Chapter 1 Introduction

INTRODUCTION

This course is designed as a first level graduate course in transport phenomena. Undergraduate courses generally start with simple example problems and lead to more complex problems. With this approach, the student must learn the fundamental principles by induction. The approach used here is to teach the fundamental principles and then deduce the analysis for example problems. The example problems are classical problems that should be familiar to all Ph.D. Chemical Engineering graduates. These problems will be presented not only as an exercise with analytical or numerical solutions but also as simulated experiments which are to be interpreted and graphically displayed for presentation.

Prerequisites and text books

Students in this class are expected to have a background corresponding to a BS degree in Chemical Engineering. This includes a course in multivariable calculus, which covers the algebra and calculus of vectors fields on volumes, surfaces, and curves of 3-D space and time. Courses in ordinary and partial differential equations are a prerequisite. Some elementary understanding of fluid mechanics is expected from a course in transport phenomena, fluid mechanics, or physics. It is assumed that not all students have the prerequisite background. Thus, material such as vector algebra and calculus will be briefly reviewed and exercise problems assigned that will require more reading from the student if they are not already familiar with the material.

The two required textbooks for this course are R. Aris, *Vectors, Tensors, and the Basic Equations of Fluid Mechanics* and Bird, Stewart, and Lightfoot, *Transport Phenomena*. Several of the classical problems are from S. W. Churchill, *Viscous Flows, The Practical Use of Theory*. The classical textbook, Feyman, Leighton, and Sands, *The Feyman Lectures on Physics, Volume II* is highly recommended for its clarity of presentation of vector fields and physical phenomena. The students are expected to be competent in MATLAB, FORTRAN, and EXCEL and have access to *Numerical Recipes in FORTRAN*.

The following table is a suggested book list for independent studies in transport phenomena.

Table 1.1 Transport phenomena book list

Author	Title	Publisher	Year
L.D. Landau and E. M. Lifshitz	Fluid Mechanics, 2^{nd} Ed.	Butterworth	1987
V. G. Levich	Physicochemical Hydrodynamics	Prentice-Hall	1962
S. Chandrasekhar	Hydrodynamics and Hydromagnetic Stability	Dover	1961
H. Schlichting	Boundary Layer Theory	McGraw-Hill	1960
H. Lamb	Hydrodynamics	Dover	1932
S. Goldstein	Modern Developments in Fluid Dynamics	Dover	1965
W. E. Langlois	Slow Viscous Flow	Macmillan	1964
J. Happel, H. Brenner	Low Reynolds Number Hydrodynamics	Kluwer	1973
G. K. Batchelor	An Introduction to Fluid Mechanics	Cambridge	1967
S.-I. Pai	Viscous Flow Theory I Laminar Flow	Van Nostrand	1956
M. Van Dyke	Perturbation Methods in Fluid Mechanics	Academic Press	1964
S. W. Churchill	Inertial Flows	Etaner	1980
S. W. Churchill	Viscous Flows	Butterworths	1988
R. F. Probstein	Physicochemical Hydrodynamics	Butterworth-Heinemann	1989
S. Middleman	An Introduction to Fluid Dynamics	John Wiley	1998
S. Middleman	An Introduction to Mass and Heat Transfer	John Wiley	1998
E. L. Koschmeider	Benard Cells and Taylor Vortices	Cambridge	1993
W.-J. Yang	Handbook of Flow Visualization	Taylor & Francis	1989
W.-J. Yang	Computer-Assisted Flow Visualization	CRC Press	1994
A. J. Chorin	Computational Fluid Mechanics	Academic Press	1989
A. J. Chorin, J. E. Marsden	A Mathematical Introduction to Fluid Mechanics	Springer-Verlag	1993
L. C. Wrobel, C. A. Brebbia	Computational Modeling of Free and Moving Boundary Problems, Vol. 1 Fluid Flow	Computational Mechanics Publications	1991
M. J. Baines, K. W. Morton	Numerical Methods for Fluid Dynamics	Oxford	1993
W. E. Schiesser,	Computational Transport	Cambridge	1997

C. A. Silebi	Phenomena		
N. Ida, J. P. A. Bastos	Electro-Magnetics and Calculation of Fields	Springer	1997
L. G. Leal	Laminar Flow and Convective Transport Processes	Butterworth	1992
W. M. Deen	Analysis of Transport Phenomena	Oxford	1998
C. S. Jog	Foundations and Applications of Mechanics, Vol. I, Continuum Mechanics	CRC Press	2002
C. S. Jog	Foundations and Applications of Mechanics, Vol. II, Fluid Mechanics	CRC Press	2002

Scalar, vector and tensor fields

Scalars, vectors, and matrices are concepts that may have been introduced to the student in a course in linear algebra. Here, scalar, vector, and tensor fields are entities that are defined over some region of 3-D space and time. It is implicit that they are a function of the spatial coordinates and time, i.e., $\varphi=\varphi(x,y,z,t)=\varphi(\mathbf{x},t)$. The spatial coordinates are expressed as Cartesian coordinates in this class. However, vectors and tensors are physical entities that are independent of the choice of spatial coordinates even though their components depend on the choice of coordinates.

Scalar fields have a single number, a scalar, at each point in space. An example is the temperature of a body. The temperature field is usually expressed visually by a contour map showing curves of constant temperature or isotherms. An alternative visual display of a scalar field is a color map with the value of the scalar scaled to a gray scale, hue, or saturation. The values of the scalar field are continuous with the exception of definable surfaces of discontinuity. An example is the density of two fluids separated by an interface. Media that are chaotic and discontinuous on a microscopic scale may be described by an average value in a *representative elementary volume* that is large compared to the microscopic heterogeneity but small compared to macroscopic variations. An example is the porosity of a porous solid.

Vector fields have a magnitude and direction associated with each point in space. An example is the velocity field of a fluid in motion. Vector fields in two dimensions can be visually expressed as field lines that are everywhere tangent to the vector field and whose separation quantifies the magnitude of the field. Streamlines are the field lines of the velocity field. Alternatively, a vector field in two dimensions can be visually expressed by arrows whose directions are parallel to the vector and having a width and/or length that scales to the magnitude of the vector. These graphical representations of vector fields are not useful in three dimensions. In general, a vector field in 3-D can be expressed in terms of its components projected on to the axis of a coordinate system. Thus, a vector field may have different components when projected on to different coordinate systems. Since a vector is a physical entity, the components in different frames of reference transform by prescribed rules. The position of a point in space relative to an origin is a vector defined by the distance and direction. Special vectors having a magnitude of unity are called unit vectors and are used to define a direction such as coordinate directions or the normal direction to a surface. We will denote vectors with bold face letters, e.g., **v, x,** or **n**.

Tensors are physical entities associated with two directions. For example, the stress tensor represents the force per unit area, each of which are directional quantities. Transport coefficients, such as the thermal conductivity, are tensors, which transform a potential gradient to a flux, each of which are vectors. The components of a tensor in a particular coordinate system are represented by a 3×3 matrix. Since the tensor is a physical entity that is independent of the coordinate system, the components must satisfy certain transformation rules between coordinate systems. In particular, a set of three directions called the principal directions can be found to transform the components of the tensor to a diagonal matrix. This corresponds to finding the eigenvectors of a matrix and the components correspond to the eigenvalues. Bold face letters will also denote tensors. The stress tensor will be denoted by **T** or τ, depending on whether discussing Aris or BSL, respectively.

Curves, surfaces, and volumes

We will be dealing with regions of space, *V*, having volume that may be bound by surfaces, *S,* having area. Regions of the surface may be bound by a closed curve, *C*, having length.

Surfaces are defined by one relationship between the spatial coordinates.

$$x^3=f(x^1,x^2),\ \text{or}\ F(x^1,x^2,x^3)=0,\ \text{or}\ F(\mathbf{x})=0$$

Alternatively, a pair of surface coordinates, u^1, u^2 can define a surface.

$$x^i=x^i(u^1,u^2),\ i=1,2,3\ \text{or}\ \mathbf{x}=\mathbf{x}(u^1,u^2)$$

Each point on the surface that has continuous first derivatives has associated with it the normal vector, **n**, a unit vector that is perpendicular or normal to the surface and is outwardly directed if it is a closed surface. Fluid-fluid interfaces need to also be characterized by the mean curvature, H, at each point on the surface to describe the normal component of the momentum balance across the interface. The flux of a vector, **f**, across a differential element of the surface is denoted as follows, i.e. the normal component of the flux vector multiplied by the differential area.

$$\mathbf{f}\bullet\mathbf{n}\ da$$

Curves are defined by two relationships between the spatial coordinates or by the intersection of two surfaces.

$$f_1(x^1,x^2,x^3)=0\ \text{and}\ f_2(x^1,x^2,x^3)=0,\ \text{or}\ f_1(\mathbf{x})=0\ \text{and}\ f_2(\mathbf{x})=0$$

Alternatively, a curve in space can be parameterized by a single parameter, such as the distance along the curve, *s* or time, *t*.

$$\mathbf{x}=\mathbf{x}(s)$$

The tangent vector is a unit vector that is tangent to each point on the curve.

$$\tau=d\mathbf{x}(s)/ds$$

The component of a vector, **f**, tangent to a differential element of a curve is denoted as follows.

$$\mathbf{f}\bullet\tau\ ds$$

If the parameter along the curve is time, the differential of position with respect to time is the velocity vector and the differential of velocity is acceleration.

$$\mathbf{v}=\frac{d\mathbf{x}}{dt}$$

$$\mathbf{a}=\frac{d\mathbf{v}}{dt}$$

Coordinate systems

Scalars, vectors, and tensors are physical entities that are independent of the choice of coordinate systems. However, the components of vectors and tensors depend on the choice of coordinate systems. The algebra and calculus of vectors and tensors will be illustrated here with Cartesian coordinate systems but these operations are valid with any coordinate system. The student is suggested to read Aris to learn about curvilinear coordinate systems. Bird, Stewart, and Lightfoot express the components of the relevant vector and tensor equations in Cartesian, cylindrical polar, and spherical polar coordinate systems.

Cartesian coordinates have coordinate axes that have the same direction in the entire space and the coordinate values have the units of length. Curvilinear coordinates, in general, may have coordinate axis that are in different directions at different locations in space and have coordinate values that may not have the units of length, e.g., θ in the cylindrical polar system. If (y^1,y^2,y^3) are Cartesian coordinates and (x^1,x^2,x^3) are curvilinear coordinates, a differential length is related to the differential of the coordinates by the following relations.

$$ds^2 = \sum_{k=1}^{3} dy^k \quad dy^k$$

$$dy^k = \frac{\partial y^k}{\partial x^i} \quad dx^i \equiv \frac{\partial y^k}{\partial x^1} \quad dx^1 + \frac{\partial y^k}{\partial x^2} \quad dx^2 + \frac{\partial y^k}{\partial x^3} \quad dx^3$$

$$ds^2 = \sum_{k=1}^{3} \left(\frac{\partial y^k}{\partial x^i} \quad dx^i \right) \left(\frac{\partial y^k}{\partial x^j} \quad dx^j \right)$$

$$= g_{ij} \quad dx_i \quad dx_j$$

$$g_{ij} = \sum_{k=1}^{3} \left(\frac{\partial y^k}{\partial x^i} \right) \left(\frac{\partial y^k}{\partial x^j} \right)$$

where g_{ij} are components of the metric tensor which transforms differential of the coordinates to differential of length. Summation is understood for repeated indices. Calculus in a curvilinear coordinate system will require the metric tensor.

A differential element of volume in curvilinear coordinate system is related to differentials of the coordinates by the square root of the determinate of the metric tensor or the Jacobian, *J*.

$$\begin{aligned} dV &= dy^1 \, dy^2 \, dy^3 \\ &= \varepsilon_{ijk} \frac{\partial y^i}{\partial x^1} \frac{\partial y^j}{\partial x^2} \frac{\partial y^k}{\partial x^3} dx^1 \, dx^2 \, dx^3 \\ &= g^{1/2} \, dx^1 \, dx^2 \, dx^3 \\ &= J \, dx^1 \, dx^2 \, dx^3 \end{aligned}$$

Henceforth, Cartesian coordinates with subscript notation will be used.

Units

Dimensional quantities will be used in equations without explicit specification of units because it is understood that they will have the SI system of units. The SI units and mks units are similar with some exceptions as in electricity and magnetism. The following table lists the SI units of the quantities used in this course and the conversion factor needed to convert the quantity from some customary units to SI units. Multiply the quantity in customary units by the conversion factor to obtain the quantity in SI units. The following is taken from, *The SI Metric System of Units and SPE METRIC STANDARD*, Society of Petroleum Engineers.

Table 1.2 SI units and conversion factors			
Quantity	SI unit	Customary unit	Conversion factor
Length	m	ft	3.048 E-01
Mass	kg	lbm	4.535 924 E-01
Time	s	s	1.0

Temperature	°K	°R	5/9
Pressure, stress	Pa	psi	6.894 757 E+03
Density	kg/m^3	g/cm^3	1.0 E+03
Force	N	lbf	4.448 222 E+00
Flow rate	m^3/s	U.S. gal/min	6.309 020 E-05
Diffusivity	m^2/s	cm^2/s	1.0 E-04
Thermal conductivity	W/(m·K)	Btu/(hr-ft^2-°F/ft)	1.730 735 E+00
Heat transfer coefficient	W/(m^2·K)	Btu/(hr-ft^2-°F)	5.678 263 E-06
Permeability	m^2	darcy	9.869 233 E-13
Surface tension	N/m	dyne/cm	1.0 E-03
Viscosity (dynamic)	Pa·s	cp	1.0 E-03

Continuum approximation

The calculus of scalar, vector, and tensor fields require that these quantities be piecewise continuous down to infinitesimal dimensions. However, quantities such as density, pressure, and velocity become ambiguous or stochastic at the scale of molecular dimensions. Thus the fields discussed here are the average value of the quantity over a *representative elementary volume, REV,* of space that is large compared to molecular dimensions but small compared to the macroscopic variation of the quantities. The size of the REV depends on the scale that a problem is being investigated. For example, suppose one is investigating a fixed bed catalyst reactor. As a first order approximation for design purposes, the reactor may be modeled as a one-dimensional system with the cross-section of the reactor approximated as the REV. However, is one is investigating instabilities and channeling, the bed may be modeled in 2-D with the REV being a volume that is small compared to the macroscopic dimensions of the reactor but large compared to the size of the catalyst particles. If one is optimizing the transport-limited kinetics of the reactor, then the REV may be small compared to the size of the catalyst particle. If one is optimizing the balance between transport-limited and surface reaction rate limited kinetics, the REV may be small enough to describe the surface morphology of the catalyst particle. However, the molecular dynamics of the surface reaction is beyond the realm of transport phenomena.

Densities, potential gradients, and fluxes

Velocity: and flux by convection. Transport or flux of the various quantities discussed in this course will be due to convection (or advection) or due to the gradient of a potential. Common to all of these transport process is the convective transport resulting from the net or average motion of the molecules or the velocity field, **v**. The convective flux of a quantity is equal to the product of the density of that quantity and the velocity. In this sense, the velocity vector can be interpreted as a "volumetric flux" as it has the units of the flow of volume across a unit area of surface per unit of time. Because the flux by convection is common to all forms of transport, the integral and differential calculus that follow the convective motion of the fluid will be defined. These will be known as the Reynolds' transport theorem and the convective or material derivative.

Mass density and mass flux. If ρ is the mass density, the mass flux is $\rho\,\mathbf{v}$.

Species concentration. Suppose the concentration of species A in a mixture is denoted by C_A. The convective flux of species A is $C_A\,\mathbf{v}$. Fick's law of diffusion gives the diffusive flux of A.

$$\mathbf{J}_A = -\mathbf{D}_A \bullet \nabla C_A$$

The diffusivity, $\mathbf{D}_A$, is in general a tensor but in an isotropic medium, it is usually expressed as a scalar.

Internal energy (heat). The density of internal energy is the product of density and specific internal energy, ρE. The convective flux is $\rho E\,\mathbf{v}$. For an incompressible fluid, the convective flux becomes $\rho C_p (T-T_o)\,\mathbf{v}$. The conductive heat flux, **q**, is given by Fourier's law for conduction of heat,

$$\mathbf{q} = -\mathbf{k} \bullet \nabla T$$

where **k** is the thermal conductivity tensor (note: same symbol as for permeability).

Porous media. The density of a single fluid phase per unit bulk volume of porous media is $\phi\,\rho$, where ϕ is the porosity. Darcy's law gives the volumetric flux, superficial velocity, or Darcy's velocity as a function of a potential gradient.

$$\begin{aligned}\mathbf{u} &= -\frac{\mathbf{k}}{\mu} \bullet \left(\nabla p - \rho\,\mathbf{g}\right) \\ &= \phi\,\mathbf{v}\end{aligned}$$

where **k** is the permeability tensor and **v** is the interstitial velocity or the average velocity of the fluid in the pore space. Darcy's law is the momentum balance for a fluid in porous media at low Reynolds number.

Momentum balance. Newton's law of motion for an element of fluid is described by Cauchy's equation of motion.

$$\rho\mathbf{a} = \rho\frac{d\mathbf{v}}{dt}$$
$$= \rho\mathbf{f} + \nabla \bullet \mathbf{T}$$

where **f** is the sum of body forces and **T** is the stress tensor. The stress tensor can be interpreted as the flux of force acting on the bounding surface of an element of fluid.

$$\iiint\limits_{V(t)} (\rho\mathbf{a} - \rho\mathbf{f})\,dV = \iiint\limits_{V(t)} \nabla \bullet \mathbf{T}\,dV$$
$$= \iint\limits_{S(t)} \mathbf{T} \bullet \mathbf{n}\,dS$$

The stress tensor for a Newtonian fluid is as follows.

$$\mathbf{T} = (-p + \lambda\Theta)\mathbf{I} + 2\mu\mathbf{e}$$
$$\mathbf{e} = \frac{1}{2}\left(\nabla\mathbf{v} + \nabla\mathbf{v}^t\right)$$

where *p* is the thermodynamic pressure, Θ is the divergence of velocity, μ is the coefficient of shear viscosity, (λ+2/3μ) coefficient of bulk viscosity, and **e** is the rate of deformation tensor. Thus the anisotropic part (not identical in all directions) of the stress tensor is proportional to the symmetric part of the velocity gradient tensor and the constant of proportionality is the shear viscosity.

Electricity and Magnetism. We will not be solving problems in electricity and magnetism but the fundamental equations are presented here to illustrate the similarity between the field theory of transport phenomena and the classical field theory of electricity and magnetism. The Maxwell's equations and the constitutive equations are as follows.

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial\mathbf{D}}{\partial t}$$
$$\nabla \bullet \mathbf{B} = 0$$
$$\nabla \times \mathbf{E} = -\frac{\partial\mathbf{B}}{\partial t}$$
$$\nabla \bullet \mathbf{D} = \rho$$

Constitutive equations:

$$\mathbf{B} = \boldsymbol{\mu}\mathbf{H}$$
$$\mathbf{D} = \boldsymbol{\varepsilon}\mathbf{E}$$
$$\mathbf{J} = \boldsymbol{\sigma}\mathbf{E}$$

where

E electric field intensity
D electric flux density or electric induction
H magnetic field intensity
B magnetic flux density or magnetic induction
J electric current density
ρ charge density
μ magnetic permeability (tensor if anisotropic)
ε electric permittivity (tensor if anisotropic)
σ electric conductivity (tensor if anisotropic)

When the fields are quasi-static, the coupling between the electric and magnetic fields simplify and the fields can be represented by potentials.

$$\mathbf{E} = -\nabla V$$
$$\mathbf{B} = \nabla \times \mathbf{A}$$

where *V* is the electric potential and **A** is the vector potential. The electric potential is analogous to the flow potential for invicid, irrotational flow and the vector potential is analogous to the stream function in two-dimensional, incompressible flow.

Reading assignment

Read Chapter 1 and Appendix A and B of Aris.