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From highly specialised to generally available modelling of shear induced particle migration for flow segregation based separation technology

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ABSTRACT

Shear induced diffusion can be used to induce particle migration in flow, and this may be a lead to novel separation technology. Under specific conditions, depending on, amongst others, the ratio between channel height and particle diameter, larger particles preferentially move to the centre of a channel. It has been demonstrated earlier that separation and fractionation can be facilitated by this, leading to lower energy and water demand, and prevention of particle accumulation on sieves that have pores that are much larger than the particles. This situation is very different from regular (cross-flow) membrane filtration, in which particles are retained by the pores, and accumulate in various layers.

Unfortunately, the underlying mechanisms of particle migration are not that well understood, and contradicting results are reported in literature. There is clearly a need for a unifying approach that can be used by many; therefore, we developed a CFD computer model that can readily be used, unlike the rather inaccessible computer models that are mostly reported in literature. We focus on particle–particle interactions of monodisperse suspensions in flow, for which we added momentum terms to the general momentum equation. We found amongst others that due to shear induced diffusion the particle volume fraction will be 1.7 times higher at the centre of the channel compared to the channel wall for a bulk particle volume fraction of 50%. Our results describe the experimental results, obtained under similar ideal conditions, to a high level of detail. Our findings are also in reasonable agreement with other modelling and experimental studies from literature, and the discrepancies are most probably due to non-ideal behaviour in the experiments and different approaches used in the models. The big advantage of using this software is that the model can be adapted readily by researchers not specifically trained in modelling or programming, but even more importantly, particle migration can now be used as a starting point in separation design since parameter and geometry studies will take less effort using this software.

1. Introduction

Concentration and segregation of suspensions is needed in different fields, such as biotechnology, water treatment, etc. [1]. Also in the food sector it plays an important role, e.g. in the dairy industry bacteria need to be separated from the product stream [2] in order to obtain a safe product, and in the beer industry yeast is separated to clarify the product [3]. Also during fermentation it would be useful to fractionate mature from not fully mature species, so they can be sent back to the fermentation vessel to obtain higher productivity.

Often the concentration and segregation of suspensions, in the range of 1–10 µm, is done by microfiltration [1–3], during which convective flow carries the particles toward the membrane that retains them, forming a layer that in turn is influenced by various back transport mechanisms, amongst which shear induced diffusion [4–6]. We would like to stress that there is a clear difference between shear induced diffusion as used for modelling of microfiltration, and for segregation in flow; therefore both processes are first discussed.

1.1. Microfiltration

During classic membrane microfiltration particles are separated from the suspension fluid by a membrane. Due to the applied transmembrane pressure both the fluid and the particles are pushed towards

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the membrane; the liquid permeates through the membrane, while the particles remain at the retentate side when the membrane pore size is smaller than the size of the particles. Since these particles cannot cross the membrane, they accumulate, pores become blocked and a (cake) layer forms [7], which results in flux reduction and a change in retention due to the presence of the (cake) layer in combination with a possible decrease in effective pore size.

Accumulation of particles can be mitigated in several ways. One solution would be to decrease the concentration of the suspension so that less particles are available to block the membrane pores, although this is not always practical to do [8,9]. A back flush can also be applied to remove the particles from the membrane [10], or a cross flow can be applied that induces back transport of particles (to some extent). Whatever option is chosen, more energy, more water or both will be needed [9], and the membrane will have to be cleaned regularly. Although this is standard procedure in industry, it would be better if particles could be kept from accumulating, leading to an environmentally and economically more sustainable situation by extension of the run period and less need for cleaning.

1.2. Flow segregation

Instead of using the membrane's size exclusion mechanism that is responsible for accumulation, the intrinsic migration mechanisms of the particles can be considered as means to facilitate fractionation or concentration of a suspension. These mechanisms include Brownian motion, inertial lift and shear-induced diffusion [7]. In short, Brownian motion describes how particles arbitrarily move around in a certain space, which does not have a specific direction. Inertial lift takes into account the influence of the fluid flowing around the particles; particle movement follows the pressure gradient over the particle, which is directed toward the centre of the channel. Shear-induced diffusion considers how particles affect the movement of other particles in flow. It is directed towards regions of lower shear (middle of the channel), and various complex relations have been given in literature as will be shown in the model development section.

Which of these mechanisms dominates depends on various parameters, that are incorporated in the dimensionless particle Reynolds number, defined as:

$$Re_p = \frac{\mathrm{v_r} \cdot a \cdot \rho_f}{\eta_f} \tag{1}$$

and the dimensionless Péclet number, defined as:

$$Pe = \frac{\dot{\gamma} \cdot a^2}{D_B} \tag{2}$$

In which v_r is the relative velocity between the phases (m/s), $\dot{\gamma}$ the shear rate (1/s), a the particle radius (m), ρ_f the fluid density (kg/m^3), η_f the fluid viscosity (Pa s), and D_B the Brownian diffusion coefficient (m^2/s) defined as:

$$D_B = \frac{k \cdot T}{6\pi \cdot \bar{\eta} \cdot a} \tag{3}$$

Here $\bar{\eta}$ is the suspension viscosity (Pa s), k the Boltzmann constant (J/K) and T the temperature (K). Inertial lift dominates when $\mathrm{Re_p} > 1$, and Brownian motion dominates when $\mathrm{Pe} < 1$. Hence, for shear induced diffusion to be dominant, $\mathrm{Re_p} < 1$ and $\mathrm{Pe} > 1$. For particles that are between 1 and 10 µm, which are most relevant for microfiltration, shear-induced diffusion is the dominant mechanism and, therefore, this study focuses on this topic.

As mentioned previously, we will use shear-induced diffusion to segregate particles flowing in a closed channel. Shear induced diffusion is a result of how particles affect the movement of other particles and it scales with the square of the particle size (Table 1). With equal volume fractions of large and small particles, the larger particles will move faster towards a region with low shear, which would be the centre of the channel [11]. In this way, the particles can migrate away from the wall in a closed channel before they are exposed to a porous section. It can be expected that this will lead to processes that are environmentally and economically more sustainable.

Table 1
Closure relations SID momentum term.

Closure relation	Reference	Equation
η	Krieger-Dougherty relation	$\eta_f \left(1 - \frac{\alpha_p}{\alpha_{max}}\right)^{[\eta]\alpha_{max}}$
M	Vollebregt et al. [13]	$\frac{2}{9}\frac{a^2}{\eta_f}\alpha_p f(\alpha_p)$
$D_{\alpha p}$	Vollebregt et al. [13]	$\frac{2}{9}\dot{\gamma}a^2(1-\alpha_p)^2 \cdot 1.5\frac{\alpha_p}{\alpha_{max}}(1 + \alpha_p(1-\alpha_p)^{-1})$
$D_{\dot{\gamma}}$	Vollebregt et al. [13]	$\frac{2}{9}a^2(1-\alpha_p)^2 \cdot 0.75\alpha_p^2$
$f(\alpha_p)$	Vollebregt et al. [13]	$(1-\alpha_p)^2(1-\alpha_p)^2$
$\dot{\gamma}$	Miller et al. [14]	$\frac{d\mathrm{v}}{dy} + \frac{a \cdot \mathrm{v}_{max}}{H^2}$

In summary, for microfiltration flux predictions are based on the build-up of various layers of particles accumulated on the membrane as a result of amongst others convective flow toward the membrane, and cross-flow over the layers that induces back transport. Therefore, Kim and Zydney [12] developed a CFD model that gives good insight in the effect of a number of transport mechanisms, but given the complexity of the filtration process, shear induced diffusivity was not investigated individually. For the flow segregation process that we propose here, shear induced diffusivity needs to be described very accurately since it is the only transport mechanism, and that puts extra weight on the accuracy of our model. To the best of our knowledge, simulation of segregation in flow, as a starting point for novel separation design, using commercially available software has not been covered in literature, which distinguishes our work from that of others.

In order to make use of the flow segregation process, we have designed the system that is shown in Fig. 1; pre-migration will take place in the closed channel, and liquid can be removed through the pores that are larger than the particles (Fig. 1) [9,11]. This implies that the chances of fouling are reduced, while at the same time higher suspension concentrations can be used (that in turn stimulate shear induced diffusion).

As a prerequisite for the design of this novel separation technology, particle migration as a result of shear induced diffusivity needs to be described at a high level of detail and ideally in a flexible way. For this, both experimental work and computer models are needed, and ideally these studies focus on exactly the same system. Previous studies have covered monodisperse [13–16], bidisperse [17–19] or polydisperse [20] suspensions, and have focused on modelling, on experimental work or both, but mostly there are notable discrepancies between experimental data and modelling results.

In case of modelling, most often the particle phase mass balance is rewritten to insert a diffusive flux term [13,21] that describes the principle of shear induced diffusion. However, it should be mentioned that the models that are currently available are mostly the author's own written code and are therefore at a level that is only accessible for experts in the field of modelling and programming. These models generally do not target to capture these effects with commercially available computational fluid dynamics (CFD) programs that are much more accessible. At the same time it should be mentioned that commercially available CFD software is not that flexible to start off with, since the governing equations cannot always be rewritten. Different studies have used CFD to study shear induced diffusivity [4,5], but not to describe flow segregation in a closed channel aiming at the development of new separation technology [22]. We use the commercial CFD software STARCCM+ to describe the diffusive behaviour of monodisperse particles