

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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Contents

Preface	xi
I Fundamental Equations	1
1 Fundamental Equations of Transport Phenomena - Field description	3
1.1 Introduction	3
1.2 Conservation laws for a control volume in differential form	3
1.2.1 Source terms and constitutive relations	8
1.2.2 Common form of the differential conservation law	10
1.3 Classification of equations	11
1.4 Boundary and initial conditions	13
1.5 Coordinate transformations	14
II Analytical Methods	17
2 Analytical Methods	19
2.1 Partial differential equations	19
2.2 Separation of variables	19
2.3 Eigenfunctions and eigenvalues	25
2.3.1 Spherical symmetry	26
2.4 Cylindrical symmetry: Bessel functions	28
2.5 Laplace-transformation	31
2.6 Error- and Gamma-function	36
2.6.1 Error function	36
2.6.2 Gamma function	37
2.7 Combination of variables and dimension analysis	38
2.8 Integral methods	40
2.9 Exercises	44
2.9.1 Heat storage in the ground	44
2.9.2 Steel cooling	45
2.9.3 Chemical reaction on a sphere	45

2.10	Answers to exercises	45
2.10.1	Heat storage in the ground	45
2.10.2	Steel cooling	48
2.10.3	Chemical reaction on a sphere	50
3	Transport in Stagnant Media	53
3.1	Stationary problems	53
3.2	Diffusion equation	55
3.2.1	Boundary conditions	55
3.2.2	Solutions for sources	56
3.2.3	Summation of sources and Green's functions	59
3.2.4	Line sources and point sources	61
3.2.5	Penetration theory and Duhamel's theorem	62
3.2.6	Contact temperature	63
3.3	Moving front problems	65
3.3.1	Non-stationary heat conduction with phase changes	65
3.3.2	Moving fronts in mass transport problems	67
3.3.3	Integral method for solidification problems with convective heat transfer	68
3.4	Diffusion equation with source terms	71
3.5	Exercises	73
3.5.1	Colour photo	73
3.5.2	Apollo heat shield	73
3.5.3	Decomposing apple	74
3.5.4	Wall temperature for type-3 boundary condition	75
3.6	Answers to exercises	76
3.6.1	Colour photo	76
3.6.2	Apollo heat shield	77
3.6.3	Decomposing apple	78
3.6.4	Wall temperature for type-3 boundary condition	80
4	Momentum Transport	83
4.1	Introduction	83
4.2	Incompressible flows	83
4.2.1	Potential flow	84
4.2.2	Creeping flow	89
4.3	Boundary layers	90
4.3.1	Boundary-layer equations	90
4.3.2	Solving the boundary-layer equations	93
5	Transport in Flowing Media	97
5.1	Stationary transport in flows with a uniform velocity profile	97
5.1.1	Transport in a plug flow along a flat plate	98
5.1.2	Diffusion of heat in a plug flow through a pipe	100

5.2	Lévêque-problem	101
5.3	Diffusion of heat in a laminar pipe flow	103
5.4	Natural convection	104
5.5	Exercises	106
5.5.1	Electrochemical detector	106
5.5.2	Infinitely long vertical tank	106
5.6	Answers to exercises	108
5.6.1	Electrochemical detector	108
5.6.2	Infinitely long vertical tank	112

III Numerical Methods 115

6	Numerical Heat and Fluid Flow	117
6.1	Introduction	117
6.2	Heat conduction	120
6.2.1	Steady one-dimensional (1D) diffusion	120
6.2.2	An iterative procedure for nonlinear equations	122
6.2.3	Boundary conditions for heat conduction	122
6.2.4	Basic principles of the discretisation procedure	123
6.2.5	Unsteady one-dimensional (1D) diffusion	124
6.2.6	Unsteady two-dimensional (2D) diffusion	126
6.2.7	Unsteady three-dimensional (3D) diffusion	127
6.2.8	Iterative solving of system of linear discretised equations	128
6.2.9	Measures for facilitating convergence	129
6.3	Convection and diffusion	129
6.3.1	Steady one-dimensional (1D) convection and diffusion	130
6.3.2	The central differencing scheme (CDS)	130
6.3.3	The upwind differencing scheme (UDS)	131
6.3.4	The hybrid (flux-blending) scheme	132
6.3.5	The exact solution	132
6.3.6	The exponential scheme	133
6.3.7	The generalised formulation of differencing schemes	134
6.3.8	Numerical ("false") diffusion	136
6.3.9	UDS versus CDS for one-dimensional convection-diffusion	138
6.3.10	Higher order differencing schemes	139
6.3.11	Total variation diminishing schemes (TVD)	141
6.3.12	Unsteady two-dimensional (2D) convection and diffusion	145
6.3.13	Unsteady three-dimensional (3D) convection and diffusion	147
6.4	Calculation of the velocity field	148
6.4.1	The discretised form of the momentum equation	150
6.4.2	The pressure-correction equation	151
6.4.3	The SIMPLE algorithm	152

6.4.4	Pressure-velocity coupling for collocated grid arrangement	153
6.5	Boundary conditions	154
6.6	Chart diagram of a numerical code for CFD	155

IV Turbulence and Transport Phenomena 159

7 Turbulence: Some Features and Rationale for Modelling 161

7.1	The phenomenon of turbulence	161
7.2	Solution to turbulence: needs for modelling and simulations	162
7.3	Statistical description of turbulence: Reynolds decomposition	166
7.3.1	Reynolds averaging	168
7.3.2	Reynolds-averaged conservation equations	170
7.4	Some features of turbulence	172
7.5	Characterisation and scales of turbulence	179
7.5.1	Measure of turbulence: intensity	179
7.5.2	Turbulence scales	180
7.5.3	Turbulence Reynolds numbers	181
7.5.4	Another look at the prospects of Direct Simulation	183
7.5.5	Two-point correlations	184
7.5.6	Turbulence Spectra.	186

8 Generic Flows and Similarity Analysis 191

8.1	Generic turbulent flows	191
8.1.1	Homogeneous turbulent flows	193
8.1.2	Thin shear flows	194
8.1.3	More complex generic flows	195
8.2	Turbulent wall boundary layer	197
8.2.1	Similarity analysis and velocity distribution	197
8.2.2	Temperature distribution	201

9 Turbulence Models for RANS 205

9.1	The closure problem and modelling principles	205
9.1.1	Scope and limitations of RANS (SPCM)	206
9.1.2	Desirable features of Turbulence Models	207
9.1.3	Some modelling principles and rules	207
9.2	Eddy-viscosity/diffusivity models (EVM, EDM)	208
9.2.1	Turbulent viscosity/diffusivity; classification of models	210
9.3	Algebraic models, mixing length	211
9.4	Differential eddy viscosity/diffusivity models	212
9.4.1	One- and two-equation differential EVM/EDM	213
9.4.2	The k -equation	214
9.4.3	The ε -equation	217
9.5	The $k - \varepsilon$ model	220

9.5.1	Modelling the k -equation	220
9.5.2	The modelled ε equation for high-Re-number flows	222
9.5.3	Determining the coefficients	223
9.5.4	Summary of the high-Re-number $k - \varepsilon$ model in integral form	225
9.5.5	Boundary conditions: Wall Functions	226
9.5.6	Low-Re-number (near-wall) $k - \varepsilon$ models	228
9.6	Other two-equation eddy-viscosity models	231
9.7	Limitations of two-equation linear EVMs	233
9.8	Non-linear eddy-viscosity models (NLEVM)	234
9.9	Second-moment closure models	236
	Literature	239
	Index	241

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:

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

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),