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CONSEQUENCES OF THE CONFINEMENT ON THE MASS OR HEAT TRANSFER ON A SPHERICAL PARTICLE IN NON-NEWTONIAN FLUIDS

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ABSTRACT

In non-Newtonian fluids, the mass or heat transfer on particles are of major interest in many industrial processes using suspensions such as fluidized beds or microfluidics reactors. In all these problems we often face hydrodynamic and mass or thermal interactions between a single particle and others or between a single particle and some walls. In this study, such confined configurations can be modeled by a spherical particle translating parallel to the axis of a cylindrical tube. As the suspending fluid may be non-Newtonian, and before examining any possible additional viscoelastic effect on suspension, the first step in the understanding of the consequences of the principal non-Newtonian behavior is the study of the shear thickening or shear thinning (power law model) regarding the transfer phenomena. Then, when the particle translates along the axis of the tube in symmetrical configuration, we numerically solved the momentum and mass (or heat) transfer equations using the stream/vorticity functions formulation coupled to the singularity technique in order to make a numerical conformal mapping for the mesh. For Newtonian fluids, the successful comparisons firstly between our numerical results and asymptotical solutions obtained by us in the lubrication regime, and secondly between our results and those obtained by other authors in unlimited medium, confirm the validity of our approach. Thereby we extended this method to power law fluids. As the geometrical distribution of particles in suspensions is not at all symmetric, we study the influence of some geometrical disturbance breaking the symmetry of the system. To answer this question, we numerically investigate, using the finite volume method, the simple configuration of single spherical particles translating parallel to and in the off-axis position in the tube.

INTRODUCTION

In various kinds of engineering processes (fluidized beds reactors for example) we are concerned by the mass or heat transfer on suspensions of spherical particles. More and more, in many processes the transporting fluid is non-Newtonian. These processes are also present in microfluidics systems (biochemical, …). The control of mass or heat transfer on spherical particles in suspensions or in microchannels implies to understand hydrodynamic and mass or thermal interactions between single particles and others or between a single particle and some plane or curved walls. These confined geometrical configurations can be modeled by a spherical particle translating at constant velocity parallel to the axis of a cylindrical tube and maintained at fixed concentration or temperature. As such configurations rarely have specific geometrical symmetries, the knowledge of the consequences of an asymmetry in the transfer on a sphere is therefore useful for optimization of this transfer. In fact, the introduction of some geometrical noise in the position of particles or in variation of their diameters (polydisperse particles) in an array of ordered monodisperse spheres could lead to a fluctuation of the transfer with amplitude that is necessary to be estimated. In order to elucidate the physics which controls the transfers involved in such geometrically disturbed situations, we focus in this work on the basic model constituted by the same sphere translating at constant velocity parallel to the axis and in different off-axis positions in the tube. As the suspending fluid may exhibit a non-Newtonian rheological behavior, and before studying the possible additional viscoelastic effects on suspensions, it is worthwhile to have a sufficient knowledge on the main behavior exhibited by almost non-Newtonian fluids which are the shear thinning or shear thickening described by Ostwald-de Waele model. In all cases, the momentum and mass or heat transfer problems are solved for Dirichlet or Neumann boundary conditions.

Let us recall that the effect of the confinement on the hydrodynamic correction factor of the drag submitted by a sphere in power law fluids, at low generalized Reynolds numbers, is solved previously [1,2] from unbounded medium to the lubrication regime. Notice also that in the case of shear thinning, our dynamical results are in good agreement with those given by Missirlis et al. [3] and by Chhabra et al. [4,5] for $0 \le k \le 0.5$. In this work, we will give the correction factor due to this confinement on the mass or heat transfer on a sphere in this non-Newtonian fluid. A comparison with an asymptotic approach in the lubrication regime is made. At low Reynolds numbers, in contrary to the Newtonian case where the thickness of the boundary layer is very high and a cutoff of this one can be introduced only by the confinement, notice that the power law behavior introduces (at low generalized Reynolds numbers) a hydrodynamic screen length $\xi \sim 1/r^{1/n}$ which can be controlled through the index of the fluid n. In this situation, it is expected that in the mass or heat transfer, the introduction of this screen length implies another cutoff permitting, in the shear thinning case ($n<1$), a decrease of the mass or thermal boundary layers in the convective regime (for high Péclet numbers) which can allow an increase of the flux.

Due to the difficulty to give an analytical solution of this non linear hydrodynamic problem despite the linearity of the mass (or heat) transfer equation, we numerically solved the momentum equations using the stream/vorticity functions formulation coupled to the singularity technique in order to make a numerical conformal mapping for the mesh. The velocity vector components are expressed in terms of the stream function in the mass or energy equation which is written in the new coordinates. For the solution of these differential equations we have used the finite differences method. We successfully verified our results by using the finite volume CFD code FLUENT.

BASIC EQUATIONS AND METHODS OF SOLUTION

The aim of this study is to determine the influence of the confinement on the mass or heat transfer on a spherical particle of radius a moving at constant velocity U_0 parallel to the axis of a tube of radius $b = a/k$ and maintained at concentration c_s (or temperature T_s) when it is placed in an off-axis position in the tube filled with a power law fluid. Firstly, the dynamic problem was solved in unbounded and confined medium and is not discussed here but all the results have been successfully verified by a comparison with our asymptotic calculations in the lubrication regime [1,2]. Let us recall that the rheological law of the Ostwald-de Waele fluid is described by $\underline{\underline{\sigma}} = -p\underline{\underline{\delta}} + 2m(2D_{II})^{(n-1)/2}\underline{\underline{D}}$ where $\underline{\underline{\sigma}}$ is the stress tensor, $\underline{\underline{D}} = (1/2)\left(\underline{\underline{\nabla\vec{u}}} + \underline{\underline{\nabla^t\vec{u}}}\right)$ is the strain rate tensor and $D_{II} = tr\left(\underline{\underline{D}}^2\right)$ is the second invariant with $\vec{u}$ the fluid velocity. This law exhibits a shear thinning behavior $\left(for\ n<1\right)$ and a shear thickening one $\left(for\ n>1\right)$. The apparent viscosity of such fluids is given by: $\mu_a = m\left(2D_{II}\right)^{(n-1)/2}$. This flow takes place at very low generalized Reynolds number $\mathrm{Re}_n = \rho U_0^{\,2-n}\left(2a\right)^n/m$. The fluids we are concerned with have sufficiently high Schmidt numbers (or high Prandtl numbers: highly viscous fluids) to reach a range of Péclet numbers $Pe = 2aU_0/D_m$ where the convective regime can take place. D_m corresponds to the molecular diffusion coefficient (in the thermal case, this coefficient must be replaced by the thermal one $D_{th} = \lambda/\rho C_p$). In spite of the dynamic non-Newtonian behavior of the fluid in this work, both diffusion coefficients are assumed to be in first approximation independent of the hydrodynamics, and then they are supposed to be constant. Besides, all the thermo-physical properties are supposed to be constant. But it is important to point out that in the lubrication regime, as the fluid elements will locally experience higher rate of shearing in the small gap, the viscous dissipation may not be negligible anymore with shear thickening fluids, necessitating to add the Rayleigh dissipation function to the energy equation and the thermodynamic laws describing the evolution of the thermo-physical properties. In these conditions, the equations which must be solved here are reduced to the Cauchy equations taking into account the rheological power law model, the continuity equation and the convective mass transfer equation (or the energy equation). The momentum equations have been solved numerically by using the stream function ψ and vorticity ω, which are written in an orthogonal system of curvilinear coordinates matching perfectly the contours of the sphere and the cylindrical wall of the tube. We express the velocity vector components in terms of the stream function in the mass (or energy) equation which is written in the new orthogonal coordinates. All these equations have been written in a dimensionless form, by the use of the respective characteristic parameters: length (a), velocity (U_0), pressure $\left(m\left(U_0/a\right)^n\right)$ and time $\left(\rho a^2/\left(m\left(U_0/a\right)^{n-1}\right)\right)$. The dimensionless concentration is defined by: $c_+ = \left(c - c_s\right)/\left(c_\infty - c_s\right)$. The generation of the grid was performed by the singularities method, corresponding to the

internal flow of an inviscid fluid [6-9]. The domain with curved borders was transformed into a rectangular domain through a numerical conformal mapping. Then a finite differences method was applied by using the successive over-relaxation (S.O.R.) and the alternating direction implicit (A.D.I.) techniques [10-13] respectively to calculate the functions ψ and ω of the fluid. For more details, this method is explained in [14]. The convergence criterion is defined as $\left|\left(Sh^{i+1}(k,n,Pe)-Sh^{i}(k,n,Pe)\right)/Sh^{i+1}(k,n,Pe)\right|<10^{-6}$. In all cases, we numerically calculated the Sherwood (or Nusselt number) $Sh(k,n,Pe)=\phi_m(k,n,Pe)/2\pi aD\,\Delta c$ for different Péclet numbers, different confinements $k=a/b$, different eccentricities $e=d/a$ and different indexes of fluidity n. Let us recall that for the thermal corresponding problem, the Nusselt number is obtained by replacing $\phi_m(k,n,Pe)$ by $\phi_s(k,n,Pe)/\rho C_p$. To check this numerical method, we successfully verified our results by using the finite volume CFD code FLUENT, where the SIMPLE algorithm was employed with a QUICK scheme on a structured mesh. The convergence criterion used is similar to the one used in our method. Nevertheless in front of this success, we used this last code to solve the asymmetric problem in 3D geometry. In fact, in this situation, the problem is fundamentally tridimensional in contrary to the axisymmetric case which possesses an axial symmetry in the range of the low Reynolds numbers considered here.
The geometry and the boundary conditions used in this problem are defined in the Fig. 1.

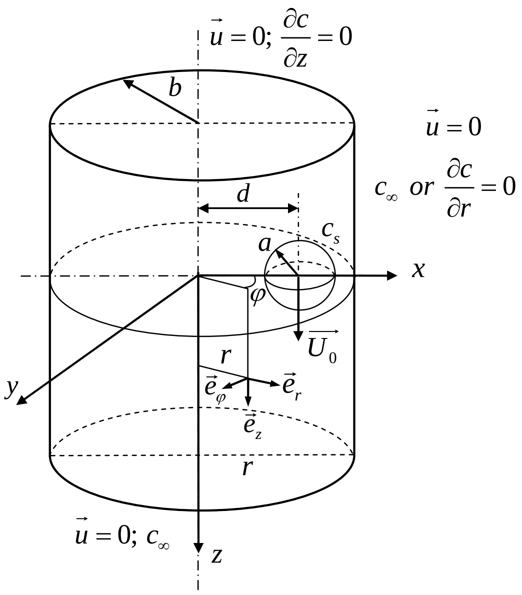

Figure 1: Sketch of the problem

RESULTS AND DISCUSSION

In this chapter, we will give and discuss our numerical and asymptotical results concerning the transfer on the sphere translating at low Reynolds numbers in the axial and off-axis position of the tube filled with an Ostwald-de Waele fluid.

Case 1: Sphere in symmetrical position

To improve our numerical method, we calculated for the Newtonian fluid the evolution of the Sherwood number (or Nusselt number in the thermal case) with the Péclet number for very low confinements until we have no influence of the tube's wall. We compare the results obtained for $k=a/b=10^{-6}$ with the well-known analytical result given by Acrivos [15] and Leal [16] for low Péclet number:

$$Sh(Pe<1)=2+\frac{Pe}{2}+\frac{1}{4}Pe^2\ln\frac{Pe}{2}+0.2073Pe^2+\frac{1}{16}Pe^3\ln\frac{Pe}{2} \quad (1)$$

and by Acrivos et al. [17] for high Péclet numbers:

$$Sh(Pe>5)=1.249\left(\frac{Pe}{2}\right)^{1/3}+0.922 \quad (2)$$

The successful comparison seen in the Fig. 2 with our results and those analytical ones confirms the validity of our code in the Newtonian case and confirms that the infinite medium is achieved for $k=10^{-6}$ and even for $k>10^{-2}$.

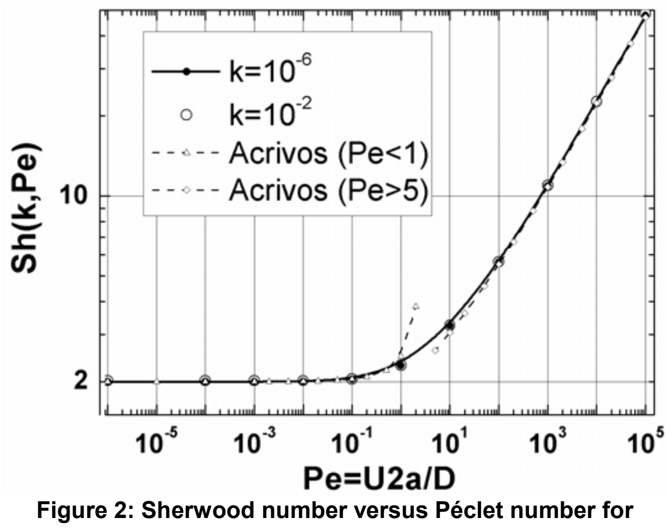

Figure 2: Sherwood number versus Péclet number for unbounded medium for the Newtonian fluid $(n=1)$

Let us remark that for the micro and nano-particles, as their radius is very low, we are not concerned by the convective regime for the transfer and all the transfer takes place in the plateau regime (pure diffusive). For this reason, we are studying the influence of the confinement in this pure diffusive regime.

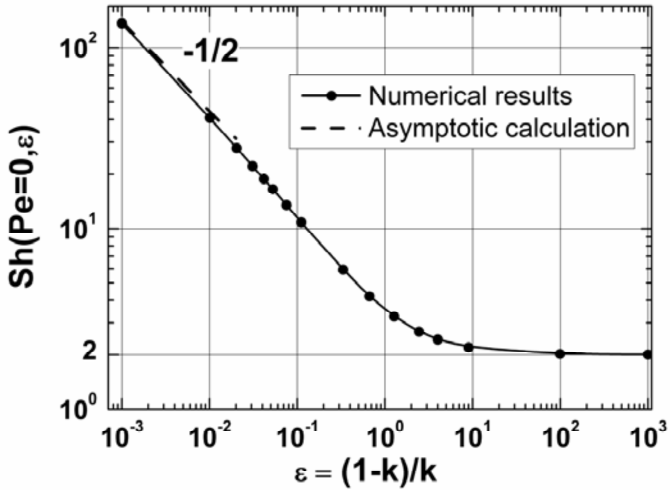

Figure 3: Evolution of the Sherwood number with the confinement (Dirichlet boundary condition)

For very low Péclet numbers, at pure diffusive regime, it is obvious that the transfer coefficient (Sherwood or Nusselt) does not depend on the Péclet number for a finite-size particle or in confined geometry. And also, it does not depend on the dynamic non-Newtonian character of the fluid as explained above. For all these reasons, we give, for a Dirichlet boundary condition, in the Fig. 3 the variation of the Sherwood number with the reduced distance between the sphere in the axial position and the tube which is valid for Newtonian and non-Newtonian fluids. In the lubrication regime, the Sherwood number varies as $\varepsilon^{-1/2}$ which is in good agreement with the asymptotic calculation giving the following relation:

$$Sh\left(k, Pe=0\right) \approx \pi\sqrt{2}\varepsilon^{-1/2} \qquad (3)$$

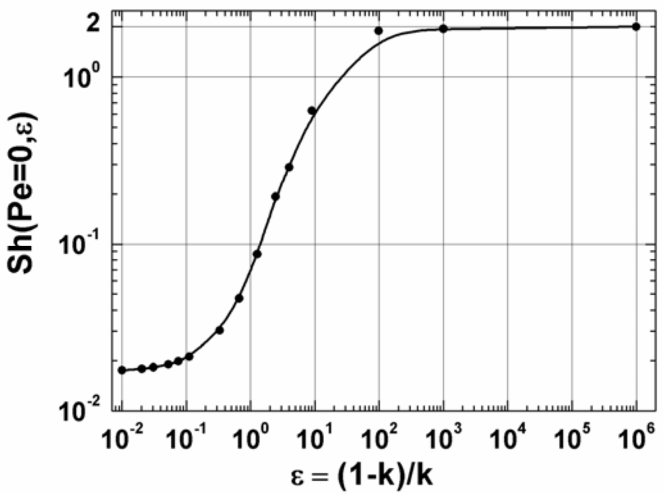

Figure 4: Evolution of the Sherwood number with the confinement (Neumann boundary condition)

But when we impose, in the same diffusive regime, the Neumann condition to the tube's wall, the transfer decreases with the confinement in contrary to the Dirichlet case for which the transfer increases with the confinement, as it is shown in Fig. 4. This decrease of the transfer, when the particle draws near the tube's wall is due to the fact that the isoconcentration lines are forced to be perpendicular to this wall, then reducing the thermal gradient on the sphere. However, one can note that a saturation regime of the transfer is reached in the lubrication regime.

For non-Newtonian fluids we give in the Fig. 5 the numerical results obtained for unbounded medium. The principal result is that the transfer is enhanced in the case of the shear thinning behavior $\left(n<1\right)$ and decreased in the shear thickening fluid$\left(n>1\right)$. In fact, in the first case as the hydrodynamic length screen ξ varies as $1/r^{1/n}$ in turn the mass transfer boundary layer decreases inducing an enhancement of the flux. The opposite scenario takes place in the shear thickening case.

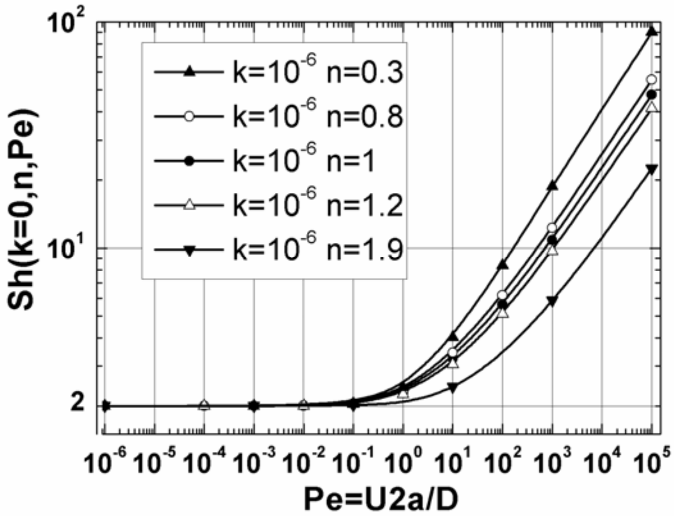

Figure 5: Sherwood number versus Péclet number for unbounded medium for a power law fluid

In the Fig. 6, we give for the mass Dirichlet condition on the tube's wall the results of the transfer on the sphere with Péclet number for different confinements k and for different fluidity indexes n. As discussed above, for the low confinements, these results can be explained by the fact that the hydrodynamic screen length in power law fluids decreases for shear thinning fluids and consequently as the flux is inversely proportional to the diffusive boundary layer thickness, the flux therefore increases. The opposite situation occurs for shear thickening fluids with the decrease of the transfer. But for high confinements, we have an additional length scale due to the confinement which is the gap between the sphere and the tube. Then when the gap is lower than the hydrodynamic screen length, the transfer is controlled principally by the confinement. Thus the insensibility of the transfer to the fluidity index n can be explained. The principal enhancement of the transfer is due to the confinement. For high Péclet numbers, the Sherwood number varies as expected by our asymptotic calculations as $Pe^{1/3}$ in any case. Notice that this dependence on the Péclet number (to the power of 1/3), due here to the fact that the Reynolds number is sufficiently low (Stokes type regime), means also that the flux varies as $Sc_n^{\;1/3}$ (or $\Pr_n^{\;1/3}$). This variation is in good agreement with the numerical and experimental results obtained for $\mathrm{Re}_n > 5$ [18-20].

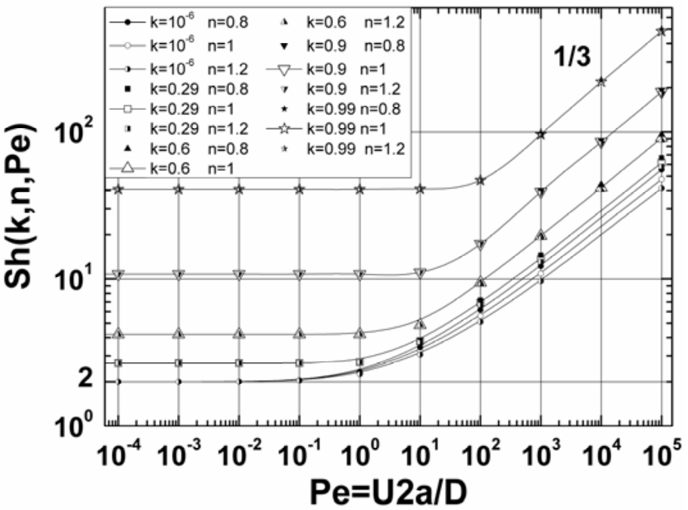

Figure 6: Sherwood number versus Péclet number for a confined medium filled with a power law fluid (Dirichlet)

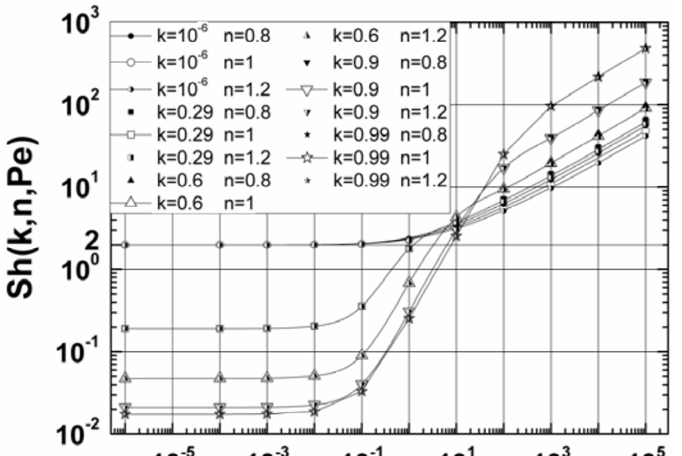

Figure 7: Sherwood number versus Péclet number for a confined medium filled with a power law fluid (Neumann)

When the tube's wall is supposed insulated, the transfer on the sphere is presented in the Fig. 7 with Péclet number. In the diffusive regime, the transfer decreases with the confinement. When the particle draws in the vicinity of the tube's wall the isoconcentration lines are forced to be perpendicular to this wall, thus we assist to a reduction of the thermal gradient on the sphere. This behavior is already discussed above in the Fig. 4. For convective regime, the transfer is independent of the boundary condition because the mass boundary layer which controls the transfer is lower than the gap between the sphere and the tube's wall.

For high Péclet number, we give in the Fig. 8 the evolution of the flux as a function of ε. All the results corresponding to this convective regime present a similar behavior and seem to be independent on the type of boundary condition for all the confinements and independent on the fluidity index of the fluid only for the high confinement. In the lubrication regime, all the results seem to be in good agreement with those obtained asymptotically for a Newtonian fluid:

$$Sh(k, Pe) \approx \frac{3^{2/3}}{2} \frac{\Gamma(1/3)}{\Gamma(2/3)} \left(\frac{Pe}{\varepsilon}\right)^{\frac{1}{3}} \qquad (4)$$

This agreement is probably due to the fact that at very low Reynolds number, $Pe = \mathrm{Re}_n\, Sc_n = \dfrac{U2a}{\nu_{ap}} \dfrac{\nu_{ap}}{D} = \dfrac{U2a}{D}$ does not depend on the index of fluidity and the flux is controlled by the cutoff of the mass or thermal boundary layer imposed by the gap between the sphere and the wall in the lubrication regime ($\varepsilon \approx 0$).

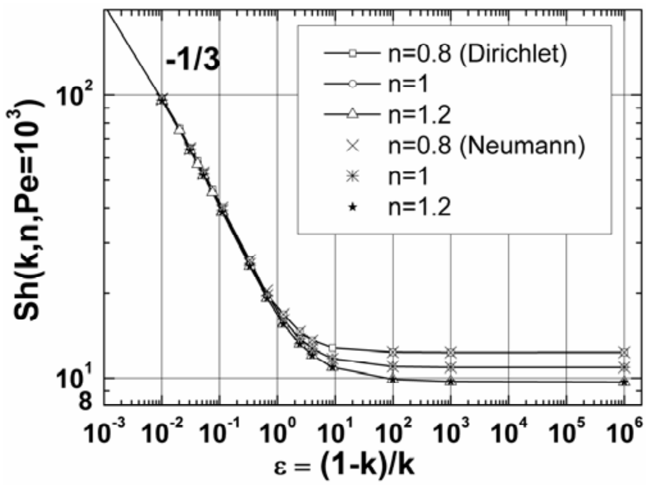

Figure 8: Evolution of the Sherwood number with the confinement for a power law fluid

Case 2: Sphere in asymmetrical position

Now we will discuss the same problem as described above, studying the influence of asymmetrical position on the transfer. We recall that this asymmetry is characterized by the eccentricity parameter $e = d/a$ where d is the distance between the axis of the tube and the center of the sphere. This parameter e varies between 0 when the sphere is in its symmetrical position and $e_{max} = 1 - k$ when the sphere touches the wall of the tube.

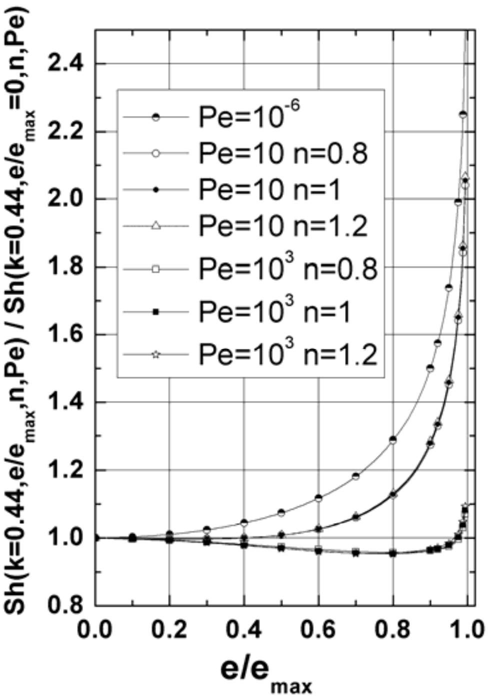

Figure 9: Evolution of the Sherwood number with the off-axis position of the particle translating in a power law fluid for various Péclet numbers (Dirichlet)

In the Fig. 9, we show, for a Dirichlet condition, the numerical results concerning the evolution of the transfer normalized by its value in the symmetrical position with the normalized eccentricity. In the diffusive regime, we assist to a monotonically increase of the transfer with the eccentricity. This enhancement is due to the cutoff of the mass boundary layer by the gap (see Fig. 10.a). For low Péclet numbers, it is obvious that the transfer in different asymmetrical positions is independent on the rheological behavior as discussed above. In the same figure, the plots corresponding to high Péclet numbers ($Pe = 10^3$) give a typical behavior in the convective regime. It shows that the flux varies non monotonically and goes through a minimum off the symmetry axis at a value $e / e_{max} \approx 0.8$. The transfer reduction is about 5% for $k = 0.44$ compared to its value in the symmetrical position. This non monotonic behavior is due to the backflow induced in the confined geometry and is similar to that obtained for the drag [21].

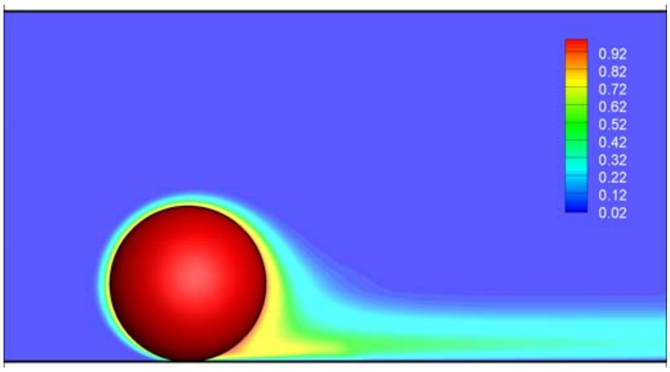

Figure 10.a: Isoconcentration profile in the vicinity of the wall at high Péclet number (Dirichlet boundary condition)

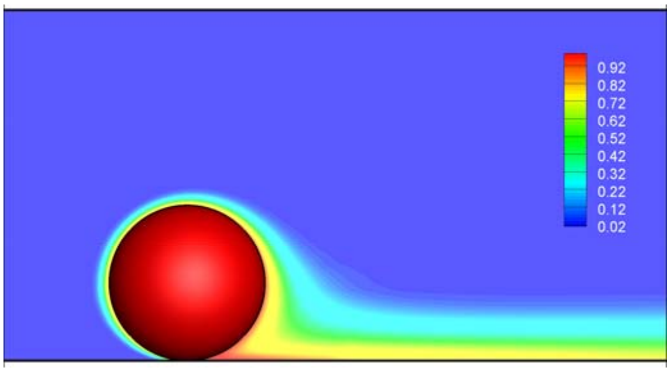

Figure 10.b: Isoconcentration profile in the vicinity of the wall at high Péclet number (Neumann boundary condition)

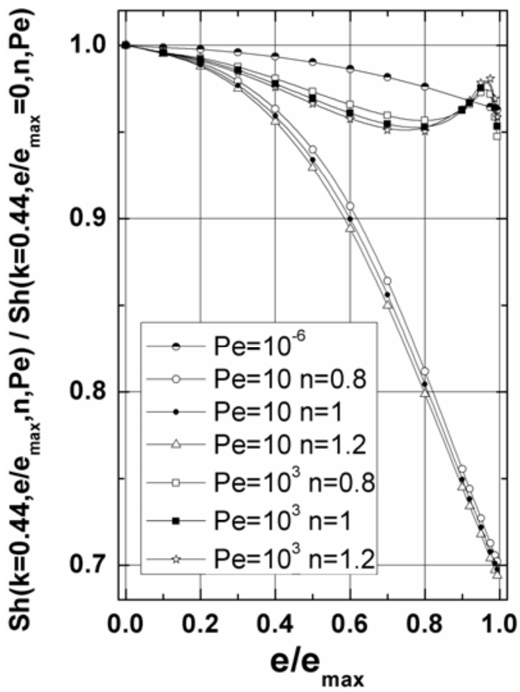

Figure 11: Evolution of the Sherwood number with the off-axis position of the particle translating in a power law fluid for various Péclet numbers (Neumann)

On the other side, when we impose a Neumann boundary condition on the tube's wall, for low Péclet numbers, we obtain in a similar way than in the symmetric configuration a monotonic decrease of the transfer with the eccentricity as shown in the Fig. 11. In the other way, in the convective regime, we get the similar behavior with the eccentricity as that obtained with a Dirichlet boundary condition shown in the Fig. 9.

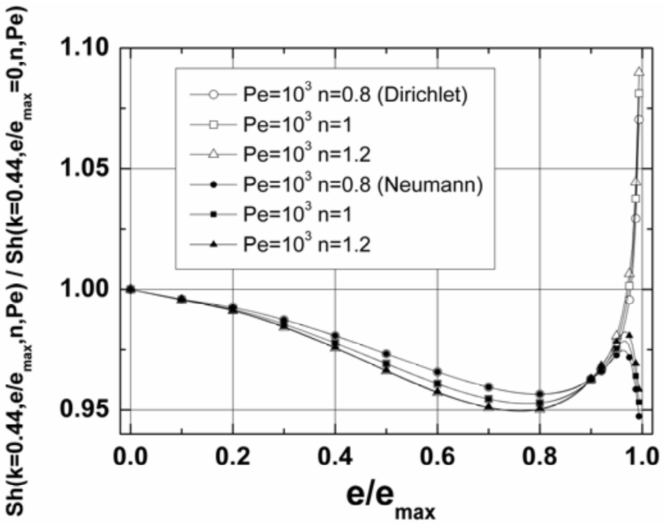

Figure 12 : Comparison between the Sherwood numbers obtained with Dirichlet and Neumann boundary conditions in the asymmetric case for high Péclet numbers

Due to the non intuitive evolution of the transfer with the eccentricity in the convective regime, we give in the Fig. 12 a comparison between the results obtained for the two boundary conditions. Firstly, far from the tube's wall, the evolution seems to be independent on the fluidity index as shown in the axisymmetric case. For the Dirichlet boundary condition, the non monotonic evolution ends by an increasing in the transfer near the wall due to the raise of the backflow convection related to the narrowest gap where the maximal transfer takes place (see the Fig. 10.a). However, when we impose the Neumann boundary condition, an additional surprising behavior of the transfer occurs by a decrease of the transfer in the vicinity of the tube's wall. This effect may be explained by the fact that the convective backflow effect is less efficient than in the decrease of the flux due to the proximity of the insulated wall as explained before in the sense that under these conditions, the isoconcentration lines are forced to be perpendicular to this wall reducing the thermal gradient on the particle. This phenomenon is illustrated in the Fig. 10.b where we can see that the concentration on the wall is slightly equal to that imposed to the particle.

CONCLUSION

In this work, we studied numerically and asymptotically the consequences of an asymmetrical confinement in the mass or heat transfer on a spherical particle moving at low Reynolds number in the tube which mass or thermal boundary conditions are of the Dirichlet or Neumann type. In the other way, we studied the influence of the rheological shear thickening and shear thinning behaviors of non-Newtonian fluid on this transfer. For Dirichlet boundary conditions in symmetrical position and at low Péclet number the results show for all fluids as expected a purely diffusive behavior and the flux increases with the confinement. The Sherwood number varies as $\varepsilon^{-1/2}$ in the lubrication regime, in good agreement with our asymptotic development. In the convective regime, the Sherwood number varies as $Pe^{1/3}$ for a given confinement k in accordance with the boundary layer theories and in the lubrication regime as $\varepsilon^{-1/3}$ for a given Péclet because of the backflow as obtained in the asymptotical approach. Notice that also the influence of the fluidity index appears principally in unbounded situation or very low confinements. For Neumann, the transfer is reduced when the confinement is increased in the diffusive regime with the same conclusion than for the Dirichlet case concerning the non-Newtonian effect. In order to study the influence of the asymmetry, we studied the evolution of the transfer with the eccentricity of the sphere. For the convective regime and for both boundary conditions, the effect of the asymmetry is characterized by the appearance of a minimum of the transfer in the off-axis position. This behavior is analogous to that observed for the drag force in the dynamic problem. This non monotonous evolution is due to the backflow related to the confinement. But it is important to mention the existence of a decrease of a transfer in the vicinity of the tube's wall when the Neumann boundary condition is imposed.

NOMENCLATURE

a	radius of the sphere, m
b	radius of the tube, m
c	solute concentration, $kg.m^{-3}$
c_s	solute concentration on the sphere's surface, $kg.m^{-3}$
c_∞	solute concentration in the fluid, $kg.m^{-3}$
C_p	specific heat of the fluid, $J.kg^{-1}K^{-1}$
D	molecular diffusion coefficient or thermal diffusivity, $m^2.s^{-1}$
$\underline{\underline{D}}$	strain rate tensor, s^{-1}
D_{II}	second invariant of the strain rate tensor, s^{-2}
d	distance between the axis of the tube and the sphere center, m
e	eccentricity
$e_{\max}$	maximal eccentricity
k	confinement coefficient

m consistancy, $Pa.s^n$
n index of fluidity
Nu Nusselt number
p pressure, Pa
Pe Péclet number
$\mathrm{Pr}_n = \dfrac{m(U/2a)^{n-1}}{\rho D_{th}}$ Prandtl number
T_s temperature on the sphere's surface, K
T_f fluid temperature, K
Re_n generalized Reynolds number
$Sc_n = \dfrac{m(U/2a)^{n-1}}{\rho D}$ Schmidt number
Sh Sherwood number
t time, s
U_0 sphere velocity, $m.s^{-1}$

Greek symbols
ε reduced distance between the sphere and the tube's wall
ϕ_m mass flux on the sphere, $kg.s^{-1}$
ϕ_s heat flux on the sphere, W
λ thermal conductivity, $W.m^{-1}.K^{-1}$
ψ stream function, $kg.s^{-1}$
ω vorticity, s^{-1}
μ_a apparent viscosity, $Pa.s$
ρ density, $kg.m^{-3}$
$\underline{\underline{\sigma}}$ stress tensor, Pa

Indexes
$+$ dimensionless quantity

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