Analysis and Modelling of Physical Transport Phenomena

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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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:

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

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):

$$\Phi = \int_s \phi\, dm = \int_s \phi \rho\, dV \tag{1.2}$$

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),