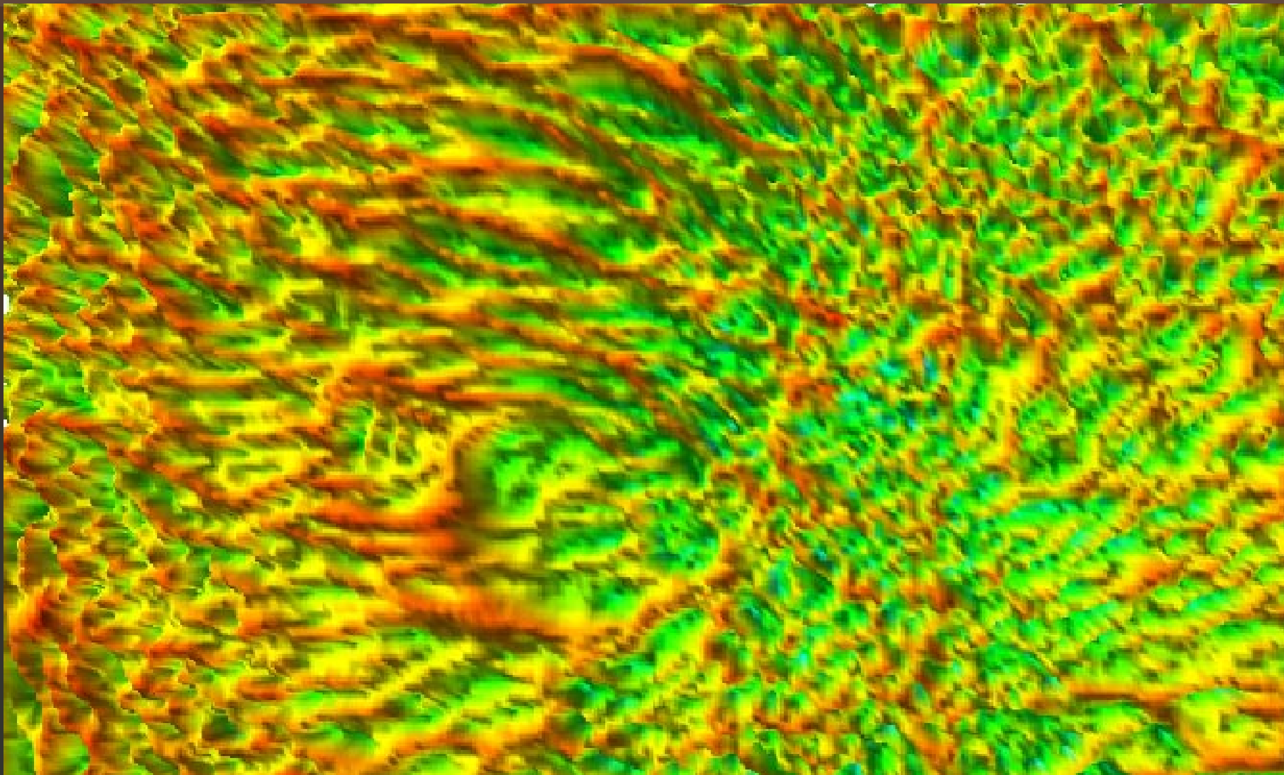
Analysis and Modelling of

Physical Transport Phenomena

K. Hanjalić S. Kenjereš
M.J. Tummers H.J.J. Jonker



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The cover pictures represent the instantaneous temperature fields in the proximity of hot and cold walls (inside thermal boundary layers) in Rayleigh-Bénard convection of air at Ra = 10^9, large-eddy simulation. S. Kenjereš, 2006.

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VSSD

First edition 2007, corrected 2009

Published by VSSD
Leeghwaterstraat 42, 2628 CA Delft, The Netherlands
tel. +31 15 27 82124, telefax +31 15 27 87585, e-mail: hlf@vssd.nl
internet: http://www.vssd.nl/hlf
URL about this book: http://www.vssd.nl/hlf/c001.htm

Printed version
ISBN-13 978-90-6562-165-8
Electronic version
ISBN-13 978-90-6562-166-5

NUR 924

Key words: physical transport phenomena

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Preface

These lecture notes contain the course material Advanced Physical Transport Phenomena, offered in the Master's programme in Applied Physics at Delft University of Technology. The notes follow in part the concept and content of the book *Fysische Transportverschijnselen II* (in Dutch) by Hoogendoorn and Van der Meer (Delft University Press, 1991). However, a significant amount of new material on turbulent flows, convective processes and numerical methods has now been included. The course aims at providing graduate students with an overview of analytical, numerical and modelling methods for solving problems of heat and fluid flow, following a unified and comparative approach.

The course is divided into four parts. The first part gives the conservation laws for mass, momentum and energy in general differential forms, accompanied with the relevant constitutive relations, physical and mathematical classification of equations, and their boundary conditions. This concise introduction is just a generalisation of the macroscopic conservation laws considered in basic courses on Physical Transport Phenomena at the bachelor's level.

Part II covers a number of classical analytical methods for solving some generic problems in heat, mass and momentum transfer. In addition to providing insight into the basic physics of transport phenomena, this part is meant to encourage students to master the analytical tools and to use analytical approaches for gaining a physical intuition by solving elementary problems in idealized situations. It also illustrates the limitations and constraints of analytical methods in solving complex problems in transport phenomena.

Part III introduces numerical methods for computer-aided solutions of complex problems that are not tractable by analytical approaches. It is, in fact, an introduction to computational fluid dynamics (CFD) and computational heat and mass transfer (CHMT), which have recently emerged as major tools for solving heat and fluid flow problems in engineering and environmental applications. With that in mind, the focus is on the finite-volume discretization of the conservation laws, which is the main approach in industrial CFD and CHMT. In addition to introducing basic concepts of equation discretization and their numerical solution, this chapter aims at illustrating the potential but also the limitations and inherent snares of computational methods. Rather than providing a full coverage of various schemes and solution methods, the chapter aims at developing a critical attitude among students and an ability to recognize potential errors and numerical contaminations.

Part IV deals with turbulent convection, considered to be the most widespread mode of transport in real life problems, but also the most challenging both for analytical and computational treatment. Basic notions on turbulence relevant to its modelling are first introduced, followed by statistical averaging of the conservation equations and their interpretation. Major features of turbulence are briefly outlined, followed by definition of the characteristic scales. A series of generic turbulent flows is then introduced, with focus on flows partially or fully bounded by solid walls. This should provide students with basic physical insight based solely on similarity and scaling arguments. Limitations of numerical simulation are also discussed, together with the need for mathematical modelling of turbulence and the associated turbulent transport of momentum, heat and mass. The last section in this part covers the basics of turbulence modelling, its scope and limitations. The practice and the rationale of turbulence modelling are illustrated by detailed derivation of the $k-\varepsilon$ model and its closure. This is accompanied by physical interpretations, which provide an insight into modelling arguments, levels of approximation and model limitations. The section is closed with a brief overview of other two-equation eddy-viscosity/diffusivity models and a brief introduction into non-linear eddy-viscosity models and second-moment closures.

The lecture notes contain a number of worked-out examples, especially in Part II (analytical methods).

Authors, December 2008, Delft, The Netherlands

Part I

Fundamental Equations

Chapter 1

Fundamental Equations of Transport Phenomena - Field description

1.1 Introduction

Physical Transport Phenomena is the common name for processes involving transfer of mass, heat and momentum. While each of these phenomena has evolved into a separate scientific (and engineering) discipline on its own, taught as separate courses and covered in numerous textbooks and monographs, they also have much in common. The fundamental principles and physical laws governing these phenomena and their mathematical description can often be treated in a unified and comparative manner. Such an approach has been adopted in this course, and is especially suited for students in general applied sciences.

The principal aim of a course in Transport Phenomena is to understand the underlying physics and to master methods that can be used to predict the effects of heat, mass and momentum transport in various situations. The prediction tasks essentially focus on evaluating heat, mass and momentum fluxes and their integrals - total heat and mass transfer and forces on target surfaces, and are usually related to solid walls bounding the system under consideration. But in order to solve the problems, we need to consider field variables such as temperature, species concentration, fluid velocity. These are governed by the conservation laws and complementary constitutive relations, from which the fundamental equations are derived. The basic conservation laws in integral form (for macroscopic systems) are considered in the undergraduate courses in Thermodynamics, Fluid Mechanics and Transport Phenomena and here we give a brief overview of the general formulation and then move on to differential forms that describe the motion of a continuum matter and associated transport of heat and mass.

1.2 Conservation laws for a control volume in differential form

We first introduce the notion of a conserved (or conservable) variable, as a quantity whose identity in the original or transformed form can be followed and described by the basic physical conservation laws:

- conservation of mass
- conservation of momentum (linear, angular) which is the main focus of Solid and Fluid Mechanics;
- conservation of energy - mechanical (kinetic, potential), thermal or total, which is in essence the First law of Thermodynamics

Other conservation laws can also be formulated, e.g. conservation of entropy (Second Law of Thermodynamics). It is noted here that the notions 'conserved' or 'conservable' quantity, is, strictly speaking, true only if the source term in the conservation equations is zero. In that case the 'conserved variable' remains indeed conserved in a closed system, just transported by fluid motion and molecular effects from one place to another within the system.

It is recalled that all conservation laws have been postulated for a certain mass (definable quantity of matter under study). Such a mass system is often referred to as a *closed system* (control mass, mass system), defined by a finite number of state properties. Conservation laws for a control mass can be formulated in a general ('generic') mathematical form defining a finite change or a time rate of the variable Φ_s associated with the mass system:

$$(\Delta\Phi)_s = \Upsilon_s \quad \text{or, in time} \quad \left(\frac{\Delta\Phi}{\Delta t}\right)_s = \frac{\Upsilon_s}{\Delta t}; \quad \text{with} \quad \lim_{\Delta t \to 0}\left(\frac{\Delta\Phi}{\Delta t}\right)_s = \left(\frac{d\Phi}{dt}\right)_s = \dot{\Upsilon}_s \quad (1.1)$$

where Φ_s is a conservable quantity in the system (an extensive property, which depends on the size of the system, i.e on the amount of matter considered), such as mass m, momentum $\vec{M}$, energy E, and Υ is the source/sink of Φ. A dot over the symbols denotes the time rate. Everything outside and beyond this system represents its environment. The control mass can be finite, in which case we talk about the integral form of the conservation law, or infinitesimally small (infinitesimal continuum element) when the conservation laws are postulated in a differential mathematical form.

Note that an extensive property can be expressed as a product of mass and the corresponding intensive property, $\Phi = m\phi$, or, if ϕ varies within the system (as it is usually the case):

$$\Phi = \int_s \phi dm = \int_s \phi \rho dV \quad (1.2)$$

where ϕ is an intensive property of a system (independent of its size or its extent).

Table 1.1 summarises the variables for the three basic conservation laws,

	Φ	ϕ	Υ	$\dot{\Upsilon}$
mass	m	1	0 (or r)	0 (or $\dot{r}$)
momentum	$\vec{M} = m\vec{v}$	$\vec{v}$	$\Sigma\vec{F}\Delta t$	$\Sigma\vec{F}$
energy	$E = me$	e	$Q - W$	$\dot{Q} - \dot{W}$

Table 1.1 Basic conservation laws.

where

- r denotes the reaction source or sink ($\dot{r}$ is the reaction rate in time) for mass m in case we consider mass conservation of a reacting substance (note that $r = 0$ for an inert substance or for the total mass),

- $\vec{v}$ denotes the fluid velocity vector and $\Sigma\vec{F}$ is the sum of all forces acting on the mass system
- Q and W denote the amount of energy exchanged with the environment in form of heat and work respectively, whereas $\dot{Q}$ and $\dot{W}$ denote the time rates of Q and W.

It is also recalled that the above formulation of the conservation laws is applicable only to a *closed* mechanical or thermodynamical system within whose boundaries, fixed or variable in time, there exists always the same mass. Studies of such systems focus essentially on the interaction of the mass (and associated momentum, energy, entropy) in the system with its environment.

Most problems of interest in transport phenomena are associated with *open systems*, identifiable with engineering or environmental systems, equipment, device, machine, or a part of them, through which a fluid flows. In such cases it is convenient to apply the conservation laws to a *control volume* bounded by the *control surface* that coincides with the boundary surface of the system (equipment, device, or part of it), which we want to study. A control volume can be fixed in the adopted coordinate frame, can move with its own velocity, expand or contract (with a local velocity of the control surface). By definition, an *open system* should have some parts of the control surface open, through which the matter (fluid) flows in and out of the control volume and caries fluid properties. Just as the control mass, the control volume can be of a finite size (macroscopic or integral systems) or be infinitesimally small, Figure 1.1. In fact, ”a point” in space at which a property is defined (e.g. fluid velocity, temperature, pressure, density) is an infinitesimally small control volume. In a continuous matter (*continuum*) the size of the infinitesimal control volume must be sufficiently small so that it can be regarded as ”a point” both in the mathematical sense (associated with the variable in differential conservation equations) and in a practical physical realm (corresponding to the size of an instrument sensor by which that property is measured). It must, however, be also sufficiently large to contain sufficient number of molecules to allow the unique definitions of fluid properties, e.g density, pressure, at a point.

The *control mass* approach, suited for describing and analysing movement of discrete mass systems (e.g. material particles, or bodies) is also called the Lagrangean description, whereas the *control volume* approach, suited for describing flow of a continuum, especially in differential form (for an infinitesimal control volume) is called the Eulerian description.

The application of the generic conservation laws (1.1) to an open system requires its transformation to account for the inflow and outflow of the considered quantity Φ into and out of the control volume by inflowing and outflowing fluid through the open parts of the system control surface. Such a transformation, or direct derivation of the conservation laws for a finite-size (macroscopic) control volume can be found in basic textbooks in Thermodynamics, Fluid Mechanics and Transport Phenomena, and here it will suffice to list the generic form of the conservation law for a control volume with identifiable inlets denoted by ”*i*” and exits denoted by ”*e*” for an extensive thermodynamic and dynamic

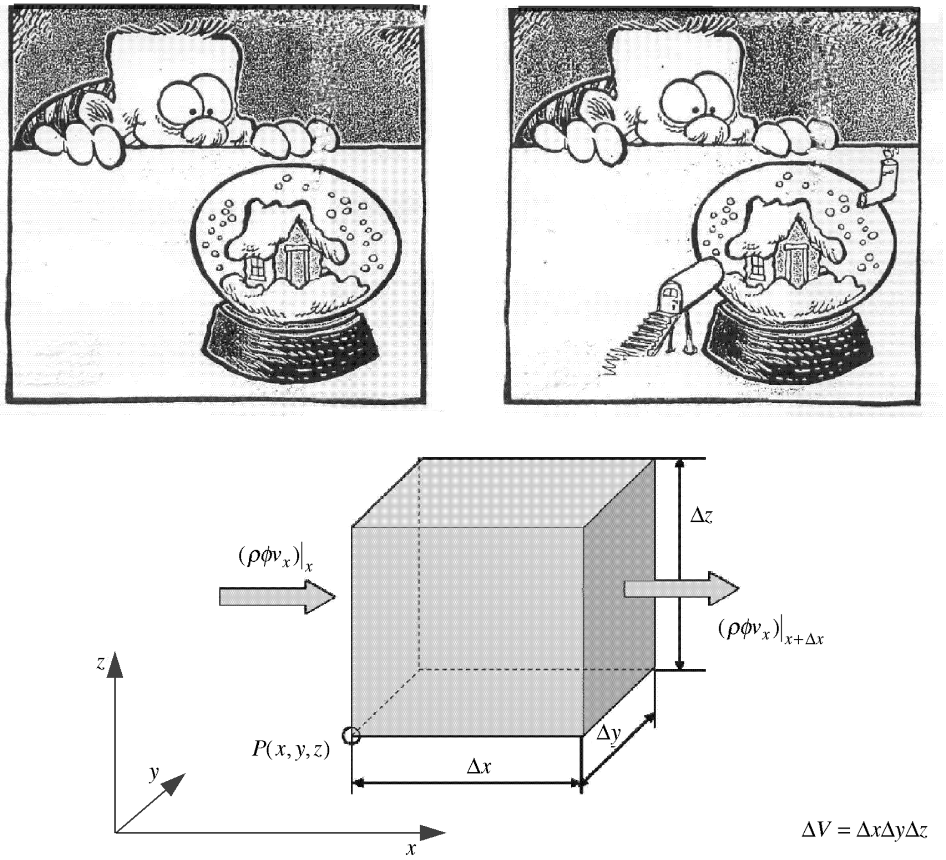


Figure 1.1 Above: macroscopic control mass (closed system) and control volume (open system); below: differential control volume

property Φ:

$$\frac{d\Phi_{CV}}{dt} = \sum_i \dot{\Phi}_i - \sum_e \dot{\Phi}_e + \dot{\Upsilon} \tag{1.3}$$

Since we are interested here in the differential form of the conservation laws, we recall first that

$$\Phi = \int_m \phi \mathrm{d}m = \int_V \rho\phi \mathrm{d}V \qquad \dot{\Phi} = \int_A \phi \mathrm{d}\dot{m} = \int_A \rho\phi \mathrm{d}\dot{V} = \int_A \rho\phi(\vec{v}\cdot \mathrm{d}\vec{A})$$

$$\Upsilon = \int_m \gamma \mathrm{d}m = \int_V \rho\gamma \mathrm{d}V \qquad \dot{\Upsilon} = \int_m \dot{\gamma} \mathrm{d}m = \int_V \rho\dot{\gamma} \mathrm{d}V$$

$$\text{where} \quad \mathrm{d}\dot{m} = \rho\,(\vec{v}\cdot\mathrm{d}\vec{A}) \qquad \text{and} \qquad \mathrm{d}\dot{V} = (\vec{v}\cdot\mathrm{d}\vec{A})$$

are the mass and volume flow rates respectively through the elementary surface $\mathrm{d}\vec{A}$.

A control volume can always be identified with a mass system at a particular time instant, hence the definition of an extensive property Φ as an integral of its intensive property ϕ over a mass or volume can be regarded as identical at that time instant, but their *changes in time*, i.e. *the time rates* are *different*,

$$\left(\frac{d\Phi}{dt}\right)_{mass\ system} \neq \left(\frac{d\Phi}{dt}\right)_{control\ volume}$$

The extensive properties in each term of the generic formulation (1.3) can now be replaced by volume/surface integrals in terms of intensive properties. So, the time rate of change term becomes

$$\frac{d\Phi_{CV}}{dt} = \frac{d}{dt}\int_{CV} \rho\phi \mathrm{d}V = \int_{CV} \frac{\partial(\rho\phi \mathrm{d}V)}{\partial t} \tag{1.4}$$

Note that the ordinary time derivative d/dt is replaced by the partial derivative $\partial/\partial t$ after commutation of the sequence with the integral because it is now applied to field properties ρ and ϕ, which depend also on space variables.

The inflow and outflow are expressed as

$$\sum_i \dot{\Phi}_i = \int_{A_i} \rho\phi(\vec{v}\cdot \mathrm{d}\vec{A}) \ \text{ and } \ \sum_e \dot{\Phi}_e = \int_{A_e} \rho\phi(\vec{v}\cdot \mathrm{d}\vec{A}) \tag{1.5}$$

or,

$$\sum_i \dot{\Phi}_i - \sum_e \dot{\Phi}_e = -\int_{A_{CV}} \rho\phi(\vec{v}\cdot d\vec{A}) = -\int_{CV} \nabla\cdot(\rho\phi\vec{v})\mathrm{d}V \tag{1.6}$$

where the integral over the control surface was converted into an integral over the control volume using the Green-Gauss theorem. Note that the sign of the surface integral is determined by the scalar product of the velocity vector and the outward-pointing unit normal vector of the surface element, yielding $(\vec{v}\cdot \mathrm{d}\vec{A})_i < 0$ and $(\vec{v}\cdot \mathrm{d}\vec{A})_e > 0$.

Equation (1.4) now becomes:

$$\int_{CV} \frac{\partial(\rho\phi\, \mathrm{d}V)}{\partial t} = -\int_{CV} \nabla\cdot(\rho\phi\vec{v})\mathrm{d}V + \int_{CV} \rho\,\dot{\gamma}\mathrm{d}V \tag{1.7}$$

For an infinitesimally small control volume (a point in space) $\mathrm{d}V = \mathrm{d}x\mathrm{d}y\mathrm{d}z$ we can omit the $\int_{CV}$ sign and divide the equation by $\mathrm{d}V$, yielding the generic *differential* form of the conservation laws[1]:

$$\frac{\partial(\rho\phi)}{\partial t} = -\nabla\cdot(\rho\phi\vec{v}) + \rho\,\dot{\gamma} \tag{1.8}$$

For convenience we will present all equations both in vector and in index notation (the latter applicable only to Cartesian coordinate systems), i.e. for velocity we shall use

---

[1] The generic differential form of the conservation laws can be derived directly from the Reynolds Transport Theorem for conservation of a continuum field variable ϕ (any continuous summable function in space and time, see advanced textbooks).

$\vec{v}(v_x, v_y, v_z)$ and $v_i(v_1, v_2, v_3)^2$:

$$\frac{\partial(\rho\phi)}{\partial t} = -\nabla\cdot(\rho\phi\vec{v}) + \rho\dot{\gamma}$$

$$\frac{\partial(\rho\phi)}{\partial t} = -\frac{\partial}{\partial x_j}(\rho\phi v_j) + \rho\dot{\gamma} \tag{1.9}$$

It is noted that equation (1.9) is given in the so-called *strong conservative form* of the differential conservation law (recognizable by the density being lumped together with the variable ϕ under all differentiation operators) implying the conservation of ϕ per unit volume. Other forms are also in use, which could be more suitable for solving problems with constant or mildly varying fluid density. For example, applying equation (1.9) to mass conservation, i.e. $\phi = \Phi/m = 1$ and $\dot{\gamma} = 0$, leads to the *continuity equation in differential form*:

$$\frac{\partial\rho}{\partial t} = -\nabla\cdot(\rho\vec{v})$$

$$\frac{\partial\rho}{\partial t} = -\frac{\partial}{\partial x_j}(\rho v_j) \tag{1.10}$$

Using the continuity equation, the differential conservation law can be transformed into a simpler, more convenient form, the so-called *weak conservative form*

$$\rho\frac{D\phi}{Dt} = \rho\frac{\partial\phi}{\partial t} + \rho(\vec{v}\cdot\nabla)\phi = \rho\dot{\gamma}$$

$$\rho\frac{D\phi}{Dt} = \rho\frac{\partial\phi}{\partial t} + \rho v_j\frac{\partial\phi}{\partial x_j} = \rho\dot{\gamma} \tag{1.11}$$

where $\frac{D}{Dt} = \frac{\partial}{\partial t} + v_j\frac{\partial}{\partial x_j}$ is the material (substantial) derivative , denoting the total rate of change of the variable ϕ along a streamline (felt by an observer traveling with the fluid element by its velocity).

1.2.1 Source terms and constitutive relations

The ”source” $\dot{\gamma}$ can be associated with the system mass, the so-called *mass* source(s) $\dot{\gamma}_m$ and with the system surface, the so-called *surface (diffusion)* source(s) $\dot{\gamma}_A$, so that the total source can be written as a sum of the two source types,

$$\dot{\Upsilon} = \int_V \dot{\gamma}_m\rho\, dV + \int_A \dot{\gamma}_A\, dA = \int_{CV}(\rho\,\dot{\gamma}_m + \nabla\cdot\dot{\gamma}_A)\, dV \tag{1.12}$$

---

[2] Note also other common notations for the velocity vector and its components: $\vec{v}(u, v, w)$ or $U_i(U, V, W)$ are used often in the analysis of simpler flows especially when one or two velocity components are zero (two- and one-dimensional flows), and $U_i(U_1, U_2, U_3)$ is more common in the treatise of turbulent flows.

For example:

- $\dot{\gamma}_m$ stands for an internal source per unit mass of heat due to chemical reaction, combustion, electric or magnetic heating in the energy equation, whereas in the momentum equation it denotes the gravitational, Coriolis, centrifugal or electromagnetic force ;
- $\dot{\gamma}_A$ represents the diffusion flux of heat through the control surface in the energy equation, and a force on control surface due to pressure and viscous stresses in the momentum equation.

The *surface source* is in essence the *molecular flux through the surface* and can often be expressed in terms of the *gradient* of the property considered , i.e.

$$\dot{\gamma}_A = -\Gamma \nabla \phi$$

where Γ is the molecular transport coefficient. The above equation connects the continuum property ϕ with their molecular (material) constitution (represented by the transport coefficient Γ) and is called the *constitutive relation or equation.* The constitutive equations associated with the three conservation laws here considered are:

▷ Conduction flux (Fourier's law):

$$\dot{\gamma}_A = -\vec{q} = \lambda \nabla T \quad \text{or,} \quad -q_i = \lambda \frac{\partial T}{\partial x_i} \tag{1.13}$$

where λ [W m^{-1} K^{-1}] is the thermal conductivity.

▷ Mass molecular diffusion flux (Fick's law):

$$\dot{\gamma}_A = -\vec{m}'' = \mathcal{D} \nabla c \quad \text{or} \quad -m_i'' = \mathcal{D} \frac{\partial c}{\partial x_i} \tag{1.14}$$

where $\vec{m}''$ [kg m^{-2} s^{-1}] is the mass flux of a species in kg (or moles) per unit area and in unit time, C [kg m^{-3}] (or [mol m^{-3}]) is the species concentration and $\mathcal{D}$ [m^2 s^{-1}] is the mass diffusivity.

▷ Momentum flux, i.e. the stress (Newton's law of viscosity)[3]:

$$\begin{aligned} \dot{\gamma}_A = \mathbf{T} &= -p\mathbf{I} + \mu [\nabla \cdot \vec{v} + (\nabla \cdot \vec{v})^T - \frac{2}{3} \nabla \cdot \vec{v} \mathbf{I}] \qquad \text{or,} \\ \tau_{ij} &= -p\delta_{ij} + \mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \frac{\partial v_k}{\partial x_k} \delta_{ij} \right) \\ &= -p\delta_{ij} + 2\mu (S_{ij} - \frac{1}{3} S_{kk} \delta_{ij}) \end{aligned} \tag{1.15}$$

---

[3] Note that the capital boldface letters denote Cartesian second-order tensors.

where μ [kg m^{-1} s^{-1}] is the dynamic molecular viscosity, $S_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)$ is the rate of strain (rate of deformation of a fluid element), and $\mathbf{I}$ denotes the unit second-order tensor with its Cartesian components δ_{ij} (known also as *Kronecker delta*).

1.2.2 Common form of the differential conservation law

Now we can write the common differential form of the conservation law:

$$\rho\,\frac{D\phi}{Dt} = \rho\frac{\partial \phi}{\partial t} + \rho\,(\vec{v}\cdot\nabla)\phi = \rho\,\dot{\gamma}_m + \nabla\cdot\dot{\gamma}_A$$

$$\rho\,\frac{D\phi}{Dt} = \rho\frac{\partial \phi}{\partial t} + \rho\,v_j\frac{\partial \phi}{\partial x_j} = \rho\,\dot{\gamma}_m + \frac{\partial\,\dot{\gamma}_A}{\partial x_j} \tag{1.16}$$

Inserting the appropriate variables and the corresponding source terms from Table 1.1, defining the unit mass sources $\dot{\gamma}_m$ and using Eqns (1.13), (1.14) and (1.15) for the surface sources $\dot{\gamma}_A$, yield the common conservation equations:

- Momentum (Navier-Stokes) equations, $\phi = \vec{v}$ or v_i:

$$\begin{aligned}
\rho\,\frac{D\vec{v}}{Dt} &= \rho\frac{\partial \vec{v}}{\partial t} + \rho\,(\vec{v}\cdot\nabla)\vec{v} = \rho\vec{g} + \nabla\cdot\mathbf{T}\\
&= \rho\,\vec{g} - \nabla p\mathbf{I} + \nabla\cdot\left(\mu\left[\nabla\cdot\vec{v} + (\nabla\cdot\vec{v})^T) - \frac{2}{3}\nabla\cdot\vec{v}\mathbf{I}\right]\right)\\
\rho\,\frac{Dv_i}{Dt} &= \rho\frac{\partial v_i}{\partial t} + \rho\,v_j\frac{\partial v_i}{\partial x_j} = \rho g_i + \frac{\partial\,\tau_{ij}}{\partial x_j}\\
&= \rho g_i - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3}\frac{\partial v_k}{\partial x_k}\,\delta_{ij}\right)\right]
\end{aligned} \tag{1.17}$$

- Energy equation, written in terms of enthalpy, $\phi = h = c_p T$:

$$\rho\,\frac{Dh}{Dt} = \rho\left(\frac{\partial h}{\partial t} + (\vec{v}\cdot\nabla)h\right) = \rho\,\dot{q}_g + \nabla\cdot(\frac{\lambda}{c_p}\nabla h)$$

$$\rho\,\frac{Dh}{Dt} = \rho\left(\frac{\partial h}{\partial t} + v_j\frac{\partial h}{\partial x_j}\right) = \rho\,\dot{q}_g + \frac{\partial}{\partial x_j}\left(\frac{\lambda}{c_p}\frac{\partial h}{\partial x_j}\right) \tag{1.18}$$

which for a constant specific heat c_p [J kg^{-1} s^{-1}] can also be written in terms of temperature $\phi = T$, by dividing Eq. (1.18) by ρc_p:

$$\frac{DT}{Dt} = \left(\frac{\partial T}{\partial t} + (\vec{v}\cdot\nabla)T\right) = \frac{\dot{q}_g}{c_p} + \nabla\cdot(\alpha\nabla T)$$

$$\frac{DT}{Dt} = \left(\frac{\partial T}{\partial t} + v_j \frac{\partial T}{\partial x_j}\right) = \frac{\dot{q}_g}{c_p} + \frac{\partial}{\partial x_j}\left(\alpha \frac{\partial T}{\partial x_j}\right) \tag{1.19}$$

where $\alpha = \lambda/(\rho c_p)$ [$\mathrm{m^2 s^{-1}}$] is the thermal diffusivity, and $\dot{q}_g$ [W $\mathrm{kg^{-1}}$] is the internal heat source.

- Concentration equation (for each species in a multi-component system) $\phi = C$:

$$\rho \frac{DC}{Dt} = \rho\left(\frac{\partial C}{\partial t} + (\vec{v}\cdot\nabla)C\right) = \rho\dot{r} + \nabla\cdot(\mathcal{D}\nabla C)$$

$$\rho \frac{DC}{Dt} = \rho\left(\frac{\partial C}{\partial t} + v_j \frac{\partial C}{\partial x_j}\right) = \rho\dot{r} + \frac{\partial}{\partial x_j}\left(\mathcal{D} \frac{\partial C}{\partial x_j}\right) \tag{1.20}$$

1.3 Classification of equations

Conservation equations in differential form can often be simplified for specific problems by omitting various terms that are negligible in that specific situation. In many cases this makes it possible to solve the equations either by analytical tools or by simpler computational methods. Moreover, simplification of equations makes it possible to identify clearly the major physical phenomenon governing the problem under investigation. In some cases the simplification leads to well established forms of equations known under separate names and used in other areas of science. We discuss classification of general partial differential equations (PDE) from two points of view, using physical criteria based on the physical meaning of terms in the equations, and mathematical criteria that primarily define the method of solution.

Physical criteria

A precise physical meaning can be assigned to each of the terms in the general differential conservation equations:

$$\underbrace{\rho\frac{D\phi}{Dt}}_{\mathcal{M}} = \underbrace{\rho\frac{\partial\phi}{\partial t}}_{\mathcal{L}} + \underbrace{\rho(\vec{v}\cdot\nabla)\phi}_{\mathcal{C}} = \underbrace{\rho\,\dot{\gamma}_m}_{\mathcal{S}} + \underbrace{\nabla\cdot(\Gamma\nabla\phi)}_{\mathcal{D}} \tag{1.21}$$

where:

$\mathcal{M}$ = material (substantial) derivative (the total change of ϕ along the streamline)

$\mathcal{L}$ = local time rate of change (felt by the observer at a fixed position in an inertial coordinate frame)

$\mathcal{C}$ = convection (rate of change felt by the observer moving with the fluid particle at local velocity $\vec{v}$)

$\mathcal{D}$ = diffusion (flux of ϕ through the surface of the elementary control volume)

$\mathcal{S}$ = source of ϕ

In the absence of various terms, the equation reduces to special forms. Assuming for clarity that in all cases the material properties remain constant, so that Γ=const, the following well-known equations are obtained:

- For stationary transport ($\partial/\partial t = 0$) without flow ($\vec{v} = 0$, solids, stagnant liquids) and without internal source, $\mathcal{M} = \mathcal{L} + \mathcal{C} = 0,\ \ \mathcal{S} = 0$, and equation (1.21) reduces to the *Laplace (potential) equation*

$$\nabla^2 \phi = 0 \tag{1.22}$$

- For non-stationary (transient) transport without flow and without source: $\mathcal{C} = 0,\ \ \mathcal{S} = 0$, we obtain the *Diffusion (Conduction) equation*

$$\rho \frac{\partial \phi}{\partial t} = \Gamma \nabla^2 \phi \tag{1.23}$$

- For stationary transport with flow, but without internal source, $\mathcal{L} = 0,\quad \mathcal{S} = 0$, equation (1.21) is known as the *Convection-diffusion equation*

$$\rho\,(\vec{v} \cdot \nabla)\phi \;=\; \Gamma \nabla^2 \phi \tag{1.24}$$

When the time-rate term $\mathcal{L}$ is added, the equation is known as the *Unsteady convection-diffusion equation.*

Mathematical criteria

In the mathematical sense, second-order partial differential equations can be classified into three types according to the equation discriminant. Consider, as an illustration, a general form of such an equation for two-dimensional flows

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu = 0 \tag{1.25}$$

where, for brevity, subscripts are used to denote differentiation with respect to particular coordinates, i.e. $u_x = \partial u/\partial x$, $u_{xy} = \partial^2 u/\partial x \partial y$

Depending on the system discriminant, equations are classified as:

1. *Elliptic*, if

   $$B^2 - 4AC < 0$$

   Example: The Laplace equation

   $$u_{xx} + u_{yy} = 0$$

2. *Parabolic*, if:

   $$B^2 - 4AC = 0$$

   Example: Diffusion equation (with $y = t$)

   $$Au_{xx} - u_y = 0$$

3. *Hyperbolic*, if:

   $$B^2 - 4AC > 0$$

   Example: wave propagation equation (e.g. momentum equation for supersonic flow)

It is noted that this classification has major implications on the selection of the appropriate numerical or analytical methods for solving the equations. For example, in problems governed by parabolic equations (e.g. fluid flow and scalar convection in wall boundary layers and jets) there is no influence of flow properties upstream from the point of consideration and one can simply march along the flow and compute all variables in one sweep, starting from the given inflow conditions and side boundary conditions. In contrast, problems governed by elliptic equations are influenced by conditions on all boundaries surrounding the solution domain and the numerical solutions are much more demanding, requiring usually an iterative solution process. Hyperbolic problems resemble the parabolic ones, but the propagation of a variable occurs along specific lines called the *characteristics*. For that reason, different numerical solvers have been developed for different families of problems governed by each type of equations, though general solution methods are also available.

1.4 Boundary and initial conditions

Transport processes are described by partial differential equations of the second order in space, and first order in time: Hence,

- two boundary conditions are needed for each dependent variable in terms of space coordinates, and
- for non-stationary problems we need to know the initial conditions.

Two types of boundary conditions can be used (depending on the problem)

- Dirichlet boundary conditions: the value of ϕ is defined on the boundary, i.e. $\phi_b = \phi_b(x,y,z,t)$
- Neumann boundary conditions: the flux of ϕ related to its gradient in the direction normal to the boundary is given, i.e.

$$\dot{\gamma}_b = -\Gamma \left(\frac{\partial \phi}{\partial n} \right)_b = f(x,y,z,t,\phi_b) \tag{1.26}$$

For the momentum equation the *no-slip* boundary condition at a solid wall implies that the fluid velocity equals the wall velocity (if any), i.e. $\vec{v}|_w = 0$ for a stationary wall, and $\vec{v}|_w = v_w$ for a wall moving with the velocity v_w. For the energy equation, the heat flux at the wall can be defined in two ways (depending on whether the heat exchange at the boundary occurs by convection or by radiation - or both)

- Convective flux

$$q_b = -\lambda \left(\frac{\partial T}{\partial n} \right)_b = f(x,y,z,t,T_b) = h(x,y,z,t)(T_b - T_0) \tag{1.27}$$

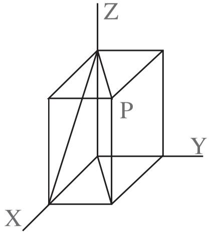
- Radiative flux

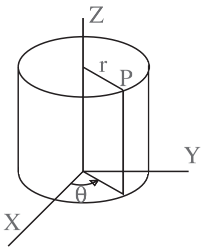
$$q_b = -\lambda \left(\frac{\partial T}{\partial n} \right)_b = f(x,y,z,t,T_b) = G(x,y,z,t)\sigma(T_b^4 - T_0^4) \tag{1.28}$$

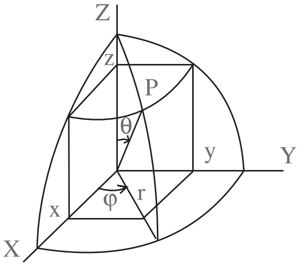
where subscript b denotes the boundary of the solution domain (a solid wall or a free surface) and T_0 is the reference fluid temperature, h [W m^{-2} K^{-1}] is the heat transfer coefficient and σ [W m^{-2} K^{-4}] stands for the Stefan-Boltzmann constant.

1.5 Coordinate transformations

The differential conservation equations for mass (1.10), momentum (1.17), energy (1.18 and 1.19), and species concentration (1.20) do not depend on the coordinate system as long as the vector notation is used. However, the conservation equations with the index notation (that are given below the vector notation) are valid only in a Cartesian coordinate system. When solving problems involving heat, mass, and/or momentum transfer, one has to select a reference coordinate system. Tables 1.2 and 1.3 give the various terms in conservation equations for Cartesian, cylindrical and spherical coordinate systems. The conservation equations on a general curvilinear coordinate system can be derived by using methods described by e.g. Bird et al. (2002), Chung (1996).







	Cartesian coordinates	cylindrical coordinates	spherical coordinates
∇T	$\vec{e}_x \frac{\partial T}{\partial x} + \vec{e}_y \frac{\partial T}{\partial y} + \vec{e}_z \frac{\partial T}{\partial z}$	$\vec{e}_r \frac{\partial T}{\partial r} + \vec{e}_\theta \frac{1}{r} \frac{\partial T}{\partial \theta} + \vec{e}_z \frac{\partial T}{\partial z}$	$\vec{e}_r \frac{\partial T}{\partial r} + \vec{e}_\theta \frac{1}{r} \frac{\partial T}{\partial \theta} + \vec{e}_\varphi \frac{1}{r \sin\theta} \frac{\partial T}{\partial \varphi}$
$\nabla \cdot \vec{v}$	$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}$	$\frac{1}{r} \frac{\partial}{\partial r} r v_r + \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z}$	$\frac{1}{r^2} \frac{\partial}{\partial r} r^2 v_r + \frac{1}{r \sin\theta} \frac{\partial}{\partial \theta} \left(v_\theta \sin\theta \right) + \frac{1}{r \sin\theta} \frac{\partial v_\varphi}{\partial \varphi}$
$\nabla^2 T$	$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}$	$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2}$ or $\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2}$	$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial T}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2 T}{\partial \varphi^2}$ or $\frac{2}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\cos\theta}{r^2 \sin\theta} \frac{\partial T}{\partial \theta} + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2 T}{\varphi^2}$
$\nabla \lambda \cdot \nabla T$	$\frac{\partial}{\partial x} \lambda \frac{\partial T}{\partial x} + \frac{\partial}{\partial y} \lambda \frac{\partial T}{\partial y} + \frac{\partial}{\partial z} \lambda \frac{\partial T}{\partial z}$	$\frac{1}{r} \frac{\partial}{\partial r} \lambda r \frac{\partial T}{\partial r} + \frac{1}{r} \frac{\partial}{\partial \theta} \frac{\lambda}{r} \frac{\partial T}{\partial \theta} + \frac{\partial}{\partial z} \lambda \frac{\partial T}{\partial z}$	$\frac{1}{r^2} \frac{\partial}{\partial r} \lambda r^2 \frac{\partial T}{\partial r} + \frac{1}{r \sin\theta} \frac{\partial}{\partial \theta} \lambda \frac{\sin\theta}{r} \frac{\partial T}{\partial \theta} + \frac{1}{r \sin\theta} \frac{\partial}{\partial \varphi} \left(\frac{\lambda}{r \sin\theta} \frac{\partial T}{\partial \varphi} \right)$
$\vec{v} \cdot \nabla T$	$v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z}$	$v_r \frac{\partial T}{\partial r} + \frac{v_\theta}{r} \frac{\partial T}{\partial \theta} + v_z \frac{\partial T}{\partial z}$	$v_r \frac{\partial T}{\partial r} + \frac{v_\theta}{r} \frac{\partial T}{\partial \theta} + \frac{v_\varphi}{r \sin\theta} \frac{\partial T}{\partial \varphi}$
$\frac{D}{Dt}$	$\frac{\partial}{\partial t} + v_x \frac{\partial}{\partial x} + v_y \frac{\partial}{\partial y} + v_z \frac{\partial}{\partial z}$	$\frac{\partial}{\partial t} + v_r \frac{\partial}{\partial r} + \frac{v_\theta}{r} \frac{\partial}{\partial \theta} + v_z \frac{\partial}{\partial z}$	$\frac{\partial}{\partial t} + v_r \frac{\partial}{\partial r} + \frac{v_\theta}{r} \frac{\partial}{\partial \theta} + \frac{v_\varphi}{r \sin\theta} \frac{\partial}{\partial \varphi}$

Table 1.2 Coordinate transformations.

	Cartesian coordinates
x-comp.	$\rho\left(\frac{\partial v_x}{\partial t}+v_x\frac{\partial v_x}{\partial x}+v_y\frac{\partial v_x}{\partial y}+v_z\frac{\partial v_x}{\partial z}\right)=-\frac{\partial p}{\partial x}+\mu\left(\frac{\partial^2 v_x}{\partial x^2}+\frac{\partial^2 v_x}{\partial y^2}+\frac{\partial^2 v_x}{\partial z^2}\right)+\rho g_x$
y-comp.	$\rho\left(\frac{\partial v_y}{\partial t}+v_x\frac{\partial v_y}{\partial x}+v_y\frac{\partial v_y}{\partial y}+v_z\frac{\partial v_y}{\partial z}\right)=-\frac{\partial p}{\partial y}+\mu\left(\frac{\partial^2 v_y}{\partial x^2}+\frac{\partial^2 v_y}{\partial y^2}+\frac{\partial^2 v_y}{\partial z^2}\right)+\rho g_y$
z-comp.	$\rho\left(\frac{\partial v_z}{\partial t}+v_x\frac{\partial v_z}{\partial x}+v_y\frac{\partial v_z}{\partial y}+v_z\frac{\partial v_z}{\partial z}\right)=-\frac{\partial p}{\partial z}+\mu\left(\frac{\partial^2 v_z}{\partial x^2}+\frac{\partial^2 v_z}{\partial y^2}+\frac{\partial^2 v_z}{\partial z^2}\right)+\rho g_z$
	Cylindrical coordinates
r-comp.	$\rho\left(\frac{\partial v_r}{\partial t}+v_r\frac{\partial v_r}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_r}{\partial \theta}-\frac{v_\theta^2}{r}+v_z\frac{\partial v_r}{\partial z}\right)=-\frac{\partial p}{\partial r}+\mu\left(\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial}{\partial r}(rv_r)\right)+\frac{1}{r^2}\frac{\partial^2 v_r}{\partial \theta^2}-\frac{2}{r^2}\frac{\partial v_\theta}{\partial \theta}+\frac{\partial^2 v_r}{\partial z^2}\right)+\rho g_r$
θ-comp.	$\rho\left(\frac{\partial v_\theta}{\partial t}+v_r\frac{\partial v_\theta}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_\theta}{\partial \theta}+\frac{v_r v_\theta}{r}+v_z\frac{\partial v_\theta}{\partial z}\right)=-\frac{1}{r}\frac{\partial p}{\partial \theta}+\mu\left(\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial}{\partial r}(rv_\theta)\right)+\frac{1}{r^2}\frac{\partial^2 v_\theta}{\partial \theta^2}+\frac{2}{r^2}\frac{\partial v_r}{\partial \theta}+\frac{\partial^2 v_\theta}{\partial z^2}\right)+\rho g_\theta$
z-comp.	$\rho\left(\frac{\partial v_z}{\partial t}+v_r\frac{\partial v_z}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_z}{\partial \theta}+v_z\frac{\partial v_z}{\partial z}\right)=-\frac{\partial p}{\partial z}+\mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 v_z}{\partial \theta^2}+\frac{\partial^2 v_z}{\partial z^2}\right)+\rho g_z$
	Spherical coordinates
r-comp.	$\rho\left(\frac{\partial v_r}{\partial t}+v_r\frac{\partial v_r}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_r}{\partial \theta}+\frac{v_\varphi}{r\sin\theta}\frac{\partial v_r}{\partial \varphi}-\frac{v_\theta^2+v_\varphi^2}{r}\right)=-\frac{\partial p}{\partial r}+\mu\left(\nabla^2 v_r-\frac{2}{r^2}v_r-\frac{2}{r^2}\frac{\partial v_\theta}{\partial \theta}-\frac{2}{r^3}v_\theta\cot\theta-\frac{2}{r^2\sin\theta}\frac{\partial v_\varphi}{\partial \varphi}\right)+\rho g_r$
θ-comp.	$\rho\left(\frac{\partial v_\theta}{\partial t}+v_r\frac{\partial v_\theta}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_\theta}{\partial \theta}+\frac{v_\varphi}{r\sin\theta}\frac{\partial v_\theta}{\partial \varphi}+\frac{v_r v_\theta}{r}-\frac{v_\varphi^2\cot\theta}{r}\right)=-\frac{1}{r}\frac{\partial p}{\partial \theta}+\mu\left(\nabla^2 v_\theta+\frac{2}{r^2}\frac{\partial v_r}{\partial \theta}-\frac{v_\theta}{r^2\sin^2\theta}-\frac{2\cos\theta}{r^2\sin^2\theta}\frac{\partial v_\varphi}{\varphi}\right)+\rho g_\theta$
φ-comp.	$\rho\left(\frac{\partial v_\varphi}{\partial t}+v_r\frac{\partial v_\varphi}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_\varphi}{\partial \theta}+\frac{v_\varphi}{r\sin\theta}\frac{\partial v_\varphi}{\partial \varphi}+\frac{v_\varphi v_r}{r}+\frac{v_\theta v_\varphi}{r}\cot\theta\right)=-\frac{1}{r\sin\theta}\frac{\partial p}{\partial \varphi}+\mu\left(\nabla^2 v_\varphi-\frac{v_\varphi}{r^2\sin^2\theta}+\frac{2}{r^2\sin\theta}\frac{\partial v_r}{\partial \varphi}+\frac{2\cos\theta}{r^2\sin^2\theta}\frac{\partial v_\theta}{\partial \varphi}\right)+\rho g_\varphi$

Table 1.3 Coordinate transformations for Navier-Stokes equations.