An Introduction to Modeling of Transport Processes Applications to Biomedical Systems

Organized around problem solving, this book gently introduces the reader to computational simulation of biomedical transport processes, bridging fundamental theory with real-world applications. Using this book the reader will gain a complete foundation to the subject, starting with problem simplification, implementation in software, through to interpretation of results, validation, and optimization. Ten case studies focusing on emerging areas such as thermal therapy and drug delivery, with easy-to-follow step-by-step instructions, provide ready-to-use templates for further applications. Solution process using the commonly used tool COMSOL Multiphysics is described in detail, useful biomedical property data and correlations are included, and background theory information is given at the end of the book for easy reference. A mixture of short and extended exercises make this book a complete course package for undergraduate and beginning graduate students in biomedical engineering, biological engineering, and other engineering curricula, as well as an invaluable self-study guide.

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An Introduction to Modeling of Transport Processes

Applications to Biomedical Systems

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Cornell University

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To my sister, Namita, and my brother, Ashis
Ashim

To my sisters, Smita, and Namrata
Vineet

Contents

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978-0-521-11924-5 - An Introduction to Modeling of Transport Processes: Applications to Biomedical Systems
Ashim Datta and Vineet Rakesh
Frontmatter
More information

Preface

Simulation is an important component of the engineering design process in many sectors. The integration of simulation into undergraduate engineering education in an appropriate manner, so that it enhances the fundamentals, and also provides students with a cutting-edge tool, has been in the forefront of education thinking, as evidenced by the interest in a recent workshop at Cornell University (ISTEC, 2008), and in a report by the National Science Foundation (NSF, 2006). The tremendous growth in biomedical engineering over the last 10–15 years has encouraged increased quantitative treatment of biomedical product, process and equipment design, and design of treatment procedures. Such quantitative treatment has made simulation into a useful tool in biomedical applications as well. The synergy between increased use of simulation and the availability of improved interfaces has brought down the barriers to the use of simulation, from only specialized modelers, to just about anyone who has the necessary prerequisite of the physical process (engineering science content such as heat transfer or mass transfer). The increased need in industry and research, and the lower barrier to modeling can be integrated further by having all the essential information under one umbrella – which is the goal for this book. This introductory book walks a person without any prior knowledge in modeling through all of the necessary steps thus helping them to join the modeling community, and thereby enabling a productivity tool for design and research.

Although more widespread use of modeling in practical terms means that a typical modeler will now have a less formal background training than in the past, training material that introduces modeling to the less well prepared is elusive. We have made our primary goal in this book to provide a smooth, easy-to-follow introduction which takes the newcomer through the entire model development, formulation from physical to mathematical, required biomedical data on all parameters, complete implementation in software, validation of the solution, making sense of the data and, finally, sensitivity analysis and optimization. It is designed for someone with a transport-phenomena background as a self-study tool, in order that they can walk through the entire process without any external help; thus making it suitable in both industry and introductory classroom situations. In academia, although the material was used as a follow-up course to heat transfer or heat and mass transfer, the gentle approach of the book will allow, without additional instruction, students to perform small projects and thus enhance an introductory transport process course.

The needs of the introductory modeler, without an elaborate background in modeling, were far from obvious when this course was started in 1996 (Datta, 2009). It is through observing the students (3rd and 4th year engineering) and the questions they asked, that we learned where they needed the most help. For example, problem formulation from a physical process to a mathematical one, was clearly somewhere they needed significant help – this led to the development of a complete chapter (Chapter 1). The instructors learned from the process just as much. For example, problem formulation is not an explicit topic in any typical curriculum, however, it made us think more about this topic, which also happens to be at the center of the engineer's ability to solve problems. Likewise, much of the book is centered around the precise information that the students needed to complete their modeling projects. Since its inception, the students on this course have completed close to 100 projects, most of which have been learning experiences for the instructors as well. This knowledge has been distilled and incorporated into the book.

Obviously, the book intends to develop a modeling background which is not meant to replace more specialized training, typically graduate coursework in computational fluid flow, heat transfer and so on (computational fluid dynamics or CFD). Rather, the intent here is that the user of the book should be able to perform less-complex simulations and, for more complex simulations, be a more effective team member. Also, the person will be sufficiently familiar with simulation methodology to be competent to take part in discussions involving simulation.

To summarize, we feel the novelties of this book are three-fold: (1) introducing modeling to an audience with less formal and specialized training in modeling, and to undergraduates; (2) bringing the context of emerging biomedical processes; and (3) to achieve this without making the process a complete blackbox. Our hope is that as modeling in biomedical processes and modeling in general become more ubiquitous, this book will serve the need for gentle introduction for the beginner and a resource that can be put to use right away in the classroom situation, academic research or industrial design and research.

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Introduction and overview

What does modeling involve? Why should we care about modeling? Do I have to be a math whiz to succeed? How can this book help me to get started in modeling (in case I do care)? These are some of the questions we try to answer in this introductory chapter. This chapter is critical and should not be skipped.

What is modeling?

By modeling, we mean developing a replica on a computer of a physical process that interests us so that we can manipulate the process on the computer. In contrast with a computer-aided design (CAD) model which deals mostly with geometric or solid modeling, shading, etc., we must include the detailed physics of the system in order to evaluate its performance. In short, such a model involves simplifying the geometry and physics of a real situation and solving the simplified equations that describe the physics, using a software that is primarily an equation solver.

You have modeled before. As a child, you learned that the area of a trapezoid is the height multiplied by the average of the two bases. If we program this on a calculator, so that we only have to input the height and the two bases and the calculator spits out the area, we have a model for area calculation. Most real areas will not be exact trapezoids, but you will have to use your intuition in simplifying the geometry to that of a trapezoid so that you can use the program you wrote for the calculator (see O'Connor and Spotila, 1992). In this book we develop models that involve more complex calculations. We have to use our understanding of the physics to simplify the geometry and the process and we tell the computer to solve for this situation. This procedure is worthwhile if the computer can quickly solve a problem that is close to reality. The ongoing revolution in computer processing speed makes it possible now to do just that.

Why model?

You don't have to model. But let's look at two scenarios – you are trying to design either medical equipment or a medical procedure. In designing medical equipment, your choice is to build a prototype, test it, and evaluate its shortcomings to guide you to an improved prototype. Building and testing physical prototypes is expensive and *time consuming*. While this procedure cannot be totally eliminated, it sure would be nice to reduce the time and money involved in prototype building. In today's industrial setting, saving time (also called development cycle time) alone can justify alternatives. With a realistic computer model, we can check out the expected performance of the equipment for different scenarios on the computer before we build the first prototype. This is often faster than building and testing physical prototypes.

Another scenario to consider would be the development of a new medical procedure. The comments made above about time and resources do apply to this case but, perhaps more importantly, the safety of the new procedure becomes more critical. Again, a realistic computer model can allow us to reduce the amount of experimentation that is typically needed to optimize a new procedure. Using a computer model, we can improve the performance and safety of the procedure before it is actually carried out on a patient.

Thus, models primarily provide vastly *improved understanding* of a process that is often not possible to achieve in other ways. The other major advantage stems from the fact that, once a model is built, it is much easier to modify. By repeated use of the model, we can check "what if" scenarios, making it much easier to *optimize* a process. Models can often (but not always) provide improved understanding and optimization in less time and with fewer resources. It is also inherently safer.

Many other engineering applications have embraced modeling as part of the design process for industries such as automotive, aeronautical, manufacturing, etc. A major push has occurred in recent years in the quantitative understanding of biomedical systems; modeling is therefore becoming a standard biomedical engineering tool.

What preparation do I need?

To develop the modeling skills presented here, one needs to have a relevant background in the fundamental physics of the processes under consideration. For the types of processes considered in this book, this means having a background in fluid flow, heat transfer, and mass transfer. In the past, one also had to learn about numerical methods and computer programming (not to mention all the time that would be involved in actually writing the programs needed). Now the time and experience needed for this has been reduced dramatically as computers continue to run faster and become more user friendly. Insofar as it is possible to model problems today that involve less complex physics, we can now almost avoid these procedures altogether. Thus, much of the mathematics is hidden and it is no longer necessary to bring knowledge of numerical methods and computer programming to the task of modeling.

So what level of preparation do I need in fluid flow, heat transfer and mass transfer? The answer to this, like that for any other subject, depends on the complexity of the physics that you want to study. For the types of problems mentioned in this book, introductory engineering or science courses in these topics are considered sufficient. The goal of this book is to help you solve problems yourself that are not overly complex. For more complex problems, this book will prepare you to work effectively in a group having members with more specialized or advanced background in those topics.

With the userfriendliness of software, one may wonder if training in the fundamental physics can be skipped since "the computer is taking care of the solution." As an example, this is akin to skipping the understanding of the sine curve since a calculator is available that can easily compute a sine curve with the touch of a button. The understanding of what a sine curve is must precede the rapid calculation of the same. Otherwise, it is hard to make sense of what is computed and one would never know if different types of error had crept in (for example, you punched a wrong button!). This analogy very much applies to modeling, as it is discussed here. Depending on the physics that your problem involves, having a background in the subject matter, such as fluid flow, cannot be avoided. For, if we do, we would not know the difference between a solution and garbage, the latter being common due to the very nature of computer (numerical) solutions.

How does modeling fit into design?

Typical steps in a biomedical design procedure (e.g., see King and Fries, 2009) are shown in Figure 0.1. As noted in this figure, several of the design steps can benefit from modeling through trying out various possibilities on the computer, or pre-optimizing.

Overview of the text

This text is intended to provide a quick start to modeling and Figure 0.2 shows how this is organized. Thus, the first five chapters walk the reader through the essential steps in modeling. *Chapter 1* deals with problem formulation, the all-important topic of how to take a real situation and simplify it in terms of equations that describe the process. *Chapters 2, 3 and 4* simply show how to tell a typical software

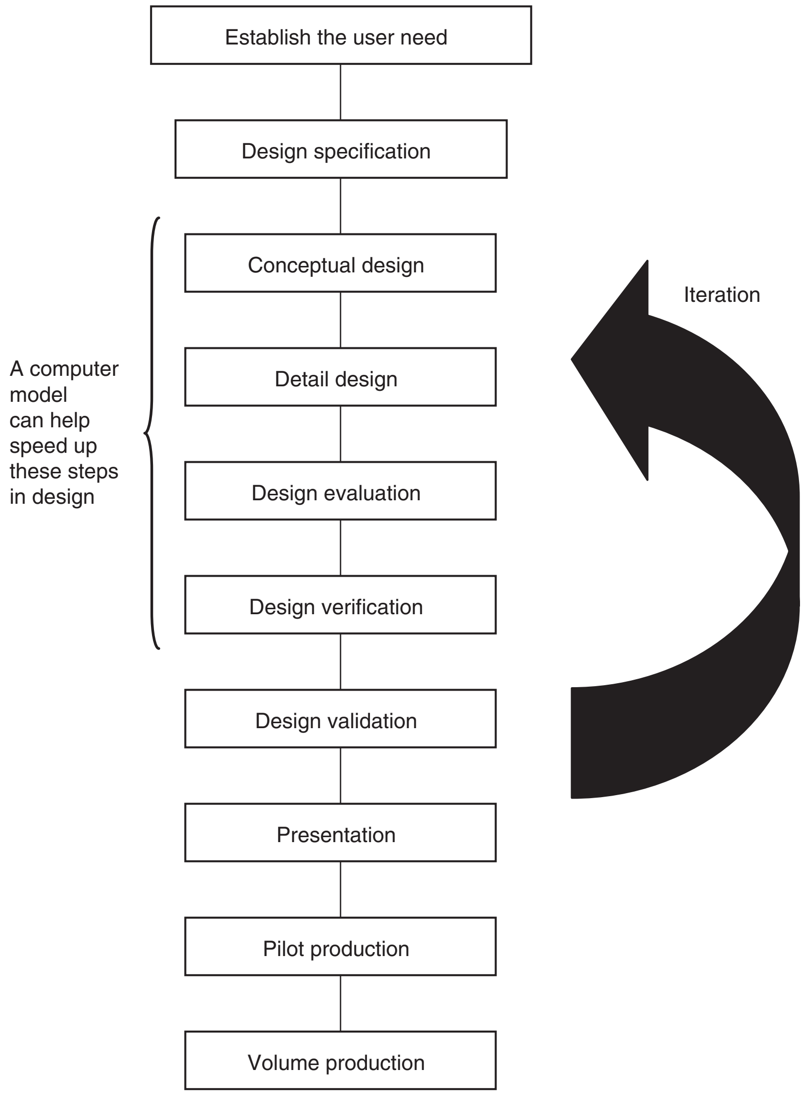

Figure 0.1

Steps in a biomedical design procedure.

application to solve the equations that we have selected (in problem formulation) and how to view the solution that we obtain. *Chapter 5* covers two important topics – validating a solution that we have just obtained, and extracting trends from the solution by changing parameters, also called sensitivity analysis, on our road to optimization of the process. *Chapter 6* provides case studies that show many examples of modeling, applying them to a number of biomedical situations. This completes the quick start to modeling. *Chapters 7–10* are provided as reference

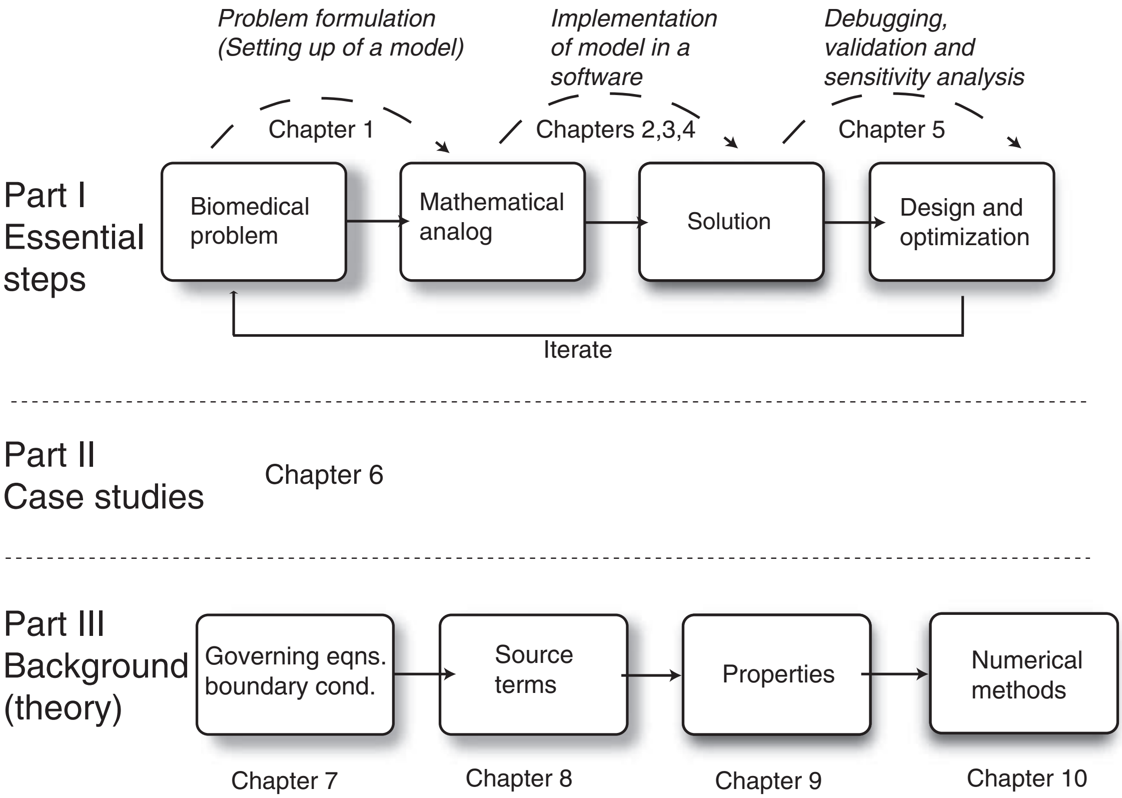

Figure 0.2

Organization of this text.

material that one can dig into, as needed. These chapters are also intended to provide, in a simple manner, the theory on which the computations are based – this should encourage the user to treat the software less as a black box. *Chapter 7* provides a quick and simple overview of how governing equations are derived. *Chapter 8* discusses how to include in the model the various modes of biomedical heating processes. *Chapter 9* is important as it discusses how one obtains the input parameters, particularly the properties, needed for the model. Finally, *Chapter 10* gently introduces the mathematical details behind numerical modeling.

Possible ways of using this text

The book is written to provide do-it-yourself training. Figure 0.3 shows another representation of the organization of this text. Depending on the user's familiarity with transport processes, two obvious approaches to using the book are:

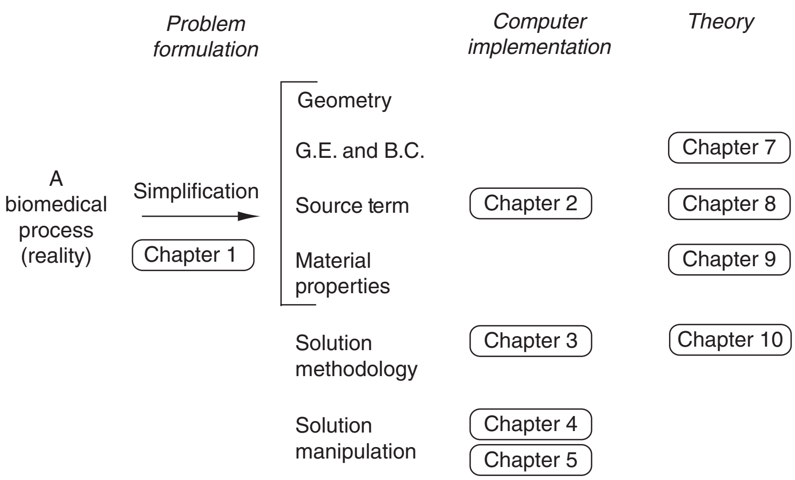

Figure 0.3

Another look at the organization of this text.

- **When familiar with transport processes** In this case, the reader can follow Chapters 1–5, using appropriate case studies from Chapter 6 as examples, turning to Chapters 7–10 only as needed.
- **When not so familiar with transport processes** In this case, the reader should first become familiarized with, or review, transport processes using Chapters 7–10. Subsequently, Chapters 1–5 are followed with appropriate case studies from Chapter 6 as examples.

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O'Connor, M. and J. R. Spotila. 1992. Consider a spherical lizard: Animals, models, and approximations. *American Zoologist*, **32**(2): 179–193.

List of symbols

a_w	water activity, dimensionless
A	area, m^2
Bi	$= hL/k$, Biot number, dimensionless
Bi_m	$= h_m K^* L/D_{AB}$, mass transfer Biot number, dimensionless
BMR	basal metabolic rate, kcal/kg/day
c	total concentration (sometimes abbreviated c_A), kg/m^3
c	speed of light in vacuum, m/s
c_*	speed of light in a medium, m/s
c_A	concentration of component A, kg of A/m^3
$c_{A,s}$	concentration of component A at a surface, kg of A/m^3
$c_{A,\infty}$	concentration of component A in the bulk fluid, kg of A/m^3
c_{av}	average concentration, kg/m^3
C_p	specific heat at constant pressure, $kJ/kg{\cdot}°C$
C_{pa}	apparent specific heat, $kJ/kg{\cdot}°C$
$CEM43$	Cumulative number of equivalent minutes at 43°C
D	diffusivity, as a general reference
D_{AB}	diffusivity of species A in species B, m^2/s
$\vec{E}$	electric field vector
E_a	activation energy, J/mole
f	force per unit volume, N/m^3
f	fraction of ice in an ice-water system
F	energy flux, W/m^2
F	force, N
Fo	$= \alpha t/L^2$, Fourier number, dimensionless
g	gravity, m/s^2
h	convective heat transfer coefficient, $W/m^2{\cdot}°C$
h_r	radiative heat transfer coefficient, $W/m^2{\cdot}°C$
h	Planck's constant, 6.625×10^{-34} J·s
h_m	convective mass transfer coefficient, m/s
H	enthalpy per unit mass, kJ/kg
H	Henry's law constant, atm/mole fraction

$\vec{H}$	magnetic field vector
I	intensity or energy flux, W/m^2
I_0	incident energy flux, W/m^2
k	thermal conductivity, $W/m \cdot °C$
k_a	absorption coefficient
k''	reaction rate constant
K	partition coefficient, units vary
L	half-thickness of a slab or characteristic length, m
m	consistency coefficient; also mass fraction
m	mass, kg
M	molecular weight, kg
M	metabolic rate, W
$\dot{m}$	mass flow rate, kg/s
n	flow behavior index, dimensionless
n	order of reaction, dimensionless
$n_{A,z}$	mass flux of species A in the z direction, $kg/m^2 \cdot s$
Nu	Nusselt number, dimensionless
p_A	partial pressure of component A, N/m^2 or Pa
P	total pressure, N/m^2 or Pa
P^*	non-dimensional pressure
P	power, W/m^2
Pe	$= \mathrm{Re} \cdot \mathrm{Pr}$, Peclet number, dimensionless
Pr	$= \mu C_p/k$, Prandtl number, dimensionless
q_x	heat flow in the x-direction, W
q''_x	heat flux in the x-direction, W/m^2
Q	volumetric heat generation, W/m^3
Q_m	metabolic heat generation per unit volume of tissue, W/m^3
Q^*	volumetric heat generation, non-dimensional
r	radial direction
r_A	rate of generation of A per unit volume, kg of $A/m^3 \cdot s$
R	universal gas constant = 8.315 $kJ/kmol \cdot K$
Ra	$= Gr \times Pr$, Rayleigh number, dimensionless
Ra_m	$= Gr_{AB} \times Sc$, mass transfer Rayleigh number, dimensionless
Re	$= \rho u_\infty L/\mu$, Reynolds number, dimensionless
Sc	$= \mu/\rho D_{AB}$, Schmidt number, dimensionless
Sh	$= h_m L/D_{AB}$, Sherwood number, dimensionless
t	time, s
T	temperature; stress
T_s	surface temperature
T_i	initial or inlet temperature

T_f	freezing point
T_R	reference temperature
T_∞	fluid or ambient temperature
u	velocity in the x-direction, m/s
u^*	dimensionless velocity in the x-direction, m/s
u_∞	free stream velocity in the x-direction, m/s
U	thermal energy per unit volume, $\mathrm{J/m^3}$
U	overall heat transfer coefficient, $\mathrm{W/m^2 \cdot {}^\circ C}$
U_m	overall mass transfer coefficient, m/s
X	source term in momentum equation, $\mathrm{m/s^2}$
v	velocity in y-direction, m/s
v_x, v_y, v_z	velocities in x, y and z-directions, respectively, m/s
$\dot{V}_b^v$	volumetric flow rate of blood per unit volume of tissue
V	volume, $\mathrm{m^3}$
w	moisture content, kg of water/kg of dry solids
x	x-coordinate, m
x_A	mole fraction of species A in liquid phase
y	y-coordinate, m
z	z-coordinate, m

Greek Letters

α	thermal diffusivity, $\mathrm{m^2/s}$
α	absorption coefficient (ultrasound)
β	coefficient of thermal expansion
β	non-linearity coefficient (ultrasound)
δ	penetration depth of microwaves
Δ	finite change
ϵ	emissivity, dimensionless
ϵ_0	permittivity of free space, $= 8.86 \times 10^{-12}$ F/m
ϵ'	relative dielectric constant, dimensionless
ϵ''_{eff}	relative dielectric loss, dimensionless
ϕ	electric potential, volts
κ	Boltzmann's constant, $1.380 \times 10^{-23}\mathrm{J/K}$
λ	latent heat, kJ/kg
λ_f	latent heat of fusion, kJ/kg
λ_{vap}	latent heat of vaporization, kJ/kg
λ	wavelength, m
λ_0	wavelength in free space, m

μ	viscosity, kg/m·s
μ_a	absorption coefficient, m^{-1}
μ_s	scattering coefficient, m^{-1}
ν	kinematic viscosity, m^2/s
ω	$= 2\pi f$, angular frequency (f is frequency, in Hz)
Ω	extent of injury in a thermal burn
ρ	density or mass concentration, kg/m^3
σ	Stefan–Boltzmann constant, 5.676×10^{-8} $W/m^2 \cdot K^4$
σ	electrical conductivity, Siemens
σ_{AB}	collision diameter, Å
$\Omega_{D,AB}$	dimensionless function, defined in Chapter 9
τ	stress, Pa
τ	thermal relaxation time
θ	non-dimensional temperature