Transport

14. Hydrodynamics

- Diffusion equations, random walks, and the Langevin equation are useful for describing transport driven by random thermal forces under equilibrium conditions or not far from equilibrium (the linear response regime).
- Fluid Dynamics and hydrodynamics refer to continuum approaches that allows us to describe non-equilibrium conditions for transport in fluids. Hydrodynamics describes flow and transport of objects through a fluid experiencing resistance or friction.

Newtonian Fluids

- Fluids described through continuum mechanics.
  - Stress: Force applied to an object. Stress is force applied over a surface area, $a$. Force has normal ($z$) and parallel components ($x$).
  - The stress can be decomposed into the normal component perpendicular to the surface $\tilde{f}_z / a$, and the sheer stress parallel to the surface $\tilde{f}_x / a$.
  - Strain: The deformation (change in dimension) of object as a result of the stress.

- Solids
  - A solid is considered Newtonian if its behavior follows a linear relationship between elastic stress and strain, i.e. Hooke’s Law.
  - Solids are stiff and will return to their original configuration when stressed, but can’t deform far (without rupture).

- Fluids
  - Fluids cannot support a strain and remain at equilibrium. Conservation of momentum dictates that application of a force will induce a flow.
  - Fluids resist flow (viscous flow).
  - Newtonian fluids follow a linear relation between shear stress and the strain rate.

Viscosity

Viscosity measures the resistance to shear forces. A fluid is placed between two plates of area $a$ separated along $z$, and one plate is moved relative to the other by applying a shearing force along $x$. At contact, the velocity of the fluid at the interface with either plate is equal to the velocity of the plate as a result of intermolecular interactions: $\tilde{v}_z(z = 0) = 0$. This is known as the no-slip boundary condition. The movement of one plate with respect to the other sets up a velocity gradient along $z$. This velocity gradient is equal to the strain rate.

The relationship between the shear velocity gradient and the force is
\[ \mathbf{f}_x = a \eta \frac{d \mathbf{v}_x}{dz} \]

where \( \eta \), the dynamic viscosity (kg m\(^{-1}\) s\(^{-1}\)), is the proportionality factor. For water at 25°C, the dynamic viscosity is \( \eta = 8.9 \times 10^{-3} \) Pa s.

**Stresses in a Dense Particle Fluid**

A normal stress is a pressure (force per unit area), and these forces are transmitted through a fluid as a result of the conservation of momentum in an incompressible medium. This force transduction also means that a stress applied in one direction can induce a strain in another, i.e. a stress tensor is needed to describe the proportionality between the stress and strain vectors.

In an anisotropic particulate system, force transmission from one region of the fluid to another results from “force chains” involving steaming motion of particles that repel each other. These force chains are not simply unidirectional, but also branch into networks that bypass unaffected regions of the system.

Stokes’ Law

How is a fluid’s macroscopic resistance to flow related to microscopic friction originating in random forces between the fluid’s molecules? In discussing the Langevin equation, we noted that the friction coefficient $\zeta$ was the proportionality constant between the drag force experienced by an object and its velocity through the fluid: $f_d = -\zeta v$. Since this drag force is equal and opposite to the stress exerted on an object as it moves through a fluid, there is a relationship of the drag force to the fluid viscosity. Specifically, we can show that Einstein’s friction coefficient $\zeta$ is related to the dynamic viscosity of the fluid $\eta$, as well as other factors describing the size and shape of the object (but not its mass).

This connection is possible as a result of George Stokes’ description of the fluid velocity field around a sphere moving through a viscous fluid at a constant velocity. He considered a sphere of radius $R$ moving through a fluid with laminar flow: that in which the fluid exhibits smooth parallel velocity profiles without lateral mixing. Under those conditions, and no-slip boundary conditions, one finds that the drag force on a sphere is

$$f_d = 6\pi \eta R v$$

and viscous force per unit area is entirely uniform across the surface of the sphere. This gives us Stokes’ Law

$$\zeta = 6\pi \eta R_h$$

(1)

Here $R_h$ is referred to as the hydrodynamic radius of the sphere, the radius at which one can apply the no-slip boundary condition, but which on a molecular scale may include water that is strongly bound to the molecule. Combining eq. (1) with the Einstein formula for diffusion coefficient, $D = k_B T / \zeta$, gives the Stokes–Einstein relationship for the translation diffusion constant of a sphere

$$D_{\text{trans}} = \frac{k_B T}{6\pi \eta R_h}$$

(2)

One can obtain a similar a Stokes–Einstein relationship for orientational diffusion of a sphere in a viscous fluid. Relating the orientational diffusion constant and the drag force that arises from resistance to shear, one obtains

$$D_{\text{rot}} = \frac{k_B T}{6V_h \eta}$$

Laminar and Turbulent Flow

- Laminar flow: Fluid travels in smooth parallel lines without lateral mixing.
- Turbulent flow: Flow velocity field is unstable, with vortices that dissipate kinetic energy of fluid more rapidly than laminar regime.

Reynolds Number

The Reynolds number is a dimensionless number is used to indicate whether flow conditions are in the laminar or turbulent regimes. It indicates whether the motion of a particle in a fluid is dominated by inertial or viscous forces.\(^2\)

\[
\mathcal{R} = \frac{\text{inertial forces}}{\text{viscous forces}}
\]

When \(\mathcal{R} > 1\), the particle moves freely, experiencing only weak resistance to its motion by the fluid. If \(\mathcal{R} < 1\), it is dominated by the resistance and internal forces of the fluid. For the latter case, we can consider the limit \(m \to 0\) in eq. Error! Reference source not found., and find that the velocity of the particle is proportional to the random fluctuations: \(v(t) = f(t) / \zeta\).

We can also express the Reynolds number in other forms:

- In terms of the fluid velocity flow properties: \(\mathcal{R} = \frac{v \rho (d \nabla / dz)}{\eta (d^2 \nabla / dz^2)}\)
- In terms of the Langevin variables: \(\mathcal{R} = f_{in} / f_d\).

Hydrodynamically, for a sphere of radius \(r\) moving through a fluid with dynamic viscosity \(\eta\) and density \(\rho\) at velocity \(v\),

\[
\mathcal{R} = \frac{rv \rho}{\eta}
\]

Consider for an object with radius 1 cm moving at 10 cm/s through water: \(\mathcal{R} = 10^3\). Now compare to a protein with radius 1 nm moving at 10 m/s: \(\mathcal{R} = 10^{-2}\).

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Drag Force in Hydrodynamics

The drag force on an object is determined by the force required to displace the fluid against the direction of flow. A sphere, rod, or cube with the same mass and surface area will respond differently to flow. Empirically, the drag force on an object can be expressed as

\[ f_d = \left[ \frac{1}{2} \rho C_d v^2 \right] a \]

This expression takes the form of a pressure (term in brackets) exerted on the cross-sectional area of the object along the direction of flow, \( a \). \( C_d \) is the drag coefficient, a dimensionless proportionality constant that depends on the shape of the object. In the case of a sphere of radius \( r \): \( a = \pi r^2 \) in the turbulent flow regime ( \( \mathcal{R} > 1000 \) ) \( C_d = 0.44–0.47 \). Determination of \( C_d \) is somewhat empirical since it depends on \( \mathcal{R} \) and the type of flow around the sphere.

The drag coefficient for a sphere in the viscous/laminar/Stokes flow regimes ( \( \mathcal{R} < 1 \) ) is \( C_d = \frac{24}{\mathcal{R}} \). This comes from using the Stokes Law for the drag force on a sphere \( f_d = 6\pi \rho v r \) and the Reynolds number \( \mathcal{R} = \rho v d / \eta \).

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