Dynamics of diatoms in a turbulent flow

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Abstract

In this project, we plan to perform a numerical study based on a Lagrangian-Eulerian approach. We model diatoms as non-spherical particles, which are transported by the flow and we neglect the effect of inertia (initially). These particles are placed in a homogeneous and isotropic turbulent flow, obtained by a direct numerical simulation of Navier-Stokes equation, in which a passive scalar field is simulated. The passive scalar represents the concentration of salt nutrients necessary for the growth of diatoms. The numerical simulation will aim to quantify the rate of the encounter between planktonic organisms and nutrients under the effect of turbulence. We will conduct a parametric study where the shape and inertia of particles, and possibly the intensity of turbulence, will be varied.
1 Introduction

The nature of suspended particles in turbulent flows is of our interest to a large number of process like collisions of water droplets in atmosphere, sediment transport and ecological processes in plankton. Planktons indeed play a major role in aquatic food chain, they are the base for the largest food web in the world by sustaining all the world’s most important fisheries and global biological cycle particularly the carbon cycle. In this project our interest is in analyzing the behavior of diatoms in a turbulent flow. Diatoms are one of the most critical group of photosynthetic platonic organism in water bodies and high altitude environment. They are unicellular but there many species which can form colonies in form of filaments also they can form long chains and this makes them an attractive model for studies on non spherical particles in turbulent flows. The diatoms are non motile which means non exhibiting the capability of movement but they have a cell wall which is made up of silica and there cell wall is denser then the sea water that permits the cell to be negatively buoyant.

Diatoms are generally smaller then or nearly same size of that of Kolmogorov length scale. So, we are more concerned in the dissipation at small scale which is independent of the production mechanism.

Here, we use a numerical model to examine whether the rotation or translation of diatoms in turbulent flow is able to quantify the rate of the encounter between planktonic organisms and nutrients under the effect of turbulence. As a prerequisite we need to develop the orientation of small spheroids settling in turbulent flow under the assumption that fluid inertia can be neglected.
Dissipation rates of turbulent kinetic energy $\varepsilon$ in the ocean vary extremely in space and in time. In open ocean, typical values range from $10^{-10}$ to $10^{-7} m^2 s^{-3}$, while coastal regions, especially influenced by tidal fronts, experience higher dissipation rates, on the order of $10^{-7}$ to $10^{-4} m^2 s^{-3}$. In the water column, turbulent kinetic energy dissipation rates are higher at the surface and decrease with depth. Given that kinematic viscosity of sea water is $v \sim 10^{-6} m^2 s^{-1}$, the characteristic Kolmogorov scale $\eta$ in the ocean is of range from $\sim 300 \mu m$ to a few millimetres.[2]

Generally speaking, diatoms are smaller than characteristic Kolmogorov scale in the ocean, and in range in size of few micro metres for small cells and range in size of hundred of micro metres in chain forming species. The various shapes of diatoms have probably evolved through natural selection since shape is likely to affect their ability to collect nutrients and reproduce.[7] M Niazi Ardekani et al 2017. Turbulence and shape are known to affect the sinking rate of particles and their eventual deposition in homogeneous isotropic turbulence.\(^1\)

\(^1\) Illustration of several size and type of diatoms
2 Theory of non spherical particles

Turbulent flows with suspended particles of non spherical shape occur most frequently in many natural and industrial processes. For instance dynamics of ice clouds, the cycle of planktons and marine snow in oceans. The problem of anisotropic particles in turbulence is more complicated. Apart from the complications of turbulence and multiphase flow with spherical particles, we have to consider the torques and forces that depend on the particle orientation. Their is a simple and rich problem at the core of non spherical particles in turbulence. Inertia-less particles passively follow the transnational fluid motion irrespective of their shape so their transnational motion is identical to Lagrangian fluid particles while spherical tracer particles rotate along their fluid vorticity. Non spherical particles are rotated randomly with respect to inertial frame of reference in homogeneous isotropic turbulence, their anisotropic shape induces a preferential alignment with local velocity gradient tensor. When non spherical particles are not density matched, they exhibiting many features of inertial particles in turbulence, such as preferential concentration, but with rich additional phenomena due to particle orientation and rotational slip.[13] Greg A Voth et Soldati, 2016

2.1 Oblate and prolate spheroids

Since a sphere is isotropic, its orientation is not important, and the translational motion can be solved independently of the rotational motion. On the other hand, for elongated particles the orientation must be considered since it influences the translational motion. In general axisymmetric ellipsoid are called spheroids. The spheroid can be specified by single aspect ratio, $\alpha=1$ corresponds to a sphere, $\alpha > 1$ corresponds to prolate spheroid and $\alpha < 1$ implies to oblate spheroid or disk. The rotation of axisymmetric particle are neutrally decomposed into a component along the symmetry axis i.e. spinning and components perpendicular to symmetry axis i.e. tumbling.
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2.2 Tracer particles

Phytoplankton eats nutrients are nutrients are more smaller then that of the size of phytoplankton. They can be modelled as passive tracer.

3 Governing equation

3.1 Modeling as passive tracer

The modeling of the diatom can be done by considering them as non motile particles which move passively by water turbulence. A commonly used simplified, but non trivial for passively advected particles is mathematically given by:

$$\frac{dx}{dt} = u$$

where,

- x is the particle position.
- u is the velocity of fluid.

This will produce translation in the particle but our aim is not only translation we want to give orientation to the particle as well. So, for orientation we are using the Jeffery’s equation.[12]Jeffery Equation

Figure 1: Illustration of oblate $\alpha < 1$ and prolate $\alpha > 1$ spheroid
The mathematical equation governing orientation of the particles is given by:

\[ \dot{p}_i = \Omega_{ij}p_j + \frac{\alpha^2 - 1}{\alpha^2 + 1} (S_{ij}p_j - p_ip_kS_{kl}p_l) \]  

where,

\[ \alpha = \frac{l}{d} \] is the aspect ratio.

\[ \Omega_{ij} \] is the rate of rotation tensor.

\[ S_{ij} \] is the rate of strain tensor.

\[ \dot{p}_i \] is the component of orientation vector which is along the axis of symmetry of particle.

Figure 2: Oblate spheroid, \( \alpha < 1 \)
3.2 Discussion

This will produce particles with complex dynamics, and particles will distribute homogeneously so their is no need of inertia, this does not reveal the orientation. Particles gets aligned due to the vorticity vector. In general it is known but many researches reveal the fact that disks like particle rotate much faster then elongated particles.[8] Parsa, Calzavarini et al 2012

In order to provide a strong example of rich dynamics of non spherical particles in turbulence, we can easily observe the trajectory of small rod in an experiment by [8] Parsa et al 2012. By the help of high speed imaging from multiple cameras, the Lagrangian trajectories of rod in a nearly homogeneous turbulence field was measured and presented in three dimensional view (3D). The trajectory reveals several important properties of anisotrophic particles in turbulence.
Figure 4: Trajectory of fiber from multiple camera high speed measurement in turbulent flow between oscillating grids at $R_\lambda = 214$.

In the three dimensional view of trajectory of fiber from multiple camera high speed measurement in turbulent flow between oscillating grids at $R_\lambda=214$, the colour of rod is representing the tumbling rate. The colour blue represents a low tumbling rate while colour red represents high tumbling rate.\(^2\)

The trajectory shows several important features of anisotropic particles in turbulence. The first important feature that can be seen is that there are regions of trajectory with vary rapid changes in the particle orientation with squared tumbling rates up to 30 times the mean square. These events come from intermittent large velocity gradients and those are the characteristics feature of high Reynolds number turbulent flows. With anisotropic particles there effects are evident in rotation of the particle.

\(^2\)Parsa et al, 2012
3.3 Results

To understand the effect of shape of particles on rotation dynamics can be analyzed by plotting mean square rate as a function of aspect ratio. In this observation we can easily observe that the mean square rotation rate of disk like particles $\alpha < 1$ is much larger then sphere $\alpha = 1$. As this can be understood as the additional contribution
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of strain $S_{ij}$ in our equation 2 to the rotation rate. While the rotation rate of rods $\alpha > 1$ is even much smaller then spheres even the rate of strain contributes to their rotation as well. For understanding the concept of rotation rate we should consider preferential alignment that occurs between velocity gradient tensor and the particles. When particles are rotated randomly, their mean square rotation rate can be calculated analytically using [12] Jeffery’s equation by extending the calculation to finite aspect ratio.

$$\langle \dot{\theta}_i \dot{\theta}_j \rangle \langle \varepsilon \rangle / \nu = \frac{1}{6} + \frac{1}{10} \left( \alpha^2 - 1 \right)^2$$

(3)

When the particles are advected by the flow, they become oriented so that their mean square rotation rates are different from randomly oriented case, with the largest difference coming for this rods as ($\alpha >> 1$)

Figure 6: Mean square rotation rate as a function of aspect ratio
The alignment with the vorticity will reduce the mean square rotation rate as only the vorticity perpendicular to the rod contributes to its rotation rate. Nevertheless, it is not known currently how to predict the effect of alignment on the mean square rotation rate.

3.4 Model considering inertia only for center of mass

Recently a group of researchers in fluid mechanics had studied about diatoms [10] Shin and Maxey 1997,[11]Siewart et al. 2014 they used direct numerical simulation to study settling velocity of heavy ellipsoid in decaying isotropic turbulence. They found preferential orientation with respect to the direction of gravity for prolate and oblate spheroid and higher sedimentation velocities then that calculated from orientation probabilities. The studies demonstrated that non spherical inertial particles experiences a preferential sweeping mechanism. The effect of turbulence on the settling of spheroids was found to be dependent on turbulence level and the aspect ratio of spheroid.

Diatoms and other phytoplankton represent the other extreme anisotropic particles that are weekly inertial. In their work they expand the modeling efforts to the parameter space at which phytoplankton operate.

The diatom was modelled as non spherical spheroids using analytical and DNS to examine if settling velocities of inertia-less diatoms are altered by turbulence and then their is introduction of flow solver and one way coupling to model turbulence used in this study to describe the particle motion in homogeneous isotropic turbulence. Finally it was examined that whether turbulence effects sinking velocities and clustering of weekly inertial particles and how they vary as a function of particular parameter.
3.5 Simple governing equations and numerical methods

The flow is considered incompressible so the incompressible turbulent velocity field, \( u \), obeys Navier stoke’s and Continuity equation.

\[
\frac{\partial u}{\partial t} + u \cdot \nabla u = -\nabla p + \frac{1}{Re} \nabla^2 u + f
\]  
\( \nabla \cdot u = 0 \)  

where,

- \( t \) is the time.
- \( p \) is the pressure.
- \( Re \) is the Reynolds number.
- \( f \) is the forcing necessary to maintain a turbulent velocity in steady state.

The equations are discretised in periodic domain at boundaries. Direct numerical simulation is employed to all the relevant flow scale without any artificial model at the smallest scale. Also, we evolve the equation in three periodic domain, it is obvious to do so in Fourier space with pseudo spectral method. The non linear terms are evaluated in physical space using classic 2/3 rule to minimize aliasing error. Time integration is done with third order low storage Runge Kutta method where diffusive terms are calculated analytically also we should not forget that in Fourier space the Laplacian operator is proportional to square of modulus of wave vector \( k^2 \). For the non linear terms Adam Bashforth like approximation is employed. The stochastic forcing is evaluated in Fourier space and it acts isotropically in first shell of wave vectors. The forcing amplitude is constant in time and field is delta correlated in time and uniformly distributed in phase and direction. We employed a resolution of \( 128^3 \) grid points with Taylor Reynolds number \( Re_\lambda = 100 \) and \( 64^3 \) grid points with Taylor Reynolds number \( Re_\lambda = 60 \). The turbulence is characterized by Taylor Reynolds number which is given as :

\[
Re_\lambda \equiv u'\lambda/\nu
\]

where,

- \( u' \) is the root mean square velocity fluctuation.
- \( \nu \) is the kinematic viscosity.
- \( \lambda \) is the Taylor micro scale.
- \( \lambda \equiv \sqrt{\epsilon/15u'^2} \)
- \( \epsilon \) is the kinetic energy dissipation rate.
3.6 Particle relaxation time

For spherical particles, the translational relaxation time is given by:

\[ \tau_p = \frac{(2\rho_p a^2)}{(9\mu)} \quad (7) \]

where,
\( \rho_p \) is particle density.
\( \mu = \rho_f \nu \) is the dynamic viscosity.
\( a \) is the particle radius.

For non-spherical particles, the particle translational relaxation time depends on direction and additional rotational relaxation time may be important.

A standard approach to define single particle relaxation time is to assume an isotropic particle orientation distribution, in which the average relaxation time for a prolate spheroid is given by : [9] Shapiro and Goldenberg 1993

\[ \tau_p = \frac{2 \rho_p a^2}{9 \mu} \frac{\alpha \ln (\alpha + \sqrt{\alpha^2 - 1})}{\sqrt{\alpha^2 - 1}} \quad (8) \]

where,
\( a \) is the particle radius perpendicular to symmetry axis.
\( \alpha \) is the aspect ratio.
For an oblate spheroid, the average relaxation time is given by : [1] Zhao et al 2015

\[ \tau_g = \frac{2 \rho_p a^2}{9 \mu} \frac{\pi - 2 \tan^{-1} \left( \frac{\alpha (1 - \alpha^2)^{-1/2}}{2 (1 - \alpha^2)^{1/2}} \right)}{2 (1 - \alpha^2)^{1/2}} \quad (9) \]

The relaxation time for prolate and oblate spheroid reduce to spherical result as \( \alpha \) goes to unity.
The relaxation times for a spheroid is given by :

\[
\tau_r = \frac{2}{15} \left( \frac{\rho_p a^2}{\mu} \right) \tag{10}
\]

For anisotropic particles, it is possible to define the rotational relaxation time tensor by the rotational resistance tensor. In particle coordinates, the rotational relaxation time tensor is diagonal with different time scale for tumbling and spinning, both of which are typically shorter then transnational relaxation time. With these operating parameter a tracer model for particular motion is suitable assumption and therefore assumes that cells behave as passive tracers with a correlation given by stokes settling velocity.

### 3.7 Translation and rotation of particles

In recent works in diatoms, the particle transnational motion obeys :

\[
\frac{dx}{dt} = u_x |x| + v_s(p) \tag{11}
\]

\[
v_s(p) = v_s^{\text{min}} \hat{e}_g + (v_s^{\text{max}} - v_s^{\text{min}}) (\hat{e}_g \cdot p) p \tag{12}
\]

where,

- \(x\) is the particle position
- \(u_x\) is the fluid velocity at specific position.
- \(v_s\) is the Stokes settling velocity.
- \(p\) is the particle orientation position.
- \(\hat{e}_g\) is a unit vector in direction of gravity.
- \(v_s^{\text{max}}\) and \(v_s^{\text{min}}\) are the minimum and maximum settling velocity in quiescent flow, corresponding to particles falling with major axis perpendicular or parallel to the direction of gravity.
The velocity $v_{s}^{\max}$ and $v_{s}^{\min}$ can be written as following:

\[ V_{s}^{\max} = \frac{(\rho_{p} - \rho_{f}) gl^{2}}{\mu_{f}} \gamma_{0}(\alpha) \]  
\[ V_{s}^{\max} = \frac{(\rho_{p} - \rho_{f}) gl^{2}}{\mu_{f}} \gamma_{1}(\alpha) \]

where,

- $g$ is the gravitational acceleration.
- $l$ is the length of spheroid major axis.
- $\mu_{f}$ is the dynamic viscosity of fluid.
- $\rho_{p}$ and $\rho_{f}$ are the densities of particle and the fluid respectively.
- $\gamma_{0}$ and $\gamma_{1}$ are the functions of aspect ratio for full expression see [3] Dahlkild 2011

For the orientation of particle it follows the Jeffery equation [12] as explained earlier which is given as:

\[ \dot{p}_{i} = \Omega_{ij} p_{j} + \frac{\alpha^2 - 1}{\alpha^2 + 1} (S_{ij} p_{j} - p_{i} p_{k} S_{kl} p_{l}) \]

where,

- $\alpha = l/d$ is the aspect ratio.
- $\Omega_{ij}$ is the rate of rotation tensor.
- $S_{ij}$ is the rate of strain tensor
- $\dot{p}_{i}$ is the component of orientation vector which is along the axis of symmetry of particle.
3.8 Results and discussion

The settling of prolate spheroidal particles of constant volume is focusing on the effect of particle aspect ratio. The parameter used are $Re_\lambda = 100$, $\rho_p/\rho_f = 1.05$ and $D_{eq} = \eta/6$, where $D_{eq}$ is the diameter of sphere having the same volume as the prolate spheroid and $\eta$ is the Kolmogorov length scale. Fixing the volume, the settling velocity varies with aspect ratio. We should not forget that for high aspect ratio $\alpha > 15$ the larger diameter of spheroid exceeds the Kolmogorov length scale $\eta$ ($\approx 1.24$ for $\alpha = 24$). This does not violate the assumption of tracer particles since rods acts as tracer when their length is less then $5\eta$ and deviation from tracer behaviour are very small until about $15\eta$ [6] Parsa and Voth 2014. In this model inertia is taking into account implicitly. This model has some limitation that model is valid only if particle is slightly heavier then flow and normally this hypothesis is not always justified.

3.9 Model considering the drag

The fact that rotational relaxation time is shorter the transnational relaxation time allows us to propose a model. It is not known in general, but recently many papers reveals this key information [7] M Niazi Ardekani et al 2017, [1] Challabotla, Zhao et al 2015

3.9.1 Modeling considering the center of mass

The transnational equation of motions given by linear momentum relation according to following equation:

$$m \frac{dv}{dt} = \mathbf{F}$$  \hspace{1cm} (16)

where,

- $m$ ............... is the mass of ellipsoid.
- $v$ ............... is the velocity vector in all three direction.
- $\mathbf{F}$ ............... is the drag force acting on ellipsoid under creeping flow condition.
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The drag force here is calculated by the equation explained below:

\[ F = \mu \pi a \cdot RKbR^T (u_f - v_p) \] (17)

where,
\( \mu \) .............. is the dynamic viscosity.
\( K \) .............. is the resistance tensor.
\( a \) .............. is the semi minor axis of ellipsoid revolution.

3.9.2 Modeling considering the orientation

Euler equation:

\[ \frac{d}{dt}(I \cdot \omega) + \omega \times (I \cdot \omega) = T \] (18)

An important parameter is the particle relaxation time, i.e. the time that the particle needs to respond to changes in the flow field due to inertia. For an ellipsoidal particles which is non isotropic the response time is not as obvious as a spherical particle. The equivalent response time based on isotropic particle orientation and the inverse of the resistance tensor.

\[ \tau_p = \frac{2 \rho_p a^2}{9 \mu} \frac{\alpha \ln (\alpha + \sqrt{\alpha^2 - 1})}{\sqrt{\alpha^2 - 1}} \] (19)

where,
\( a \) ...................... is the particle radius perpendicular to symmetry axis.
\( \alpha \) ...................... is the aspect ratio.
Orientation is governed by Jeffery equation which is explain in earlier models as well. \cite{Jeffery1922} Jeffery equation 1922

\[ \dot{p}_i = \Omega_{ij}p_j + \frac{\alpha^2 - 1}{\alpha^2 + 1} (S_{ij}p_j - p_i p_k S_{kl}p_l) \]  

where,
\[ \alpha = l/d \] is the aspect ratio.
\[ \Omega_{ij} \] is the rate of rotation tensor.
\[ S_{ij} \] is the rate of strain tensor
\[ \dot{p}_i \] is the component of orientation vector which is along the axis of symmetry of particle.

### 3.9.3 Particle acceleration

To describe a heavy and a spherical particles with a radius smaller then then Kolmogorov length scale only the drag and buoyancy forces are important. Based on the above assumptions the equation of motion can be demonstrated as: \cite{Shchekinova2018} 

\[ \frac{dv}{dt} = \frac{1}{\tau_p}[u(x_p, t) - v(t)] \]  

where,
\[ v(t) = dx_p/dt \] is the turbulence velocity.
\[ \tau_p \] is the relaxation time 

\[ \tau_p = \frac{2\rho_p a^2}{9\rho_f \mu} \]  

\[ \rho_p & \rho_f \] are diatomic cell and water densities respectively.
\[ a \] is the radius of the diatom.
\[ \mu \] is the water kinematic viscosity.

### 3.9.4 Explicit equation for coefficient of spheroidal particles

In the point-particle approximation, the force \( f \) and torque \( T \) on a spheroid are given by \cite{Marchioli2010, Gustavsson2014} 

\[
\begin{bmatrix}
  f \\
  T
\end{bmatrix}
= m\gamma 
\begin{bmatrix}
  M^{(t)} & 0 & 0 \\
  0 & M^{(r)} & M^{(2)}
\end{bmatrix}
\begin{bmatrix}
  u - v \\
  \Omega - \omega \\
  s
\end{bmatrix}
\]
where,
\( v \) is particle velocity.
\( S \) is strain rate matrix.
\( M(r) \) and \( M(t) \) are rotational and translational resistance.
\( \Omega \equiv \frac{1}{2} \nabla \wedge u \) is the half of turbulent vorticity.

Explicit expressions for the coefficient of \( C \) for spheroidal particles, as functions of the particle aspect ratio \( \alpha \) is given as:

\[
M_{ij}^{(t)} = C_\perp^{(t)} \delta_{ij} + \left( C_\parallel^{(t)} - C_\perp^{(t)} \right) p_ip_j
\]

(23)

The tensor \( M(t) \) relates the force on the particle to the slip velocity, the difference between the fluid and the particle velocities. The superscript refers to the translational \( (t) \) degrees of freedom. The equation for \( C \) perpendicular is given as follows as per [4]

\[
C_\perp^{(t)} = \frac{8 (\alpha^2 - 1)}{3\alpha ((2\alpha^2 - 3) \beta + 1)}
\]

(24)

The equation for \( C \) parallel is given as follows as per [4]

\[
C_\parallel^{(t)} = \frac{4 (\alpha^2 - 1)}{3\alpha ((2\alpha^2 - 1) \beta - 1)}
\]

(25)

The aspect ratio is the ratio of a perpendicular to the a parallel given by following relation.

\[
\alpha \equiv \frac{a_\parallel}{a_\perp}
\]

\[
\beta = \frac{\ln \left[ \alpha + \sqrt{\alpha^2 - 1} \right]}{\alpha \sqrt{\alpha^2 - 1}}
\]

3.10 Discussion and some result

In the plot in the X axis we have considered the aspect ratio and in Y we considered resistance tensor, \( K \) which is the coefficient of \( C_\perp \) and \( C_\parallel \) as a function of aspect ratio \( \alpha \). The plot show the behaviour of the drag force as a function of the particle shape.
Summary

We begin with defining the diatoms and planktons explaining its contribution to the largest food web in the world by sustaining all the most important fisheries and global ecological cycle. Here we use a numerical model to examine the whether rotation or translation of diatoms in turbulent flow is able to quantify the rate of the encounter between planktonic organisms and nutrients under the effect of turbulence. In general, diatoms are smaller then the Kolmogorov scale in the ocean and in range in size of few micro metres for small cells and in range of hundred of micro meter in chain forming species. We discover some basic theory of non spherical particles and later we built a parameter called aspect ratio to understand about prolate $\alpha > 1$ and oblate spheroid $\alpha < 1$. Phytoplankton eats nutrients are nutrients are more smaller then that of the size of phytoplankton. They can be modelled as passive tracer. So, we modelled diatom as a passive tracer which gives translation motion to diatom and for orientation we use Jeffery equation. [12]

We observe the trajectory of anisotropic particles in turbulence from paper of [8] Parsa et al 2012. The first important feature that can be seen is that there are regions of trajectory with vary rapid changes in the particle orientation with squared
tumbling rates up to 30 times the mean square. These events come from intermittent large velocity gradients and those are the characteristics feature of high Reynolds number turbulent flows. With anisotropic particles these effects are evident in rotation of the particle. To understand the effect of shape of particles on rotation dynamics can be analyzed by plotting mean square rate as a function of aspect ratio. In this observation we can easily observe that the mean square rotation rate of disk like particles $\alpha < 1$ is much larger than sphere $= 1$.

Later, we build a model considering inertia only for the center of mass and we consider the effect of gravity in this model. The diatom was modelled as non spherical spheroids using analytical and DNS to examine if settling velocities of inertia-less diatoms are altered by turbulence and then their is introduction of flow solver and one way coupling to model turbulence used in this study to describe the particle motion in homogeneous isotropic turbulence. We developed a concept that rotational relaxation time is shorter than translational relaxation time.
In recent works on diatoms, the particle transnational motion obeys fluid velocity plus Stokes settling velocity which depends on orientation of particle with respect to gravity and also for the orientation the famous Jeffery equation can be used.[12]. In this model inertia is taking into account implicitly. This model has some limitation that model is valid only if particle is slightly heavier then flow and normally this hypothesis is not always justified.

Based on the fact that rotational relaxation time is shorter the transnational relaxation time allows us to propose a model. The fact is not known in general, but recently many papers reveals this key information and also it can be calculated numerically by data available in those papers. We propose a model considering anisotropic drag and the equation for the center of mass and particles force and torques are explained in the section for the orientation we are using the Jeffery equation [12] and equation for acceleration is described. We present the explicit expression for coefficient of C for spheroidal particles, as a function of particle aspect ratio. We define the tensor M(t) which relates the force on particle to slip velocities. We compared the coefficients C\text{perpendicular} and C\text{parallel} as a function of the aspect ratio alpha, in order to show the behaviour of the drag force as a function of the particle shape.
5 Appendix

5.1 Appendix I

Jeffery equation:[12]

We want to evolve a vector; these vector will be rotated by the velocity gradients. Let us assume the matrix that rotate the vector is $K$
So, we apply $K$ to vector $\vec{P}$ and we get $\vec{P}$

We know that aspect ratio is given by,

$$Aspectratio = \frac{\alpha^2 - 1}{\alpha^2 + 1}$$

$$\vec{P} = \overrightarrow{K\bar{P}}$$

The constraint is that $p^T p = 1$ and

$$K = \Omega + f(\alpha)\vec{S}$$

We introduce a normalizing parameter $\gamma$, so

$$\vec{P} = K\bar{P} + \gamma \bar{P}$$

Evolution of equation that preserve the norm of $\vec{P}$
Computing the explicit equation for $\gamma$
\[ P^T P = 1 \]
\[ \frac{d}{dt} (P^T P) = 0 \]
\[ P^T \dot{P} + P^T \dot{P} = 0 \]
\[ \dot{P}^T = P^T k + \gamma P^T \]
\[ P^T k^T P + \gamma P^T P + p^T K P + \gamma P^T P = 0 \]
\[ P^T \left( K^T + K \right) P + 2\gamma = 0 \]
\[ \gamma = P^T \frac{1}{2} \left( K^T + K \right) P \]

Since in general \( K = \Omega + f(\alpha)S \)

\[ \gamma = f(\alpha)P^T SP \]

\[ \vec{P} = \Omega P + f(\alpha)(SP + P^T SP P) \]
5.2 Appendix II

Development of codes in C

We calculate the drag force for the spherical and non spherical particles.

```c
if((tracer+ipart)- tau_drag = 0.0)
{
  if((tracer + ipart) − tau_drag 0.0)
  {
    Why 0 ?

  }

  This is because == 0 is a tracer and 0 is an eulerian probe.
```

```c
#ifndef LAGRANGE_ORIENTATION_DRAG
The Stokes drag acceleration on a sphere is given by:
invtau = 1.0 /
(tracer+ipart)- tau_drag;
(tracer + ipart) − ax =
((tracer + ipart) − ux −
(tracer + ipart) − vx) * invtau;
(tracer + ipart) − ay =
((tracer + ipart) − uy −
(tracer + ipart) − vy) * invtau;
(tracer + ipart) − az =
((tracer + ipart) − uz −
(tracer + ipart) − vz) * invtau;
#else
```

The Stokes drag force on a NON spherical (axisymmetric ellipsoidal) particle is given by:
The notation is same as in PRL 119, 254501 (2017) see also its supplementary materials
The aspect ratio is a_par / a_perp

```c
alpha = (tracer+ipart)- aspect_ratio;
```
The meaning of the parameter \( \tau_{\text{drag}} \) in our code is \( \frac{\rho_p^2 a_{\text{perp}}^2}{9 \nu_f} \)

The particle relaxation time however is:
\[
\frac{\rho_p^2 a_{\text{perpa}} a_{\text{par}}}{9 \nu_f} = \tau_{\text{drag}} \alpha
\]

\( \text{invtau} = \frac{1}{(\text{tracer}+\text{ipart}) - \tau_{\text{drag}} \alpha} \);

We calculate the prefactors as following:

if (alpha == 1)
{
    beta = c_{\text{perp}} = c_{\text{par}} = 1.0;
}
else
{

    if (alpha > 1) beta = \log(\alpha + \sqrt{\alpha^2 - 1.0}) / (\alpha \sqrt{\alpha^2 - 1.0})
    if (alpha < 1) beta = \frac{\cos(\alpha)}{(\alpha \sqrt{1.0 - \alpha^2})}
    c_{\text{perp}} = \frac{8.0*(\alpha^2 - 1.0)}{3.0 \alpha ((2.0*\alpha^2 - 3.0)*\beta + 1.0)}
    c_{\text{par}} = \frac{4.0*(\alpha^2 - 1.0)}{3.0 \alpha ((2.0*\alpha^2 - 1.0)*\beta - 1.0)}
}
This part of code is responsible for assigning vector \( \mathbf{P} \) which is along the axis of rotation of the particle.

Vector \( \mathbf{p} \) can be calculated as:
vecP[0] = (tracer+ipart)-px;
vecP[1] = (tracer + ipart) - py;
vecP[2] = (tracer + ipart) - pz;

We build drag tensor here:
matM[0][0] = c_{\text{perp}} + (c_{\text{par}} - c_{\text{perp}})*vecP[0]*vecP[0];
matM[1][1] = c_{\text{perp}} + (c_{\text{par}} - c_{\text{perp}})*vecP[1]*vecP[1];
matM[2][2] = c_{\text{perp}} + (c_{\text{par}} - c_{\text{perp}})*vecP[2]*vecP[2];
matM[0][1] = matM[1][0] = (c_{\text{par}} - c_{\text{perp}})*vecP[0]*vecP[1];
matM[0][2] = matM[2][0] = (c_par - c_perp)*vecP[0]*vecP[2];
matM[1][2] = matM[2][1] = (c_par - c_perp)*vecP[1]*vecP[2];

We compute the velocity difference here:

\[
\begin{align*}
uvx &= (\text{tracer} + \text{ipart}) - ux - (\text{tracer} + \text{ipart}) - vx; \\
uvy &= (\text{tracer} + \text{ipart}) - uy - (\text{tracer} + \text{ipart}) - vy; \\
uvw &= (\text{tracer} + \text{ipart}) - uz - (\text{tracer} + \text{ipart}) - vz;
\end{align*}
\]

We compute the acceleration here:

\[
\begin{align*}
(\text{tracer} + \text{ipart}) - ax &= (matM[0][0] * uvx + matM[0][1] * uvy + matM[0][2] * uvz) * invtau; \\
(\text{tracer} + \text{ipart}) - ay &= (matM[1][0] * uvx + matM[1][1] * uvy + matM[1][2] * uvz) * invtau; \\
(\text{tracer} + \text{ipart}) - az &= (matM[2][0] * uvx + matM[2][1] * uvy + matM[2][2] * uvz) * invtau;
\end{align*}
\]

#ifdef LAGRANGE_GRAVITY
This part of code works only if LB_FORCING_GRAVITY is defined.

We add: -g to acceleration.

#ifdef LAGRANGE_GRAVITY_VARIABLE
(\text{tracer} + \text{ipart}) - ax = \\
(\text{tracer} + \text{ipart}) - gravitycoeff * property.gravity_x; \\
(\text{tracer} + \text{ipart}) - ay = \\
(\text{tracer} + \text{ipart}) - gravitycoeff * property.gravity_y; \\
(\text{tracer} + \text{ipart}) - az = \\
else(\text{tracer} + \text{ipart}) - ax = property.gravity_x; \\
(\text{tracer} + \text{ipart}) - ay = property.gravity_y; \\
(\text{tracer} + \text{ipart}) - az = property.gravity_z;
#endif
#endif
Dynamics of diatoms in a turbulent flow

References


Dynamics of diatoms in a turbulent flow

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