Inertial microfluidics with multi-particle collision dynamics

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Abstract. Using the method of multi-particle collision dynamics (MPCD), we investigate inertial focussing in microfluidic channels that gives rise to the Segré-Silberberg effect. At intermediate Reynolds numbers, we model the motion of a spherical colloid in a circular microchannel under pressure-driven flow. We determine the radial distribution function and show how its width and the location of its maximum are strongly influenced by the colloid size and the Reynolds number of the Poiseuille flow. We demonstrate that MPCD is well suited for calculating mean values for the lift force acting on the colloid in the cross-sectional plane and for its mean axial velocity. We introduce a Langevin equation for the cross-sectional motion whose steady state is the Boltzmann distribution that contains the integrated lift force as potential energy. It perfectly coincides with the simulated radial distribution function.

1 Introduction

In 1962 Segré and Silberberg investigated the behavior of dilute particle suspensions in tube flows at intermediate Reynolds numbers ranging from 7 to 1400 [1, 2]. They observed that the distribution of particles in the cross-section of the tube changed with the distance from the inlet. Even though the injected particles were uniformly distributed, the particles while traveling along the channel moved across streamlines and formed a thin annulus about the centerline of the tube. While the formation of the annulus has been observed previously, Segré and Silberberg were the first to attribute it to fluid inertia. At vanishing Reynolds numbers, where fluid inertia is negligible, rigid particles cannot cross streamlines due to the kinematic reversibility of the Stokes equations [3]. Hence, an annulus as observed by Segré and Silberberg cannot form.

Following the experiments of Segré and Silberberg, inertial migration of particles was extensively studied both in experiments [4, 5] and in theory by semi-analytical [6–8] and numerical calculations [9–11]. Recently, interest into inertial cross-streamline migration has been renewed by its application to microfluidic devices [12]. In particular, inertial focusing in straight [13–15] and curved [16–18] channels has been demonstrated. This offers potential applications in separation of bioparticles, such as red blood cells, and filtration [18, 16, 19].

The motion across streamlines can be understood in terms of the so-called lift force that drives the particles towards the annulus. The lift force is due to two contributions resulting from the external shear flow and the

channel walls [20]. For small particle radii, Saffman used the method of matched asymptotic expansion and investigated lateral motion of a particle in an unbounded, linear shear flow [21]. In the presence of external forces (non-buoyant particles), he identified a force that drives the particle towards larger shear velocities measured relative to the particle velocity. However, to explain the Segré-Silberberg effect, one had to extend the analysis based on the matched asymptotic expansion to neutrally buoyant particles in channel flow and also use numerical means to explore the effect of walls [6–8]. The results reproduce the lift force especially in the case of intermediate Reynolds numbers in the range studied here. Yet, as studies based on the matched asymptotic expansion assume small particles and are restricted to plane Poiseuille flow, they are only indirectly applicable if particle sizes become comparable to the channel cross-section [22].

To overcome this restriction, one ultimately has to use numerical methods for solving the full Navier-Stokes equation. Previous studies for three-dimensional channel systems employed the finite-element method [11, 22, 23] and lattice Boltzmann simulations [10]. They investigated lift forces and corresponding equilibrium positions for rectangular [22, 10] and circular channels [11, 23]. Here, we use multi-particle collision dynamics (MPCD) [24], a mesoscopic simulation method, to address inertial microfluidics. Similar to the finite-element and lattice Boltzmann methods, it solves the full Navier-Stokes equations but has a number of advantages. Without any modification, it includes thermal fluctuations [24] which are ultimately necessary to understand the particle distributions observed in experiments [13]. Furthermore, its algorithmic design makes it very efficient and at the same time

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Fig. 1. A two-dimensional schematic of the system showing the plane spanned by the centerline of the circular channel (dashed line) and the colloid with radius a . The undisturbed parabolic flow profile, the axial velocity v_z of the colloid, and the lift force f_{lift} acting on the colloid (see sect. 3.2) are shown.

allows for an easy implementation of channels and colloidal particles [24,25]. Commonly, MPCD has been used to study fluid flow at low Reynolds number but it was also successfully applied at intermediate and high Reynolds numbers in 2D [26,27].

In this article, we investigate inertial migration of single colloidal particles in microchannels at intermediate Reynolds numbers using MPCD. We will show that colloids are focussed onto an annulus in the circular cross-section of the channel and determine the corresponding radial distribution function. Its width and the location of its maximum are strongly influenced by the particle size and the Reynolds number of the Poiseuille flow. We furthermore determine lift force and particle velocity as a function of the radial coordinate by fixing the colloid position in the cross-section of the channel. We introduce the potential of the radial lift force and demonstrate that the corresponding Boltzmann distribution reproduces the simulated radial distribution function.

The paper is organized as follows. In sect. 2 we describe our system, introduce the MPCD method and how we couple the colloid to the MPCD fluid, and explain the choice of the MPCD parameters. We review the method of kernel density estimate to construct the radial distribution functions from the simulated data and finally explain how we determine the radial lift force and the axial colloid velocity as a function of the radial coordinate. We present and discuss our results in sect. 3 including the radial distribution function, the lift forces and colloid velocities, and show how we recover the distribution function from the Boltzmann distribution. We close with a summary and final remarks in sect. 4.

2 Methods

2.1 The system

We study a circular channel with radius $R = 25$ and length $L = 10R$ given in the unit length of the MPCD method which we introduce below and employ periodic boundary conditions along the channel axis. In the following we choose a cylindrical coordinate system with coordinates (r, ϕ, z) , where the channel axis is oriented along the z -axis, and attach to each space point the unit vectors (e_r, e_ϕ, e_z) of the coordinate basis. Figure 1 shows a sketch of the geometry. The channel is filled with a Newtonian

fluid with density ρ and kinematic viscosity ν and exhibits the pressure-driven Hagen-Poiseuille flow profile [28]

$$\mathbf{u}(r) = u_{\text{max}} (1 - (r/R)^2) \mathbf{e}_z. \quad (1)$$

In sect. 2.2 we explain how we implement this flow profile with the MPCD method. The maximum flow velocity u_{max} in the channel center determines the Reynolds number $\text{Re} = 2Ru_{\text{max}}/\nu$ [28]. The fluid contains a spherical particle with radius a and mass $M = 4/3\pi a^3 \rho$. In the following we investigate its behavior for Reynolds numbers $\text{Re} = 0.1, 1, 10, 20, 30, 40$ and particle radii of $a/R = 0.2, 0.3, 0.4, 0.5$.

2.2 Multi-particle collision dynamics

Multi-particle collision dynamics (MPCD) is a mesoscopic simulation method invented by Malevanets and Kapral in 1999, which they originally called stochastic rotation dynamics [24]. In this section we discuss the details of our implementation of a variant of the original method based on the Andersen thermostat. For an extensive review we refer to the article by Gompper *et al.* where they describe algorithmic details, the resulting fluid properties, and the application of MPCD to a wide range of systems [29].

MPCD describes fluid flow by coarse-grained or effective fluid particles with mass $m = 1$ in MPCD units that interact via a collision rule. The algorithm is divided into two steps [24]. In the streaming step, particles move according to Newton's equation of motion during a time interval Δt_c without any explicit interaction between the particles. We apply a constant force to each fluid particle to mimic a constant pressure gradient which together with the no-slip boundary condition (see below) generates the Hagen-Poiseuille flow profile in the cylindrical channel. In the collision step one sorts the particles into cubic cells with edge length l_c and assigns to particle i in a cell a new velocity $\mathbf{v}'_i$ according to the collision rule [30]

$$\mathbf{v}'_i = \mathbf{v}_c + \mathbf{v}_i^{\text{therm}} - \mathbf{v}_i^{\text{corr}}. \quad (2)$$

Here, $\mathbf{v}_c$ is the mean or center-of-mass velocity of all particles in one cell and the components of $\mathbf{v}_i^{\text{therm}}$ are random numbers drawn from a Gaussian distribution with zero mean and variance $k_B T/m$. This collision rule is taken from the Andersen thermostat and has the advantage of keeping temperature constant. Furthermore, the collision rule has to preserve linear momentum so that the MPCD method reproduces a solution of the Navier-Stokes equation on length and time scales larger than l_c and Δt_c , respectively [24]. One therefore subtracts the correction velocity

$$\mathbf{v}_i^{\text{corr}} = \frac{1}{N_c} \sum_{j \in \text{cell}} \mathbf{v}_j^{\text{therm}} - m\theta^{-1} \sum_{j \in \text{cell}} [\mathbf{r}_{j,c} \times (\mathbf{v}_j - \mathbf{v}_j^{\text{therm}})] \times \mathbf{r}_{i,c}, \quad (3)$$

where the first term on the right-hand side preserves linear momentum and, in addition, the second term ensures

conservation of angular momentum. We have introduced the number of particles in the cell, N_c , the particle position vector $\mathbf{r}_{i,c}$ relative to the center of mass of the cell at $\mathbf{r}_c$, and the moment of inertia tensor $\boldsymbol{\theta}$ of all the particles in the cell again relative to $\mathbf{r}_c$.

If the mean free path of fluid particles is small compared to the cell size l_c , correlations may arise [29]. To remove these correlations and restore Galilean invariance, we perform a random shift of all collision cells. For each collision step, the components of the shift vector are drawn with equal probability from the interval $[-l_c/2, l_c/2]$ [31].

The advantage of the MPCD algorithm is that one can calculate analytic expressions for the material parameters of the Newtonian fluid in terms of the parameters Δt_c , l_c , and the average number n of fluid particles in each cell. For the collision rule used in our work, analytic expressions for the kinematic viscosity ν and the self-diffusion constant D of a fluid particle are given in ref. [32]:

$$\nu = \frac{k_B T \Delta t_c}{m} \left(\frac{1}{c(n)} - \frac{1}{2} \right) + \frac{l_c^2}{24 \Delta t_c} d(n), \quad (4)$$

$$D = \frac{k_b T \Delta t_c}{m} \left(\frac{1}{s(n)} - \frac{1}{2} \right). \quad (5)$$

We use the abbreviation $d(n) = 1 - \frac{1}{n}(\frac{7}{5} + e^{-n}[\frac{7}{5} + \frac{2n}{5} + (\frac{1}{3} - \frac{3}{10})n^2])$ and $s(n)$, $c(n)$ are given, respectively, in formulas (35), (36) in ref. [32]. All these terms do not strongly depend on n . For $n = 10$, we find $d = 0.86$, $s = 0.80$, $c = 0.87$.

To implement the no-slip boundary condition at the channel wall, we use the procedure described in ref. [33]. We divide the streaming step in two steps of duration $\Delta t_c/2$ and check for each of these steps whether a fluid particle has passed the channel boundary. If so, we move the particle back along its trajectory for a time $\Delta t_c/4$ and place it along the normal onto the surface. We update the velocity of the fluid particle according to the bounce-back rule, $\mathbf{v}'_i = -\mathbf{v}_i$, and then move it forward in time during the time step $\Delta t_c/4$. This procedure only approximately fulfills the no-slip boundary condition which Lamura *et al.* traced back to the cells which overlap with the system boundaries [27]. To improve the validity of the no-slip condition, Lamura *et al.* introduced so-called ghost particles in the regions of these cells which lie outside the system [27]. Their center of mass velocity is Gaussian distributed and contributes to the mean velocity of the cell during the collision step. However, since we use a collision rule that conserves angular momentum (see eq. (3)), we have to assign explicit random positions and Gaussian-distributed velocities to the ghost particles to perform the collision step [34]. By driving the fluid particles with a constant force during the streaming step, we indeed reproduce the Hagen-Poiseuille flow profile (see fig. 2), where the slip velocity at the channel wall is always around 1% of $u_{\max}$ (the flow velocity at the centerline) as illustrated by the inset of fig. 2.

We model the colloidal particle as a perfect sphere, which moves without external force through the channel. The colloid has a center-of-mass position $\mathbf{r}_c$, a velocity $\mathbf{v}_c$,

Fig. 2. (Colour on-line) The Hagen-Poiseuille flow profile for $Re = 40$. Full line: from MPCD simulations averaged over 89×10^3 snapshots, dashed line: parabolic fit. The inset shows the relative slip velocity $u_{\text{slip}}/u_{\text{max}}$ at the channel wall plotted versus Re .

and an angular velocity $\boldsymbol{\omega}_c$. Each point of the colloid at position $\mathbf{r}$ moves with the local velocity $\mathbf{v}_{\text{loc}}(\mathbf{r}) = \mathbf{v}_c + \boldsymbol{\omega}_c \times (\mathbf{r} - \mathbf{r}_c)$. To implement the interaction with the fluid, we use the same procedure as with the wall-fluid interaction. First, we use the bounce-back rule for the fluid particle in the streaming step but implement it relative to the local surface velocity of the colloid [35]. The new velocity of the fluid particle then amounts to $\mathbf{v}'_i = 2\mathbf{v}_{\text{loc}} - \mathbf{v}_i$. Second, we introduce ghost particles inside the colloid that take part in the collision step of the respective cells. Their velocities are Gaussian distributed about the local colloid velocity $\mathbf{v}_{\text{loc}}(\mathbf{r})$, where $\mathbf{r}$ is the ghost particle position within the colloid [35]. In both the streaming and collision step, the reflected or the ghost fluid particles change their linear and angular momentum (relative to the colloid center). This change is transferred to the colloid in order to preserve linear and angular momentum.

2.3 Choice of parameters

The MPCD algorithm as described has five parameters: the cell size l_c , the average number of particles per cell n , the time between two collisions Δt_c , the particle mass m , and the temperature T . Typically, one chooses $m = 1$ and also sets the thermal energy $k_B T = 1$. The properties of the MPCD fluid can be described by a set of dimensionless numbers [36]. For our system, the Mach and the Schmidt number constrain the choice of the parameters, especially in the case of non-zero Reynolds number.

The Mach number $Ma = v_{\text{max}}/c_s$ compares the maximum fluid velocity v_{max} to the speed of sound $c_s = (\frac{5}{3} \frac{k_B T}{m})^{\frac{1}{2}}$. In the following, we control the Reynolds number Re so that $v_{\text{max}} = Re \nu / 2R$. To ensure the incompressibility of the fluid, the Mach number should be much smaller than one, otherwise the fluid has to be regarded as compressible. The Schmidt number $Sc = \nu/D$ compares the diffusion constant of fluid momentum, the kinematic viscosity ν , to the self-diffusion constant of fluid

Fig. 3. (Colour on-line) Lines of constant Mach and Schmidt numbers as a function of l_c and λ for $Re = 40$, $n = 10$, and $R = 25$. The solid lines indicate the bounds on Ma and Sc and the gray region the parameters for staying within these bounds.

Table 1. MPCD parameters, Reynolds numbers, the resulting Mach and Schmidt numbers, and the kinematic viscosity used in this article.

Δt_c	l_c	n	m	T	Re	Ma	Sc	ν
0.1	1.25	10	1	1	10	0.10	8.3	0.62
0.1	1.25	10	1	1	20	0.19	8.3	0.62
0.1	1.25	10	1	1	30	0.29	8.3	0.62
0.1	1.00	10	1	1	40	0.26	5.6	0.42

particles or mass diffusivity D . For fluids the Schmidt number should be larger than one. To describe an incompressible fluid within MPCD, typical bounds are mentioned in the literature: $Ma < 0.3$ [26, 27] and $Sc > 5$ [36]. Using eqs. (4) and (5) for ν and D , respectively, we find the following expressions:

$$Ma = \sqrt{\frac{3}{20}} \frac{Re}{R} \left[\lambda \left(\frac{1}{c} - \frac{1}{2} \right) + \frac{l_c^2}{\lambda} \frac{d}{24} \right], \quad (6)$$

$$Sc = \frac{l_c^2}{\lambda^2} \frac{d}{24} + \frac{2c^{-1} - 1}{2s^{-1} - 1}, \quad (7)$$

where we have introduced the mean free path $\lambda = \Delta t_c (k_B T / m)^{1/2} = \Delta t_c$ of the fluid particles. For $Re = 40$ we illustrate the region where the bounds on Ma and Sc are satisfied as a function of λ and l_c (see fig. 3). Since $Ma \propto Re$, the lower bound $Ma = 0.3$ (full blue line) shifts downwards with decreasing Re and the region expands.

Up to $Re = 30$ we satisfy the bounds on Ma and Sc by setting $l_c = 1.25$, $\Delta t_c = 0.1$, and $n = 10$. To stay within the bounds for $Re = 40$, we decreased the cell size to $l_c = 1$. All the parameters for the Reynolds numbers used in this article are summarized in table 1.

2.4 Probability distribution and kernel density estimate

We are interested in the radial probability distribution $P(r)$, where $P(r)2\pi r dr$ is the probability of finding the

Fig. 4. (Colour on-line) Probability distribution $P(r)$ determined as a histogram and by the method of kernel density estimate (KDE) for $Re = 10$ and $a/R = 0.5$. The bin width for the histogram and the kernel width h are both 0.02. We also show the full width at half-maximum b .

colloid at a radial distance r from the centerline in a shell of thickness dr . In the simulations we determine the distribution

$$W(r) = 2\pi r P(r), \quad (8)$$

by counting the colloids within the shell. After the system has reached a steady state, we record radial (r) and angular (ϕ) positions of a colloid at every 1000th time step and for more than 15 independent simulation runs, so that as a total we record about 5000–10000 samples (r_i, ϕ_i) .

As already stated, a straightforward way to determine $P(r)$ is to sort the samples into bins of radial thickness dr . The number of samples in each bin gives $W(r)$ from which we calculate $P(r) = w(r)W(r)$, where $w(r) = 1/(2\pi r)$ is called weight. Figure 4 illustrates the resulting histogram for $P(r)$ for typical values of our simulations. Such histograms provide a discontinuous representation of $P(r)$, whereby slight shifts in the data points may lead to strong changes in the histogram when the data points are sorted into neighboring bins [37].

An alternative method which provides a much smoother representation of $P(r)$ is the Kernel Density Estimate (KDE) [37]. We use an extended version which allows different weights $w_i = 1/(2\pi r_i)$ for each data point [38]. According to this method, we estimate the contribution of each sample r_i to the density $P(r)$ by a weighted sum over all samples

$$P(r) = \frac{1}{N} \frac{\sum_{i=1}^N w_i K_h(r - r_i)}{\sum_{i=1}^N w_i}, \quad (9)$$

where K_h is a Gaussian kernel. We systematically determine its width h using the Sheather-Jones plug-in method [39] modified for weighted data [38]. Typical values range from $h/R = 0.003$ at $Re = 40, a/R = 0.5$, when the distributions are narrow, to $h/R = 0.02$ at $Re = 10, a/R = 0.2$, when their width is larger. Clearly, the resulting distribution in fig. 4 is much smoother than the histogram.

In the following we also give the full width at half-maximum b of our distributions. When $r_{\pm 1/2}$ are the positions where the distribution $P(r)$ assumes half the value

of its maximum, then

$$b = r_{+1/2} - r_{-1/2}. \quad (10)$$

2.5 Measuring forces and velocities

In sect. 3.2 we will interpret the radial distribution function $P(r)$ in terms of a lift force f_{lift} in radial direction and also look at the colloids axial velocity $\bar{v}_z$ as a function of r . The distribution functions reported in sect. 3.1 are peaked at a radial position meaning that the colloid rarely visits other radial positions. To determine $f_{\text{lift}}(r)$ and $\bar{v}_z(r)$ by averaging over a sufficient number of sample values, we constrain the colloid to a fixed radial and azimuthal position r, ϕ by simply disregarding any motion in radial and azimuthal direction. The colloid freely moves along the channel or z axis and is not constrained in its rotation. The axial velocity is then simply the average $\bar{v}_z = \langle v_z \rangle = \langle \Delta z / \Delta t_c \rangle$. To measure the lift force, we record the momentum transfer on the colloid in radial direction during streaming and collision step: $f_{\text{lift}} = \langle \Delta p_r / \Delta t_c \rangle$.

Since MPCD includes thermal fluctuations, we determine the mean values by averaging over ca. $(2-5) \times 10^5$ time steps for each simulation run and, in addition, average over $N_{\text{sim}} \geq 5$ independent simulation runs; for $a/R = 0.2$ we choose $N_{\text{sim}} \geq 7$. Each simulation run took ca. 160 hours on several CPUs. For $\text{Re} = 40$, the number of simulated time steps was approximately halved compared to $\text{Re} < 40$ since the total number of fluid particles doubled due to the reduced cell size (see table 1).

To estimate the standard error of the mean values, we calculate the time averages $\hat{f}_{\text{lift},i}$ and $\hat{v}_{z,i}$ for each independent simulation run once the colloid has reached its steady state. The standard error of the lift force then follows from the square root of the variance [40]:

$$\sigma_{f_{\text{Lift}}}^2 = \frac{1}{N_{\text{sim}} - 1} \sum_{i=1}^{N_{\text{sim}}} \left(\hat{f}_{\text{lift},i} - f_{\text{lift}} \right)^2. \quad (11)$$

The standard error of the axial velocity is estimated in the same way.

3 Results

3.1 Probability distributions

In the limit of zero Reynolds number and zero thermal noise, a colloid in Poiseuille flow does not cross streamlines [3]. It moves with the imposed external flow but is slowed down by drag forces due to its finite extent. However, due to thermal motion the colloid diffuses in radial direction across streamlines and ultimately its radial probability distribution $P(r)$ becomes uniform. For increasing Reynolds number, when inertial forces are no longer negligible, the shape of $P(r)$ changes. Figure 5 shows the cross-sectional positions of the colloid at different times and for several independent simulation runs. Clearly, the probability distribution is nonuniform and shows the hallmark

Fig. 5. Illustration of the full probability distribution $P(r, \phi)$ by plotting the colloid's radial and angular positions at different times. Top row: $\text{Re} = 20$, bottom row: $\text{Re} = 40$. Left column: $a/R = 0.2$, right column $a/R = 0.5$.

of inertial focusing: the Segré-Silberberg annulus [1]. We observe that for increasing Re and colloid radius a/R the annulus becomes narrower.

To analyze the properties of the annulus in more detail, we construct the radial distribution function $P(r)$ from simulated data using the method of kernel density estimate as described in sect. 2.4. In fig. 6, we plot $P(r)$ for increasing Reynolds number Re at constant colloid radius a/R (a) and for increasing a/R when Re is fixed (b)¹. With increasing Reynolds number, the distribution becomes narrower and the Segré-Silberberg annulus is more pronounced. At the same time, the maximum of the distribution shifts closer to the wall. However, for increasing colloid size (fig. 6(b)), the maximum moves towards the center. This is expected since larger colloids have to be farther away from the channel walls due to their larger excluded volume but also due to larger hydrodynamic interactions with the wall. In addition, the distribution becomes narrower for increasing a/R in accordance with the cross-sectional distributions illustrated in fig. 5. The shift of the peak with increasing colloid size might be interesting for particle sorting with inertial microfluidics. We summarize the two main characteristics of the distribution

¹ In our simulations the kinematic viscosity ν at $\text{Re} = 40$ is different from the viscosity at the other Reynolds numbers (see table 1). As a result the force scale for the lift force, $\hat{f} = \rho\nu^2$, introduced in sect. 3.2 differs. In sect. 3.3 we show how the Boltzmann distributions for the potential of the radial lift force reproduce the radial distribution functions. This justifies the following procedure. To compare the distributions at $\text{Re} = 40$ to the distributions at other Re values, we renormalize them by $P(r)^{\hat{f}/\hat{f}_{40}}$, where $\hat{f}_{40}$ and $\hat{f}$ are the respective force scales for $\text{Re} = 40$ and the other Reynolds numbers.

Fig. 6. (Colour on-line) Radial distribution function $P(r)$ (a) for increasing Reynolds number Re at reduced colloid sizes $a/R = 0.5$ and $a/R = 0.2$ (inset), (b) for several reduced colloid sizes a/R at $Re = 40$ and $Re = 20$ (inset).

function $P(r)$ in fig. 7 by plotting its full width at half-maximum b introduced in sect. 2.4 and the position of its maximum $r_{\max}$ versus the colloid radius a/R (see inset). From the scaling law of the radial lift force discussed in sect. 3.2, we expect a power law dependence of the width b in both the Reynolds number and particle size. The fitted dashed line follows $b/R = 7.84(a/R)^{-1.75}Re^{-0.92}$, which we will motivate in sect. 3.3, and is in good agreement with the scaling law for the lift forces. The dependence of $r_{\max}$ on a/R is approximately linear in the recorded size range. Note that the data point on the $Re = 20$ curve at $a/R = 0.2$ has a larger uncertainty than the other points and therefore deviates from the straight line.

While the colloid changes its radial position under the influence of thermal noise, it still follows the Poiseuille flow. However, we expect the instantaneous axial velocity $v_z(r)$ to also fluctuate in time around a position-dependent mean value. To explore this feature, we plot the joint probability function $P(r, v_z)$ for $Re = 20$ and $a/R = 0.2$ in fig. 8. The mean axial velocity $\bar{v}_z^P(r)$ as a function of r is then calculated from $\bar{v}_z^P(r) = \int dv_z P(r, v_z) v_z$ and plotted in fig. 8 as red line. Here a problem arises since outside the peak region the distribution is small and it is not known with a sufficient accuracy to calculate reliable mean values. In order to determine position-dependent mean values in the full range of the radial coordinate, we apply the

Fig. 7. (Colour on-line) Characteristics of the radial distribution function $P(r)$: Full width at half maximum b plotted versus reduced colloid radius a/R for $Re = 20$ and 40 . The dashed line shows the scaling law $b/R = 7.84(a/R)^{-1.75}Re^{-0.92}$. Inset: Position $r_{\max}$ of the maximum of $P(r)$ versus a/R for $Re = 20$ and 40 .

Fig. 8. (Colour on-line) Gray-scale representation of the joint probability distribution $P(r, v_z)$ for $a/R = 0.2$ and $Re = 20$. The green lines show contours of equal probability. Solid red line: mean value $\bar{v}_z^P(r)$ calculated with $P(r, v_z)$, dashed blue line: mean value $\bar{v}_z(r)$ calculated in sect. 3.2.

method outlined in sect. 2.5. The dashed line in fig. 8 shows the mean axial velocity $\bar{v}_z(r)$ determined with this method in sect. 3.2. It agrees with the mean value $\bar{v}_z^P(r)$ calculated in the peak region of the distribution.

3.2 Lift forces and axial velocity

We can understand the radial distribution function $P(r)$ discussed in the previous section in terms of a radial lift force acting on the colloid and its Brownian motion. We first determine the lift force introduced in sect. 2.5 and then calculate $P(r)$ in sect. 3.3.

Figure 9 shows the radial dependence of the lift force for two Reynolds numbers and several colloid sizes a/R . All the curves have the same shape. They display two radial positions where the force is zero. One position is on the channel axis where the radial force vanishes due to the

Fig. 9. (Colour on-line) Lift force f_{lift} in units of $\rho\nu^2$ plotted versus radial position r/R for several colloid sizes a/R at Reynolds numbers $\text{Re} = 40$ (a) and $\text{Re} = 20$ (b). The error bars show the standard error $\sigma_{f_{\text{lift}}}$ defined in eq. (11). The lines serve as a guide to the eye.

circular symmetry of the channel. However, the position on the channel axis is unstable since close to $r = 0$ the lift force points away from the channel axis. With increasing radial coordinate, f_{lift} goes through a maximum, reaches the second radial position r_{eq} with $f_{\text{lift}} = 0$, becomes negative, and ultimately diverges close to the channel wall. The second position with zero force is stable since the forces of nearby locations drive the colloid back to this equilibrium position. It agrees with the maximum of the radial distribution function as we will explain in the following section. Note also that around r_{eq} the force curve is asymmetric with a larger curvature towards the wall.

Since the equilibrium position r_{eq} agrees with the location of the maximum in $P(r)$, it shows the same behavior as r_{max} in the inset of fig. 7. It slightly shifts closer to the wall with increasing Reynolds number. This shift was predicted in analytic works that calculated f_{lift} by an asymptotic expansion [7, 8]. It was also observed in numerical works on rectangular channels [10, 22]. In addition, the shift to smaller radial positions with increasing colloid size was also reported in ref. [22].

Figure 9 also illustrates how the magnitude of the lift force increases with both colloid size and Reynolds num-

Fig. 10. (Colour on-line) All lift forces normalized by the scaling factor $\text{Re}^2(a/R)^{3.13}$ plotted versus radial position r/R . Near the centerline of the channel the forces collapse onto one master curve. Note that the force values for $a/R = 0.2$ and $\text{Re} = 20$ were not used to determine the scaling exponent $m = 3.13$.

ber. Asmolov predicted such a behavior by deriving the scaling law

$$f_{\text{lift}}(r)/(\rho\nu^2) = \text{Re}^2(a/R)^m f_g(r), \quad (12)$$

with the help of a matched asymptotic expansion for small colloid sizes, where the exponent was $m = 4$ [8]. The factor $f_g(r)$ gives the radial dependence. Finite-element studies on channels with circular cross-sections found an exponent $m = 3.28$ for the lift forces close to the channel axis where the influence from the channel walls is negligible [22]. Using our data on the lift forces up to a radial position of $r/R = 0.2$, we determined an exponent $m = 3.13$ in good agreement with ref. [22], where similar colloid sizes were studied. In fig. 10 we plot all our lift force data normalized by the scaling factor $\text{Re}^2(a/R)^{3.13}$ and indeed observe that close to the centerline the forces collapse onto a single master curve. At larger radial positions the channel wall becomes important and the scaling law is no longer valid. The curves for $a/R = 0.2$ deviate stronger from the master curve since the corresponding force values have a larger relative standard error.

Similar to the lift force we also measure the mean axial velocity $\bar{v}_z(r)$ of the colloid as outlined in sect. 2.5. Figure 11 plots the axial velocity normalized by the flow velocity $u_z(r)$ of the Poiseuille flow at the same radial position. Several features are visible. First, the graphs are nearly horizontal close to the centerline meaning that the colloid velocity also has a parabolic profile as the Poiseuille flow. Towards the channel wall the colloids slow down due to hydrodynamic friction with the wall and a deviation from the parabolic profile occurs. The effect is more pronounced for larger colloids. Second, the ratio $\bar{v}_z(r)/u_z(r)$ is always smaller than one meaning that the colloids lack behind the Poiseuille flow. This effect becomes stronger with increasing colloid size. To quantify it, we plot $1 - \bar{v}_z(0)/u_{\text{max}}$ versus a/R in the inset of fig. 11 and find the scaling law $1 - \bar{v}_z(0)/u_{\text{max}} \propto (a/R)^{1.68}$. Third, the flow profiles for $\text{Re} = 20$ and 40 fall on top of each other

Fig. 11. (Colour on-line) Axial colloid velocity $\bar{v}_z$ normalized by the velocity $u_z(r)$ of the undisturbed Poiseuille flow for several colloid sizes a/R with $\text{Re} = 20$ (lines and open symbols) and $\text{Re} = 40$ (filled symbols). Inset: double logarithmic plot of $1 - \bar{v}_z(0)/u_{\max}$ against a/R ; dashed line: fit to the power law $\propto (a/R)^{1.68}$.

when normalized by the maximum flow velocity or Re . We indicate this behavior by the filled and open circles in fig. 11 which lie on the same curve for one colloid radius.

We will now demonstrate how the lift forces determine the radial distribution functions recorded in the simulations.

3.3 From lift forces to radial distribution functions

It makes sense to assume that the stochastic motion of the colloid in the cross-section of the channel is completely determined by the lift force but otherwise independent from the colloid motion along the channel axis. We use the lift force f_{lift} to formulate a Langevin equation for the position vector $\mathbf{x}_{\perp}$

$$M \frac{d^2}{dt^2} \mathbf{x}_{\perp} + \xi \frac{d}{dt} \mathbf{x}_{\perp} = \mathbf{e}_r f_{\text{lift}}(r) + \mathbf{\Gamma}(t), \quad (13)$$

where M is the colloidal mass, ξ the friction coefficient, and $\mathbf{e}_r$ a unit vector in radial direction. The thermal force $\mathbf{\Gamma}(t)$ has a zero mean value $\langle \Gamma_{\alpha}(t) \rangle = 0$ and its second moment obeys the fluctuation-dissipation theorem, $\langle \Gamma_{\alpha}(t) \Gamma_{\beta}(t') \rangle = 2\xi k_B T \delta_{\alpha\beta} \delta(t - t')$. We include here the inertial term in the Langevin equation since the colloid Reynolds number $\text{Re}_c = \text{Re} a/R$ quantifying the importance of the colloid inertia ranges from 0.02 to 20.

Langevin equation (13) describes the thermal motion of the colloid in the cross-sectional plane of the channel. Here we are only interested in the steady state. If we assign a potential

$$U(r) = - \int_0^r f_{\text{lift}}(r') dr' \quad (14)$$

to the lift force, the stationary distribution for the particle's radial position and its cross-sectional velocity is the conventional Boltzmann distribution

$$P(r, \mathbf{v}_{\perp}) = P_0 \exp[-U(r)/k_B T] \exp\left[-\frac{M}{2k_B T} \mathbf{v}_{\perp}^2\right]. \quad (15)$$

Fig. 12. (Colour on-line) Radial distribution functions calculated from the spatial part of the Boltzmann distribution in eq. (15) (solid lines) and determined from the particle trajectories in the simulations (dashed lines) for $\text{Re} = 40$ and $\text{Re} = 20$ (inset). The symbols indicate the positions for which the lift forces are known.

The normalization factor P_0 is chosen such that $P(r, \mathbf{v}_{\perp})$ integrates to one. Alternative approaches for eq. (15) are given in refs. [6,41].

Figure 12 compares the radial distributions calculated from the spatial part of the Boltzmann distribution (15) (solid lines) and determined from the simulated particle trajectories (dashed lines). The agreement is remarkably good considering also the fact that the lift forces are only known at a few positions indicated by the symbols in fig. 12. To calculate the potential $U(r)$, we used a linear interpolation of the lift force curves of fig. 9. Remarkably, this is sufficient to reproduce the narrow distributions for $a/R = 0.5$ with three points. By analyzing the colloidal trajectories from the simulations, we also checked that the velocity part of the Boltzmann distribution is perfectly Gaussian as expected.

In the end we comment on the scaling of the width of the radial distribution function, $b/R = 7.84(a/R)^{-1.75} \text{Re}^{-0.92}$, which we observed in fig. 7. In fig. 10 we find that the magnitude of the lift force f_0 scales as $\text{Re}^2(a/R)^{3.13}$. If we apply a harmonic approximation around the zero value of the lift force, where the magnitude again scales as f_0 , we obtain a Gaussian distribution for $P(r)$ around its maximum. The width of the Gaussian then scales as $1/\sqrt{f_0} = \text{Re}^{-1}(a/R)^{-1.56}$, which comes close to the observed scaling for b/R .

3.4 Mapping to physical units

In MPCD units the force value $\rho \nu^2$ gives the right order of magnitude of the recorded lift forces as demonstrated in fig. 9. For example, if we take the MPCD parameters at $\text{Re} = 40$ from table 1, we find $\rho = n/l_c^3 = 10$ and therefore $\rho \nu^2 = 1.8$. Multiplying with the MPCD unit length, which here equals the linear cell size $l_c = 1$, gives the characteristic energy 1.8. This is nearly equal to the thermal energy in MPCD units, which we set to $k_B T = 1$,

and explains the observed widths of the distributions for a channel radius of $R = 25$.

In physical units the force scale with density $\rho = 10^3 \text{ kg/m}^3$ and kinematic viscosity $\nu = 10^{-6} \text{ m}^2/\text{s}$ of water is $\rho\nu^2 = 1 \text{ nN}$ which agrees with typical force values mentioned in ref. [22]. The typical energy when taking the MPCD length scale as $l_c = 1 \mu\text{m}$ or a channel radius $R = 25 \mu\text{m}$ (in accordance with ref. [22]) amounts to $1 \text{ nN} \mu\text{m}$ which should be equal to $1.8k_B T$. This means that the temperature is by a factor of 10^5 larger than room temperature. So, in reality at room temperature the distributions are sharply peaked for $\text{Re} = 40$.

Keeping the total number of fluid particles fixed, one can show that the large Reynolds number together with the constraint on the Mach number forbids to lower the temperature and an increased thermal motion occurs. This is a typical artifact of the MPCD method, which becomes particular obvious at high Reynolds numbers [36]. One can only achieve a lower temperature by increasing the number of fluid particles and thereby the total simulation time. Nevertheless, as we have shown, using the MPCD method, we are able to determine the lift force acting on the colloid. We could then use it to construct the radial distribution function at the correct temperature without performing simulations.

4 Conclusion

In this article we addressed inertial microfluidics using the method of MPCD. In particular, we modeled the motion of a spherical colloid in a circular microchannel under pressure-driven flow. We discussed in detail how to tune the MPCD parameters in the range of intermediate Reynolds numbers under the constraint of keeping the Mach number sufficiently small. We determined the radial distribution function for various Reynolds numbers and colloid sizes using the method of kernel density estimate. In particular, we showed that the width of the distribution decreases with increasing colloid size and Reynolds number, whereas the position of its maximum shifts to smaller radial positions when the colloid radius increases and when the Reynolds number decreases. These features are interesting for particle sorting. Furthermore, we showed that MPCD is well suited for calculating lift forces acting on the colloid while drifting towards the Segré-Silberberg annulus and also for calculating the colloid's axial velocity. Based on a Langevin equation for the cross-sectional motion, we demonstrated that the radial distribution function is linked to a Boltzmann distribution that uses the integrated lift force as a potential energy.

Although the temperature in our MPCD simulations assumes unrealistically high values, a typical artifact of the MPCD method [36], MPCD is well suited to determine the mean values of the lift force and axial velocity. For example, we are currently calculating the radial lift force when an additional external force along the channel axis is applied which gives rise to the Saffman force. This will enable us to tune the steady-state radial position of the colloid in the microchannel. Using the lift force in

the corresponding Langevin equation, we are then able to study how the colloid assumes its steady state or to steer the colloid towards the prescribed position by applying an appropriate feedback control mechanism. One of the great strengths of MPCD is the easy implementation of complex geometries. We will therefore extend our work on inertial microfluidics to explore curved channels or the effect of undulating cross-sections. Finally, we also plan to study the collective dynamics of colloids with special emphasis on the reported formation of particle trains [5, 10].

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