

Introduction

Micro- and nanofabricated devices have led to revolutionary changes in our ability to manipulate tiny volumes of fluid or micro- and nanoparticles contained therein. This has led to countless applications for chemical and particulate separation and analysis, biological characterization, sensors, cell capture and counting, micropumps and actuators, high-throughput design and parallelization, and system integration, to name a few areas. Because biological and chemical analysis is typically concerned with molecules and bioparticles with small dimensions (some examples are shown in Fig. 0.1), the tools used to manipulate these objects are naturally of a similar scale, and the developments in micro- and nanofabrication in recent decades has brought engineering tools to a scale that easily matches these objects.

From a fluid-mechanical standpoint, our ability to manufacture micro- and nano-scale devices creates a number of challenges and provides matching opportunities, some of which are denoted schematically in Fig. 0.2. If we focus on liquid-phase devices, which have dominated most bioanalytical applications, shrinking the length scales makes interfacial phenomena and electrokinetic phenomena much more important, and reduces the importance of gravity and pressure. The no-slip boundary condition, safely assumed for macroscopic flows, can be inaccurate when the length scale is small. Although the low-Reynolds-number characteristic of most of these flows eliminates the challenges of nonlinearity in the convective term and the associated difficulty in modeling turbulent flows, we are instead forced to consider the nonlinearity of the source term in the Poisson–Boltzmann equation, nonlinearity of the coupling of electrodynamics with fluid flow, and uncertainty in predicting electroosmotic boundary conditions. Often, the microfluidics researcher worries not about *how* to solve the relevant governing equations and boundary conditions, but rather *what* those equations and boundary conditions are and how his or her analytical goals can be reconciled with fabrication

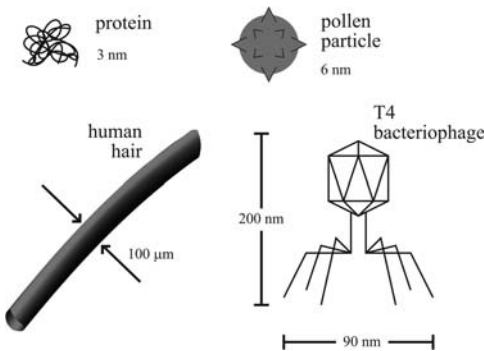


Fig. 0.1 Length scales of some biological objects ranging clockwise from top left from nano- to microscale.

2 Introduction

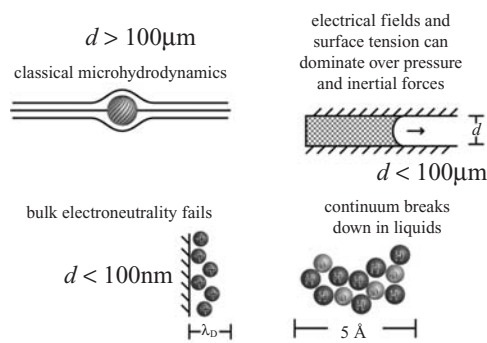


Fig. 0.2

Some fundamental changes in fluid physics and the length scales at which this occurs.

and experimentation concerns. Microscale problems are approached by use of continuum modeling and analysis, but the continuum governing equations must be modified to account for forces that are routinely ignored in macroscale systems. Figure 0.3, for example, highlights the general structure of a microfluidic device and some of the parametric inputs and fluid issues attendant with their use. Nanoscale problems are approached with a mix of continuum and atomistic approaches, depending on the the problem.

General properties of micro- and nanoscale flows. This text considers flow in micro- and nanofabricated devices, typically fabricated by photolithographic patterning combined with etching or molding processes evolved from microcircuit fabrication processes. The nature of the geometries, length scales, and materials used in these processes leads to a specialized set of physical phenomena and flow regimes, which have their own interesting properties and applications. Microscale flows are typically laminar owing to the short length scales, but can have large mass transfer Peclet numbers owing to the low diffusivity of macromolecules and particles of interest. These flows can be driven with

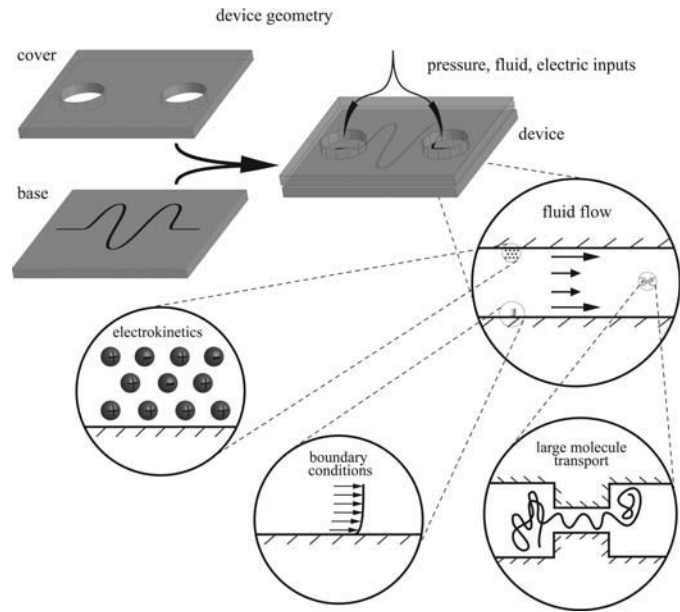


Fig. 0.3

A microfluidic device, its inputs, and some aspects of the fluid and analyte flow therein.

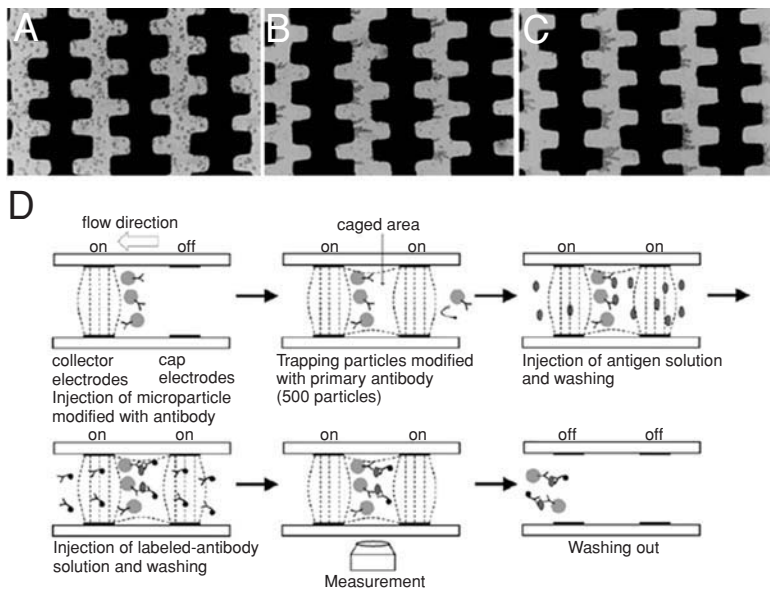


Fig. 0.4 (a) Patterned interdigitated electrodes used [1] to isolate leukemia cells from diluted blood. (b) A dilute blood suspension flows through a channel, and dielectrophoresis (Chapter 17) is used to capture both leukemia cells and erythrocytes (red blood cells) while (c) subsequently the frequency applied to the electrodes was decreased to retain the leukemia cells and elute the erythrocytes. (d) Microsystems are also used as [2] “microbeakers” whereby particles are caged from a flow stream by use of dielectrophoresis while chemistry and analysis are conducted by flowing various solutions over the captured particles on a microscope stage. Used with permission.

pressure, but applied electric fields are often more convenient or elegant to actuate these systems. Even if not applied, intrinsic electric fields exist at interfaces in all cases, driven usually by chemical reaction. Thus electrodynamics, chemistry, and fluid mechanics are inextricably intertwined, so that electric fields can create fluid flow and fluid flow can create electric fields, with a degree of coupling driven by the surface chemistry. The flow coupling is described by electrostatic source terms in the Navier–Stokes equations or particle transport equations. Many useful tools arise from these forces, such as electrokinetic pumps and dielectrophoretic manipulation of cells.

Boundary conditions become much more of an issue in microsystems, owing to high surface area–volume ratios. Boundary conditions that are taken for granted at the macroscale (e.g., the no-slip condition) can often fail in these systems. Further, microscale fluid mechanics is often closely related to chemical issues at surfaces. Multiphase implementations, designed to optimize certain aspects of transport, lead to additional interfacial concerns. Here, our boundary conditions must vary based on electric fields or chemistry.

Our ability to engineer and model microdevices is often limited by fabrication issues and instrumentation. Typical geometries resulting from microfabrication influence our discussion of transport issues in these systems – for example, most micro- and nanodevices are quasi-2D, and thus many of our analytical techniques will be used with quasi-2D structures in mind. The small scale requires specific instrumentation and techniques that facilitate inquiry into microscale flows. Our microfluidic devices are often implemented to study bioanalytes such as proteins or DNA, and bioparticles such as cells (Fig. 0.4) or virions. Often, we need to work in non-Newtonian systems, which requires a modification of the constitutive relation used in the Navier–Stokes equations.

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Excerpt

[More information](#)**4** Introduction

Outline of the material covered in this text. To a great extent, the material in this text is specified by the incompressibility condition for mass conservation, the Navier–Stokes equations for fluid flow and momentum conservation, the Nernst–Planck equation for species transport, and the Poisson equation for electrostatics, combined with boundary conditions for microchannel walls, inlets and outlets, particle/droplet/bubble interfaces, and electrodes. We combine these equations in various ways throughout, starting with low-Reynolds-number fluid mechanics described by incompressibility and Navier–Stokes, and then folding in the effects of electrodynamics first with equilibrium systems (defined by the Poisson equation and Boltzmann statistics) and later with nonequilibrium systems (defined by the Poisson equation and the Nernst–Planck equation). By their nature, the results of these analyses lend themselves naturally to the use of boundary-layer theory and matched asymptotic techniques (for the electrical double layer) and a coupling matrix formulation for electromechanical coupling (owing to the linearity of the Stokes equations). Throughout, additional results of condensed matter physics and chemistry are included as needed to describe unique aspects of these flows.

The text begins with low-Reynolds-number fluid mechanics, to ensure that the treatment stands on its own and to put these classical topics in a micro- or nanoscale context. For those cases in which the Reynolds number is low, boundary conditions are classical, solutes are small, and no electric fields are applied, classical undergraduate fluid-mechanical tools apply. Chapters 1 and 2 represent primarily classical material, with the notable exception being the discussion of Navier slip models in Chapter 1 – although this model is itself classical, experimental measurements of slip lengths have mostly been performed in the last twenty years. Chapter 3 on hydraulic circuits has focused relevance owing to the prevalence of long narrow channels in microdevices and the utility of circuit analysis in designing massively parallel microfluidic circuits. This chapter also leads into Chapter 4, which combines standard undergraduate mass transfer with the generally graduate level topic of the kinematics of mixing and chaos. It also highlights the particular importance of the low- Re , high- Pe limit found in many microfluidic devices, including both its detrimental effect on mixing and its benefits to laminar-flow-patterning devices.

The text then addresses the effect of electric fields on flow far from walls, with particular attention given to electroosmosis. Chapter 5 includes an elementary treatment of electrostatics and electrodynamics, which allows Chapter 6 to present an integral analysis of electroosmosis that highlights flow-current similitude outside the electrical double layer. Because purely electroosmotic flows with thin double layers are potential flows, Chapter 7 provides a discussion of potential flow. Because Chapters 3, 5, and 7 all use complex numbers, Appendix G provides a reference for key concepts. Chapter 8 presents Stokes flow relations, with specific attention to the motion of small particles. Although the flows in Chapter 8 are not primarily driven by electric fields, the material in this chapter builds on analytical techniques from Chapter 7 and is thus positioned immediately after it. Readers at this point are directed to Appendix F, which introduces the multipolar theory for the Laplace and Stokes equations, and prepares for later subjects, in particular multipolar models of dielectrophoretic forces. Electrokinetic pumps (Section 6.5) are discussed as an early application, as much of the work on electrokinetic pumps requires only the material in these introductory chapters.

The attention then turns to the boundary layer close to micro- and nanodevice interfaces. With background information on electrolyte solution properties from Appendix B, Chapter 9 introduces the details of the Gouy–Chapman electrical double layer, as well as modified Poisson–Boltzmann equations. Appendix H provides background on interaction potentials and facilitates expansion on these ideas. Chapter 10 summarizes experimental observations of the surface potential that is the boundary condition that

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[More information](#)**5** Introduction

drives the EDL models. With this description, the text proceeds to nonequilibrium description of species and charge distributions (Chapter 11) with applications to microchip separations, particularly protein separations (Chapter 12). These skills enable discussion of electrophoresis of small particles (Chapter 13), which is the first case in which the double-layer thickness plays a primary role and the fluid mechanics and the ion distribution in the double layer exhibit two-way coupling. Macromolecule transport follows, building on the descriptions of small ion and microparticle transport – we choose to discuss this by using DNA (Chapter 14). This segues into nanofluidics, in particular a discussion of electrokinetic effects with full two-way coupling (Chapter 15).

Finally, we explore solutions for which interfacial charge is no longer in equilibrium – here, the dynamics of charge caused by interfacial potential or interfacial discontinuities in current are critical. We discuss, in turn, the dynamics of electrical double layers at electrodes and polarizable materials (Chapter 16) and nonlinear electrokinetic manipulation of particles or droplets by using dielectrophoresis, magnetophoresis, and electrowetting (Chapter 17).

Supplementary reading. Throughout the text, supplementary reading is provided in each chapter to expand on the material of that chapter. By necessity, some topics have been omitted, and the reader is pointed here to excellent source material for a few of these topics. This text omits gas-phase microfluidic flows, for which Karniadakis [3] is a thorough source. We also omit microfabrication; general microfabrication details can be found in [4, 5], and treatments with a focus on microfluidics can be found in [6, 7]. This text is primarily focused on analytical techniques and avoids numerical simulation approaches. Some useful sources for numerical techniques include [8, 9, 10, 11, 12, 13, 14, 15]; Refs. [12, 13, 14] have stressed accessibility and are recommended for those seeking an introduction to numerical work.

1 Kinematics, Conservation Equations, and Boundary Conditions for Incompressible Flow

This text describes liquid flow in microsystems, primarily flow of water and aqueous solutions. To this end, this chapter describes basic relations suitable for describing the flow of water. For flows in microfluidic devices, liquids are well approximated as *incompressible*, i.e., having approximately uniform density, so this text describes incompressible flow exclusively.

This chapter describes the kinematics of flow fields, which describes the *motion* and *deformation* of fluids. As part of this process, key concepts are introduced, such as streamlines, pathlines, streaklines, the stream function, vorticity, circulation, and strain rate and rotation rate tensors. These concepts provide the language used throughout the text to communicate the modes of fluid motion and deformation. We discuss conservation of mass and momentum for incompressible flows of Newtonian fluids. Finally, we discuss boundary conditions for the governing equations, including solid and free interfaces with surface tension, and in particular we give attention to the no-slip condition and its applicability in micro- and nanoscale devices. This chapter assumes familiarity with vector calculus, which is reviewed in Appendix C. Importantly, Appendix C also covers the notation and coordinate systems used throughout.

We define a fluid as a material that deforms continuously when experiencing a nonuniform stress of any magnitude. We are primarily interested in a *continuum* description of the fluid flow, meaning that we are interested in the macroscopic manifestation of the motions of the individual molecules that make up the fluid, i.e., the velocity and the pressure of the fluid as a function of time and space. We also consider continuum field properties such as the temperature of the fluid or concentrations of chemical species in solution.

1.1 FLUID STATICS

In the case in which the fluid is assumed motionless, the equilibrium of fluid is determined by the interplay between the fluid pressure and the body forces:

$$\nabla p = \sum_i \vec{f}_i, \tag{1.1}$$

where p is the pressure [Pa] and \vec{f}_i is a body force per unit volume [N/m³]. Thus, in the presence of body forces, the fluid-static equations predict that pressure varies spatially. The most common fluid-static result relates to the pressure in a static column of liquid. For liquid in a gravitational field, $\vec{f}_i = -\rho g \hat{z}$, where $g = 9.8 \text{ m/s}^2$. Integrating this in the z direction, we obtain

$$p - p_0 = -\rho g z, \tag{1.2}$$

7 1.2 Kinematics of a Fluid Velocity Field

where p_0 is the pressure at $z = 0$. Similar relations can be determined for fluid in other potential fields, for example, charged fluids in an electric field.

1.2 KINEMATICS OF A FLUID VELOCITY FIELD

If we consider fluids *in motion*, we benefit from *kinematic relations*, which describe motion and deformation of a fluid. Because kinematics describes fluid motion but not the forces that generate that motion, kinematic relations are properties of the continuum velocity field alone. This velocity field gives the velocity at any point in space and time and is denoted by $\vec{u}(\vec{r}, t)$, where t is time and \vec{r} is a position vector specifying a location in space. Kinematics provides language that helps us understand velocity fields as well as the mathematical relationships that frame the physics of the system. Kinematic relations and definitions that classify types of flows often provide insight into which governing equation should be used.

1.2.1 Important geometric definitions

This subsection defines a number of curves that relate to the velocity field, namely *pathlines*, *streaklines*, *streamlines*, and *material lines*, each of which can facilitate our analysis. Streamlines are the most common tool used analytically to understand flows, because streamlines are analytically simple to generate and provide a clear image of the instantaneous velocity in a system. Pathlines and streaklines, in contrast, are straightforward to reproduce in the laboratory and are thus the most common experimental tools used for visualization. In particular, compelling simplifications for two-dimensional (2D) flows are achieved with the *stream function*, which is related to the streamlines in the system. Two-dimensional flows with plane symmetry are often relevant in microfluidic devices, because the devices created with lithography and etching often have a uniform depth. These lines describe the motion of a *fluid particle*, i.e., a point that moves in a fluid flow with a velocity equal to the local fluid velocity.

PATHLINES

Pathlines are the loci of points traced out by the motion through the flow of a fluid particle that was at location \vec{r}_0 at time t_0 (see Fig. 1.1). We can envision a pathline by imagining inserting a small fluorescent particle into a point in a fluid flow and then taking a long exposure of the particle as a function of time. Pathlines experimentally are a temporal record of the path of a point marker. The starting point and time of the fluid particle as well as the time history of the velocity field influence the resulting pathlines.

STREAKLINES

Streaklines are the loci of fluid particles that have passed through a point \vec{r}_0 . We can envision a streakline by imagining inserting a small tube into a point in a fluid flow, releasing fluorescent dye from this tube starting at t_0 , and then taking a snapshot of the dye at a later time. In this sense, streaklines experimentally are an instantaneous record of a curvilinear marker. As was the case with pathlines, the starting point and time of the dye release as well as the time history of the velocity field influence the resulting pathlines. Figure 1.2 contrasts pathlines and streaklines.

STREAMLINES

Streamlines are lines that are everywhere tangent to the instantaneous velocity. Unlike pathlines and streaklines, streamlines are properties of the *instantaneous* velocity field.

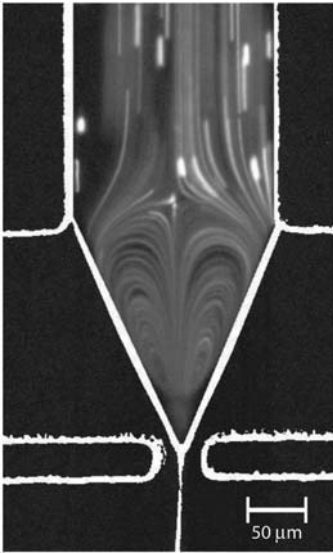


Fig. 1.1 Microparticle pathlines for a multiphase oil–water flow. Water inflow is from top, oil inflow from left and right. The resulting tipstreaming flow is used to generate micron-sized oil droplets. Fluorescent particles in the aqueous phase form pathlines on the camera, illustrating the recirculation induced by the fast oil flow on the slower water flow (Reproduced with permission from [16]).

For steady flow, all particles that pass through \vec{r}_0 follow the same trajectory. This trajectory is always tangent to the local velocity, and thus streamlines are identical to pathlines and streaklines for steady flows.¹

Importantly, for 2D flows, we can define a scalar function that defines these streamlines without integration. We define the stream function (which we denote as ψ for plane-symmetric flows and ψ_S for axially symmetric flows) such that its isocontours are always tangent to the velocity.² The stream function used depends on the nature of the symmetry in the flow, whereas the mathematical form of the velocity–stream function relationship is dependent on the coordinate system. In a plane 2D flow defined with Cartesian variables, we define the stream function by using

$$u = \frac{\partial \psi}{\partial y}, \tag{1.3}$$

$$v = -\frac{\partial \psi}{\partial x}. \tag{1.4}$$

The same plane 2D flow and stream function just described can be written in terms of cylindrical coordinates as follows:

$$u_z = \frac{1}{z} \frac{\partial \psi}{\partial \theta} \tag{1.5}$$

and

$$u_\theta = -\frac{\partial \psi}{\partial z}. \tag{1.6}$$

¹ For all of these curves, the integration terminates at stagnation points (points of zero velocity). For flows with stagnation points, generating complete streamlines sometimes requires that integration commence from multiple starting points.

² In fact, the preceding velocity–stream function relation satisfies two requirements: (1) that isocontours of the stream function are streamlines, and (2) that any velocity field specified by the stream function also satisfies the conservation of mass equation (1.21) discussed in Section 1.3. Using ψ or ψ_S to satisfy conservation of mass can greatly simplify fluid problems.

9 1.2 Kinematics of a Fluid Velocity Field

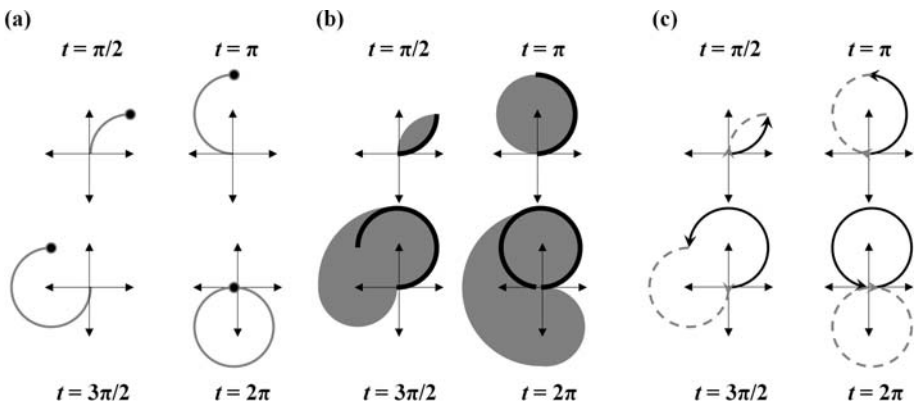


Fig. 1.2 Streaklines and pathlines. A particle released from the origin at time $t = 0$ is denoted in black, and a stream of dye released continuously from the origin starting at $t = 0$ is denoted in gray. The flow is the time-varying uniform flow $u = \cos t$, $v = \sin t$, which causes fluid particles to follow circular orbits. (a): location of the particle and dye stream at four instants (as would be visualized experimentally by a short-exposure image). The instantaneous location of the dye stream is the streakline associated with the origin and $t > 0$. (b): locus of particle and dye stream locations for $t > 0$ (as would be visualized experimentally by a long exposure starting at time $t = 0$). The time history of the particle traces out a pathline associated with the origin and $t = 0$. (c): pathlines (solid black lines) and streaklines (dashed gray lines) are shown by extracting the instantaneous dye contour from (a) and the particle time history from (b). Streamlines at any instant (not shown) are all straight lines aligned at an angle $\theta = t$ with respect to the x axis.

For axisymmetric flows, we define the *Stokes stream function* ψ_S , and the velocity–stream function relationships are written in cylindrical coordinates as

$$u_\theta = \frac{1}{r} \frac{\partial \psi_S}{\partial z}, \tag{1.7}$$

$$u_z = -\frac{1}{r} \frac{\partial \psi_S}{\partial \theta}, \tag{1.8}$$

whereas in spherical coordinates, these relationships are given by

$$u_r = \frac{1}{r^2 \sin \vartheta} \frac{\partial \psi_S}{\partial \vartheta}, \tag{1.9}$$

$$u_\vartheta = -\frac{1}{r \sin \vartheta} \frac{\partial \psi_S}{\partial r}. \tag{1.10}$$

The stream function for plane flows has units of square meters per second and is different from the Stokes stream function for systems with axial symmetry, which has units of cubic meters per second. The volumetric flow rate between two streamlines is related to the difference between the stream functions of the two streamlines. For plane-symmetric flow, the difference in stream function between two streamlines is equal to the volumetric flow per unit depth; for axisymmetric flow, the difference in the Stokes stream function between two streamlines is equal to the volumetric flow per radian.

MATERIAL LINES

Material lines trace the location of a curve in a flow field at specific instants in time. We can envision them by considering small fluorescent lines embedded in a fluid flow. Given a curve C_0 defined at a time t_0 , the material line C as a function of time is simply the curve through the fluid particles that C_0 originally comprised.

1.2.2 Strain rate and rotation rate tensors

For our purposes, a fluid is a material that responds to forces by deforming at a measurable rate, and a fluid’s unloaded state is defined by motionlessness but not by a specific configuration. This is in contrast to a solid, which responds to an applied force by acquiring a finite deformation from its unloaded state. For fluids the stresses (forces per unit area) in the material are related to the *rate of strain*. The rate of strain or *strain rate* of a fluid flow at a point is a measure of the velocity gradients at that point or, equivalently, the rate at which fluid elements are being deformed by a flow. The response of fluids is inherently *viscous*. For solids, the stresses (forces per unit area) in the material are related to the *strain*. The strain of a solid material is a measure of its static deformation from its unloaded state. In this sense, the response of solids is inherently *elastic*.

This subsection shows that the velocity gradients (expressed through the velocity gradient tensor) can be rewritten in terms of a *strain rate tensor* and a *rotation rate tensor*. Section 1.4 shows that the viscous forces or stresses in a Newtonian fluid (such as water or air) are linearly proportional to the strain rates as expressed by the strain rate tensor. The magnitude of the vorticity or, equivalently, the magnitude of the rotation rate tensor dictates what analytical tools we use to treat a specific flow problem.

STRAIN RATE FOR UNIDIRECTIONAL FLOWS

Consider a unidirectional flow $u = u(y)$ moving in the x direction. In this simple case, the scalar strain rate magnitude $\dot{\gamma}[\text{s}^{-1}]$ is given by

$$\dot{\gamma} = \frac{1}{2} \frac{\partial u}{\partial y} . \tag{1.11}$$

This unidirectional flow is simple, and this result is not general; however, it does illustrate two basic ideas – that the strain rate is a measure of how rapidly the fluid elements are deformed and that this property is related to the local velocity gradients. If the velocity is uniform, fluid elements are not distorted. If u varies spatially, then a fluid element is sheared, extended, or both.

GENERAL STRAIN RATE FOR THREE-DIMENSIONAL FLOWS

Equation (1.11) is simple and gives a scalar that measures the strain rate of a unidirectional flow; however, its result is not general. For a general three-dimensional (3D) flow, a scalar is not enough information to describe the deformation of fluid flow. The strain rate tensor $\bar{\epsilon} [\text{s}^{-1}]$ is a convenient way to record the detailed structure of the instantaneous fluid deformation. It also classifies two ways that a flow deforms: by extension and by shear.

In Cartesian coordinates, the strain rate tensor is defined as

strain rate tensor,
Cartesian
coordinates

$$\bar{\epsilon} = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{bmatrix} = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & \frac{1}{2} \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \\ \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & \frac{\partial v}{\partial y} & \frac{1}{2} \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \\ \frac{1}{2} \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) & \frac{1}{2} \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) & \frac{\partial w}{\partial z} \end{bmatrix} . \tag{1.12}$$