Prediction of Concentration Profiles of Dispersed Particles through Horizontal Cylindrical Channels

Herbert Loría Molina, Pedro Pereira-Almao, Carlos Scott

Abstract— **Deposition of dispersed and ultradispersed solid particles in cylindrical channels has received considerable attention due to its practical significance and direct application in industry. However, an adequate mathematical expression that studies the separation and suspension of dispersed and ultradispersed particles present in a horizontal cylindrical channel in unsteady state is still missing. In this paper we developed and solved a time-dependent, two-dimensional convective/dispersive model. This model simulates the transient deposition and suspension of dispersed and ultradispersed particles immersed in a stagnant fluid medium inside the cross section of a horizontal cylindrical channel. The results of the modeling are compared with images taken from a series of experiments especially designed for this work. The conditions which permit to control the suspension of the solid particles inside a liquid medium with cylindrical geometry are unveiled by the presented model. The experiments conducted in this work can be a simple way for obtaining values of the dispersion coefficient, via measuring the time required by the particles to reach the steady state. The model so far developed can now be further expanded to consider flow movement.**

Index Terms— **Dispersed and Ultradispersed Particles, Suspension, Horizontal Cylindrical Channels, Modeling.**

I. Introduction

Mass transfer and deposition of fine particles in cylindrical channels has received considerable attention for a long time due to its practical significance and direct application in industry. For example, this knowledge is helpful in aerosol classification and its deposition under electrical fields, formation of deposits in heat exchangers and pipelines, hydrodynamic field chromatography, thrombus formation in organs, ultradispersed catalysis, etc. [1]. A theoretical prediction of the particle deposition in such systems would be very useful for the design and optimization of these processes.

The study of the particles behavior immersed in fluids began hundreds of years ago, when Archimedes introduced the concepts that made it possible to determine the forces acting on objects immersed in liquids. The next significant advance on the mechanics and dynamics of immersed objects was not accomplished until the late 17^{th} century with Newton's publication *Principia* [2]. However, it was not until the last few decades when significant advancement was made in the understanding about particle sedimentation in vertical and horizontal channels.

These advances began with the study of the motion and settling of a single rigid particle in various media and also under boundary layer effect [3]. Forney and Spielman [4] investigated the phenomenon of the sedimentation of particles in vertical flow and gave expressions for their sedimentation velocity for a wide range of diameters. Around the same time, Sehmel [5] and Yoshioka et al. [6] reported their study on the settling of large particles (with diameters larger than 200 μm) in horizontal flow. Laurinat and Hanratty [7] took into account the motion of the particles in different directions and proposed an empirical fit to a representative deposition flux profile as a function of the angle around the cylindrical channel cross-section in horizontal flow. The determination of the driving forces present in the settling of particles immersed in fluids has been recently studied by Molls and Oliemans [8]. They have modeled the dispersion and deposition as a combined process of turbulent diffusion and gravitational settling fluxes of particles in a one-dimensional problem between two horizontal plates.

To summarize, we now realize that the sedimentation phenomenon in horizontal channels is more complex as compared to those in vertical channels due to the additional effect of the gravitational force. Investigations have shown that due to the gravitational pull the sedimentation velocity of the particles in horizontal cylindrical channel is nonsymmetrical along the cross-section of channels [9].

It is generally believed that the sedimentation velocity in a horizontal cylindrical channel essentially depends on the fluid properties and the position of the particles around the channel cross-section. Also the effect of the gravitational force cannot

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be neglected. However, an adequate comprehensive physical model that evaluates the effect of the separation and suspension of the particles present in a horizontal cylindrical channel is still missing in literature.

The aim of this paper is to present a study on the mechanical separation and suspension of dispersed (particle diameters: 1 μm – 100 μm) and ultradispersed particles (particle diameters: < 1 μm) based on their motion through a medium in a horizontal cylindrical channel. The objective of this work is to develop and solve a time-dependent, two-dimensional convective/dispersive model to simulate the deposition and suspension of dispersed and ultradispersed particles immersed in a fluid inside the cross section of a cylindrical channel. The model is combined with an expression that represents the velocity of these particles. This velocity is dependent on the size and density of the particle as well as on the viscosity and density of the medium. The results of the modeling are compared with images taken from a series of experiments especially designed for this work.

In some systems, it is important to ensure that the particles present in the fluid medium remain suspended in it. Because of this; one aspect that is studied in this work is to obtain the conditions (particle diameter and dispersion coefficient) that are necessary to maintain particle suspension in a fluid enclosed by the cross-section of a cylindrical geometry.

II. Development of the Mathematical Model

A. Sedimentation velocity of solid particles

When a particle settles down in a liquid medium, it accelerates until the forces that cause the sedimentation equilibrate with the resistance or drag forces offered by the medium. Once this equilibrium is achieved, the particle has a constant sedimentation velocity called terminal sedimentation velocity, v_{pT}, which can be represented by [10]

$$v_{pT} = \frac{g(\rho_p - \rho_L) d_p^2}{18 \mu_L}, \qquad (1)$$

where g is the acceleration due to gravity, ρ_p is the density of the particle, ρ_L is the density of the liquid, d_p is the diameter of the particle and μ_L is the viscosity of liquid medium.

An expression for the time that the particle needs to reach certain sedimentation velocity can be calculated by

$$t_s = \frac{1}{36} \frac{\rho_p d_p^2}{\mu_L} \ln\left(\frac{v_{pT} + v_p}{v_{pT} - v_p} \right), \qquad (2)$$

where t_s is the necessary time to reach certain sedimentation velocity, v_p.

The Stokes law applicability is well accepted for predicting sedimentation velocity of a particle in a fluid medium; several limitations start to arise when having several particles in the system and the equation becomes non-applicable when high concentrations of particles are present [11]. At substantial concentration, particles start to interact with each other and the sedimentation velocity changes.

B. Analysis of the particle distribution across the cylindrical channel circumference

A continuity equation for the particle concentration, C_P, in a fluid medium can be obtained by carrying out a mass balance on a differential element of mass [12]. Considering that the effective dispersion coefficient, D_E, is constant (it is called effective because includes the turbulence effects caused by the particles and the gravity force in all directions) and that the particles have a velocity field **v;** then the continuity equation can be written as:

$$\frac{\partial C_P}{\partial t} + (\mathbf{v} \cdot \nabla C_P) = D_E \nabla^2 C_P. \qquad (3)$$

In order to develop a mathematical convection-dispersion model for the ultradispersed particles present in a fluid medium, consider a laminar incompressible flow which contains ultradispersed particles that flow inside a horizontal cylinder of radius R and length L. Therefore, cylindrical coordinates will be used in order to develop the model. The continuity equation in cylindrical coordinates is the following:

$$\frac{\partial C_P}{\partial t} + \left(v_r \frac{\partial C_P}{\partial r} + v_\theta \frac{1}{r} \frac{\partial C_P}{\partial \theta} + v_z \frac{\partial C_P}{\partial z} \right) = D_E \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_P}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 C_P}{\partial \theta^2} + \frac{\partial^2 C_P}{\partial z^2} \right]. \qquad (4)$$

The sedimentation of the ultradispersed particles affects the distribution of the particle concentration at each point of the horizontal cylinder. However, in this model only fully developed flow is considered, meaning that the model is taking on account a cross-section far enough from the entrance of the channel and consequently, the concentration profile does not change with the axial direction (z direction).

Thus, the particle concentration inside the horizontal channel will be modeled as a function of the position of the particles in the cross-section of the channel and the time, $C_P = C_P(r, \theta, t)$.

Equation (4) can be further simplified. This simplification would involve the assumption that the particle concentration is only a function of the radius r, and the angle θ. Also the angular velocity of the particle, v_θ, is small as compared to the radial velocity, v_r; therefore, it can be neglected. Equation (4) can be written as:

$$\frac{\partial C_P}{\partial t} + v_r \frac{\partial C_P}{\partial r} = D_E \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_P}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 C_P}{\partial \theta^2} \right]. \qquad (5)$$

The expression for the radial particle sedimentation velocity, v_r, is considered to be the projection of the vertical terminal velocity of the particle into the radial direction, that is, $v_r = v_{pT}\cos\theta$. Equation (5) can now be expressed as:

$$\frac{\partial C_P}{\partial t} + v_{pT}\cos\theta\frac{\partial C_P}{\partial r} = D_E\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_P}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C_P}{\partial\theta^2}\right]. \quad (6)$$

In the beginning of the process (t = 0) all the particles are well dispersed inside the cross section of the cylindrical channel. This means that the particle concentration is uniform everywhere inside the cross-section of the cylindrical channel. This concentration is the initial concentration of the particles, C_{P0}.

At $t = 0$, $\quad C_P(r, \theta, 0) = C_{P0}, \quad 0 \le r \le R,\ 0 \le \theta \le 2\pi.$ (7)

In the vertical axis there are symmetry boundary conditions that can be represented as:

$$-D_E\left(\frac{1}{r}\frac{\partial C_P}{\partial\theta}\right) + v_\theta C_P = 0\,. \quad (8)$$

Previously it was assumed that the angular velocity of the particle, v_θ, is neglected, therefore:

At $\theta = 0$, $\quad \frac{\partial C_P}{\partial\theta} = 0\,, \quad 0 \le r \le R.$ (9)

At $\theta = \pi$, $\quad \frac{\partial C_P}{\partial\theta} = 0\,, \quad 0 \le r \le R.$ (10)

In the center of the cylindrical channel the particle concentration does not vary with respect to the radius around all the angles:

At $r = 0$, $\quad \frac{\partial C_P}{\partial r} = 0\,, \quad 0 \le \theta \le 2\pi.$ (11)

The walls of the channel represent a physical boundary where there is no mass exchange between the interior and exterior of the cylinder. This is an insulation boundary that will prevent any particle from leaving the channel and gather all them at the bottom. The insulation boundary means that there is no convective or dispersive flux across that boundary. This can be represented by:

$$-D_E\left(\frac{\partial C_P}{\partial r}\right) + v_r C_P = -D_E\left(\frac{\partial C_P}{\partial r}\right) + \left(v_{pT}\cos\theta\right)C_P = 0\,. \quad (12)$$

Then:

At $r = R$, $\quad -D_E\frac{\partial C_P}{\partial r} + \left(v_{pT}\cos\theta\right)C_P = 0\,, \quad 0 \le \theta \le 2\pi.$ (13)

The convective/dispersive model is a linear second order parabolic partial differential equation and cannot be solved analytically by the method of separation of variables. Since in the convective term of Equation (6) there is a variable coefficient (the term v_r is a function of the angle θ), it is not possible to divide the variables into two ordinary differential equations. However, the equation can be solved by a large variety of numerical methods: finite differences, finite element, finite volume, characteristics methods, discontinuous Garlekin methods, etc.

As a complimentary study for this research, the convective/dispersive model was solved at steady state. Two different numerical solutions for the model were presented and compared: one based in finite differences equations and the other in the finite element method. The solution based on the finite element method presented better convergence and stability properties due to the regular grid structure and its flexibility with respect to the adaptation to the geometry domain. Based in these results, the finite element method was used to solve the convective/dispersive model. Computational fluid dynamics software was used in order to apply the finite element method. The solution of the convective/dispersive model is presented in the Results section of this work.

III. Experiments

The objective of the experiments is to observe the behavior of dispersed particles immersed in a fluid media. Alumina particles with an average size of 75 μm were used. The fluid medium was a 50:50 (v/v) mixture of water and glycerol. The alumina particles were painted with a dye in order to enhance the visibility in the fluid medium.

The experiments were performed in a custom made plexiglass cylinder (that was designed for this work) with an internal diameter of 4.44 cm and 6.45 cm in length. These dimensions represent 100 ml of volume inside the cylinder. The cylinder was closed at both ends with two small square plexiglass slabs glued to the open ends of the cylinder. For these experiments the relation of particles-fluid used was 1 g of particles in 100 ml of fluid. The molar concentration of the particles in the cylinder is 97.8313 mol/m^3 if the density of the alumina is taken as 3970 kg/m^3 [13].

The cylinder was filled with the solution of water and glycerol. Then the solid particles were introduced from a small orifice in the top of the cylinder. The orifice was covered with a plug and the cylinder was agitated. The cylinder was then left in repose and the phenomenon was photographed and recorded with a digital camera. A series of photographs that show the complete process of the particles deposition is presented in Fig. 1.

One important parameter measured during the experiments was the time that the particles need to sediment completely. This is the time that was necessary to reach the steady state, that is, when there was no change in the particle concentration. In this set of experiments the time needed to reach the steady state was about 74 s.

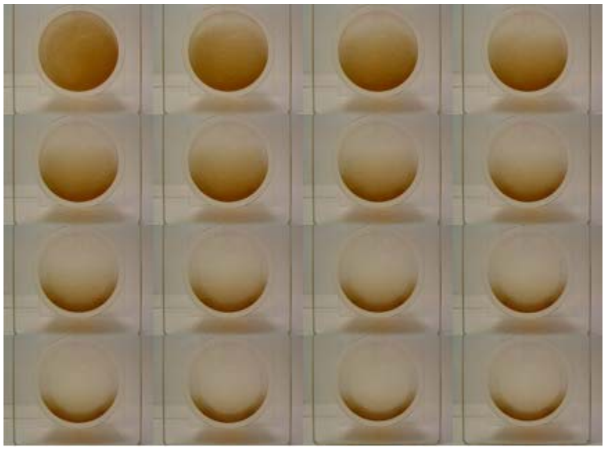

Fig. 1 Series of photographs of the particle sedimentation process

IV. Results and Discussion

A. Parameters of the model

In Equation (6) (which represents the convective/dispersive mathematical model) it can be seen that there are two important parameters: the radial velocity, v_r, and the effective dispersion coefficient, D_E.

The radial velocity is related to the vertical velocity by an angular projection of the latter over the radius of the cylinder ($v_r = v_{pT} \cos\theta$). The vertical velocity is considered to be the particle sedimentation velocity, v_p. If v_p stays constant during the sedimentation of the particle, then it is equal to the terminal particle sedimentation velocity, v_{pT}, which depends on parameters such as the density of the particles, ρ_p, and of the fluid, ρ_L, the viscosity of the fluid, μ_L, the diameter of the particles, d_p, and the acceleration due to gravity, g.

The data obtained from experiments in our lab was used as the input parameters to obtain a numerical solution of the convective/dispersive model. The density of the alumina particles (ρ_p) was 3970 kg/m^3 [13], and the diameter of the particles (d_p) was 75 µm. The fluid medium is a 50:50 (v/v) mixture of water and glycerol. The density of this mixture (ρ_L) at 25°C is 1261 kg/m^3, and the viscosity (μ_L) is 6.05×10^{-3} Pa s [14].

With these values it is now possible to calculate the terminal velocity of the particles. Using the Stokes law (Equation (1)) the obtained value is $v_{pT} = 1.37 \times 10^{-3}$ m/s. The Stokes law is valid for solutions with small values of solid volume fraction [11] and Reynolds numbers below 2 [10]. The solid volume fraction in this case was 0.002513 and the Reynolds number associated to the terminal velocity is calculated to be 0.0214, which confirms the validity of the use of the Stokes law for the terminal velocity.

Equation (2) can be used to know how long it takes to reach the terminal sedimentation velocity. The time to reach the 99.99% of the terminal velocity was calculated to be 1.015×10^{-3} s. Since the time to reach the terminal sedimentation was very short, it can be considered that the particle sedimentation velocity on Equation (6) was practically constant.

The effective dispersion coefficient of the particles, D_E, depends on the characteristics of the turbulent flow and the size of the channel. It can be calculated using various empirical equations for various Reynolds numbers [15-17]. However, these empirical relations are only valid for certain materials and ranges of particle size. The best way to obtain this value is to perform an adjustment of this parameter using concentration values from experimental data and the results of the mathematical model at different points of the cross-section of the cylinder and then apply nonlinear parameter estimation.

Since there are no experimental data or empirical correlations reported in literature for the materials used in this work, the following procedure was performed in order to obtain the value of the effective dispersion coefficient of the particles.

As a first approximation, a particular value of the dispersion coefficient was used to solve the convective/dispersive model. Once a solution was obtained, the time at which the simulation did not give any more changes in the concentration (the time at which the steady state is reached) was recorded and compared with the one obtained from the experiments. Then, the dispersion coefficient was changed in the simulation, until the time necessary to reach the steady state in the simulation became equal to the one obtained from the experiments.

The value of dispersion coefficient used in the simulation, as an initial guess, was the one reported by Snyder and Lumley [18]. It was calculated for solid particles with similar density and size than the ones used in this work for Reynolds numbers below 5 in an air flow. The value of the reported effective dispersion coefficient of the particles, D_E, was 1.38×10^{-4} m^2/s.

B. Solution of the convective/dispersive model using the finite element method implemented with computational fluid dynamics

A mass transfer time-dependent two dimensional convection-dispersion simulation was carried out using computational fluid dynamics software (COMSOL MULTIPHYSICS™). The results were obtained as follows.

The initial concentration, C_{P0}, considered for the solution was the same one that was used for the experiments (97.8313 mol/m^3). As mentioned above a first guess of the dispersion coefficient, D_E, was used to initially solve the model and compare the results with the experiments. After several comparisons it was found that the dispersion coefficient that produced the closest solution to the experiments was 7.88×10^{-6} m^2/s.

The modeled cross-section of the cylinder has the same diameter (4.44 cm) as the one used in the experiments. The selected boundary condition from the computational fluid dynamics software was the insulation/symmetry boundary condition for all the boundaries present in the model, that is, the complete circumference of the channel. For the solution of the model 2968 grid points were used. The solution of the time dependent convective/dispersive model at different times is presented in Fig. 2.

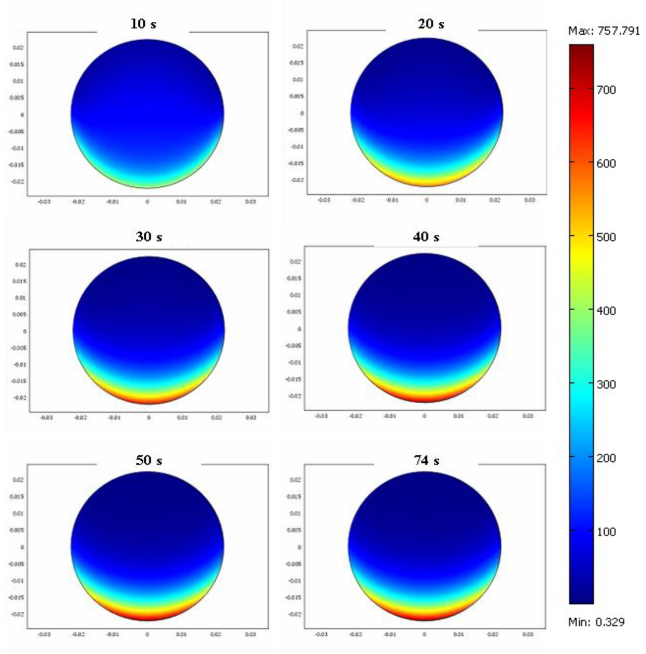

Fig. 2 Surface response of the results of the sedimentation mathematical model at different times. Concentration in mol/m^3

C. Discussion of the results

The solution of the model shows that the particles gathered at the bottom of the cylinder. Therefore, the concentration in this part increases to values higher than the initial concentration. On the other hand, the particles rapidly leave the top of the cylindrical channel, resulting in very low values of concentration in this zone.

According to the solution of the model, the maximum concentration at the bottom of the cylinder at steady state was 757.791 mol/m^3. This concentration decreases as the angle increases from 0 to π, at the top of the cylinder the minimum concentration was 0.329 mol/m^3.

The photographs of the experiments (Fig. 1) show that the shape in which the particles are distributed in the cross-sectional part of the cylinder is the same as predicted by the convective/dispersive model (Fig. 2).

D. Effect of the dispersion coefficient and particle diameter in the deposition of particles inside a horizontal cylinder

One of the targets of this research is to unveil the conditions that are necessary to maintain particle suspension inside a medium with cylindrical geometry. In this part of the work the convective/dispersive simulation model is applied to a system of interest for the petroleum upgrading and refining industry: MoO_3 hydroprocessing catalytic particles (density = 4500 kg/m^3) flowing in Athabasca bitumen. The physical properties of this bitumen can be calculated with thermodynamic models that were developed by us in a parallel research [19].

The objective of these simulations is to find the critical values of particle diameter and dispersion coefficient that permits that the MoO_3 particles flowing in Athabasca bitumen remain suspended in the cross-section part of a horizontal cylinder (which can represent a pipeline).

Fig. 3, 4, 5 and 6 show the results of several simulations carried out with different particle diameters and dispersion coefficients. The maximum particle concentration inside a horizontal cylinder, that is, the concentration at the bottom of the cylinder for a very long time (steady state) is represented in the vertical axis. Each figure represents the results of the simulations at different temperatures (and therefore different densities and viscosities of the bitumen) with an initial concentration of 100 mol/m^3, thus, the fact that the maximum concentration tends to this value means that there is not particle deposition at the bottom of the pipe.

The first effect that can be seen in the simulations is that as the dispersion coefficient increases the concentration of the particles tends to the initial one, that is, for high dispersion coefficients settling of particles will not occur. In the case of the particle diameter there is a zone for values lower than 1×10^{-7} m (100 nm) where the maximum concentration is the initial one independently of the dispersion coefficient value, this means that particles smaller than 100 nm will remain suspended in the fluid for any temperature, viscosity or dispersion coefficient in the medium.

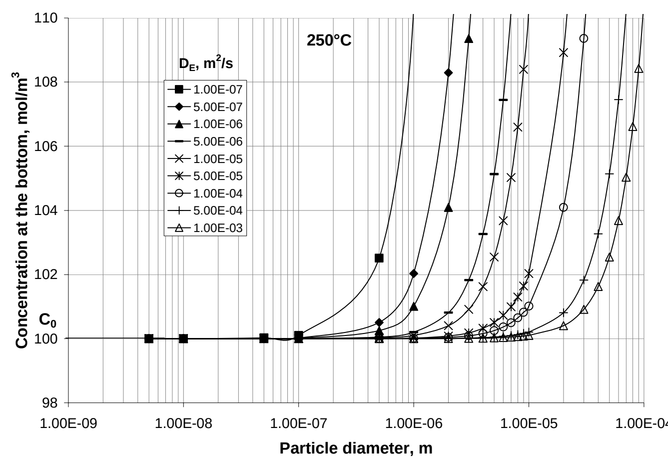

Fig. 3 Effect of the dispersion coefficient and particle diameter. Athabasca bitumen properties at 250° C: Density = 938.08 kg/m^3, Viscosity = 4.27 mPa s

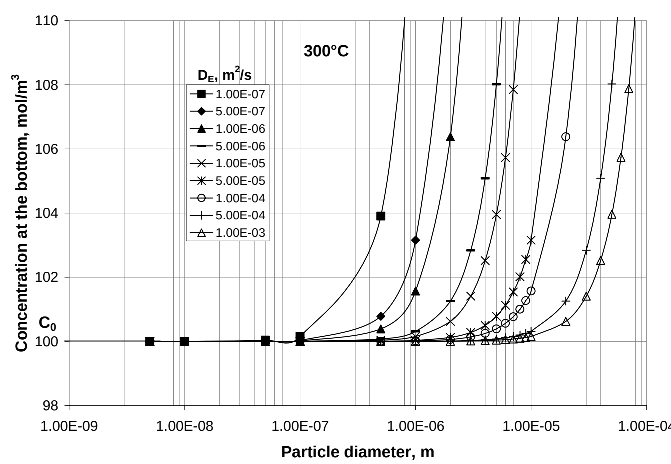

Fig. 4 Effect of the dispersion coefficient and particle diameter. Athabasca bitumen properties at 300° C: Density = 911.1 kg/m^3, Viscosity = 2.78 mPa s

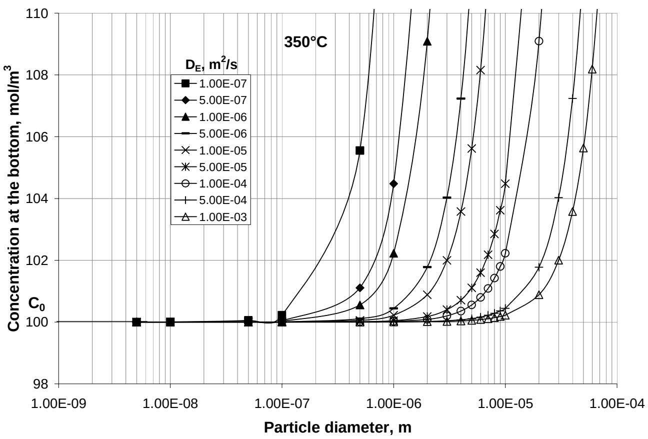

Fig. 5 Effect of the dispersion coefficient and particle diameter. Athabasca bitumen properties at 350° C: Density = 877.21 kg/m^3, Viscosity = 1.98 mPa s

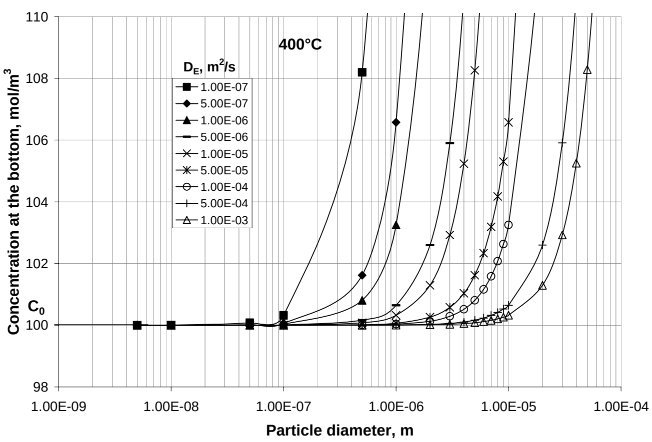

Fig. 6 Effect of the dispersion coefficient and particle diameter. Athabasca bitumen properties at 400° C: Density = 826.28 kg/m^3, Viscosity = 1.38 mPa s

V. Conclusions

The proposed convective/dispersive model is a useful tool for determining the concentration distribution of ultradispersed particles at different times in a given zone of a cylindrical channel.

As confirmed by the experiments and the model for particles sizes in the micrometer range, the concentration of particles in horizontal cylindrical channels has a nonsymmetrical distribution due to the effect of the gravity force.

The experiments conducted in this work are a new alternative for obtaining values of the dispersion coefficient. It was demonstrated that the dispersion coefficient can be determined by simply measuring the time required by the particles to reach the steady state. This is an easier method than the typical parameter adjustment, which consists on the use of the concentration values from experimental data and the results from the mathematical model at different points of the cross-section of the cylinder to apply nonlinear parameter estimation. This procedure is complex in the case of models that deal with partial differential equations.

The convective/dispersive simulation model can predict the ranges of particle sizes and dispersion coefficients at which sedimentation of the particles will not occur. In the system analyzed in this work (MoO_3 particles flowing in Athabasca bitumen) it was found that particles smaller than 100 nm will remain suspended in the fluid for any temperature, viscosity or dispersion coefficient present in the medium.

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