2	94.6	5.4



(a) 1D solution for Case 04 (b) 1D solution for Case 06 (c) 1D solution for Case 07

Figure 3. 1D solution for Case 04, 06 and 07

The analysis of Fig. 3 which are the profiles of concentrations along $\tilde{Y}$ in some points of the axial direction for each case associated with the values in Tab. 3 allows conclude that the deposition decreased as the D_p increase. This result agrees with the Brownian motion theory, in which in short, as Seinfeld and Pandis (2016) comments, that the movement of the smaller particles is faster and more vigorous than the movement of the heavier ones. Therefore, it shows that Brownian diffusion and deposition is greater in particles with a smaller diameter, which impacts on deposition.

To complement the quality-quantitative visualization of the results, it is possible to illustrate the 2D profile dimensionless. For example, for the solutions of cases 04 (Fig. 4). In addition, the oscillations present in Fig. 2(a) and 3(c) are visible due to the use of the solution by series, but for the cases analyzed here they are not considered of significance, since the interest here is to determine the deposition, therefore. $\overline{\tilde{C}(\tilde{Z}=1)}$. In addition, they can be smoothed with the use of more eigenvalues in the solution.

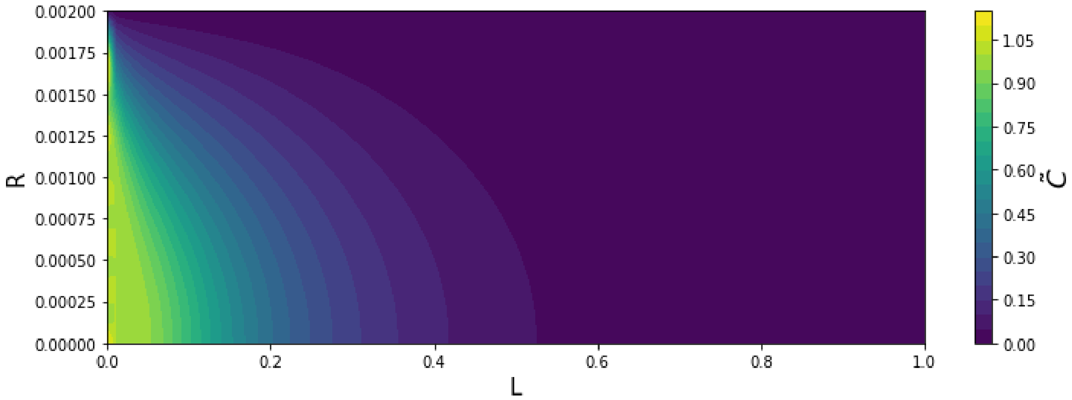


Figure 4. 2D solution for Case 04

4. CONCLUSION

The modeling of a phenomenon is an extremely important tool and requires a good understanding of the variables, their inter-dependencies, in addition to the laws that govern the phenomenon of interest. It also seeks to provide results that can be replicated and reproduced and in line with what is observed.

According to the proposed physical scheme, in the analysis, it is considered that the tube is long enough, which allows admitting that the flow is fully developed throughout the analysis region, being w a parabolic profile is given by the

Poiseuille equation and the concentration C_p and C_0 the uniform concentrations in the wall and in the entrance region, respectively.

The results of the previous section show that the tests address what is expected from the physical problem in relation to the deposition of particles in cases of variation in the average speed and in the diameter of the particles. Particles of the same size tend to deposit more at low speeds, while larger particles have more significant advective effects than diffusive effects and, therefore, deposit less at the same average speed.

In the figures presented, it can be noted that the more parabolic and sparse profile of the curves indicates greater deposition to the point that the deposition will be 100 %, that is, most of the particles do not survive diffusion.

In the case of ongoing research, the proposal for a new stage and sequence of this work is the adoption of a numerical method to be statistically analyzed together with the analytical results presented here.

5. ACKNOWLEDGEMENTS

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