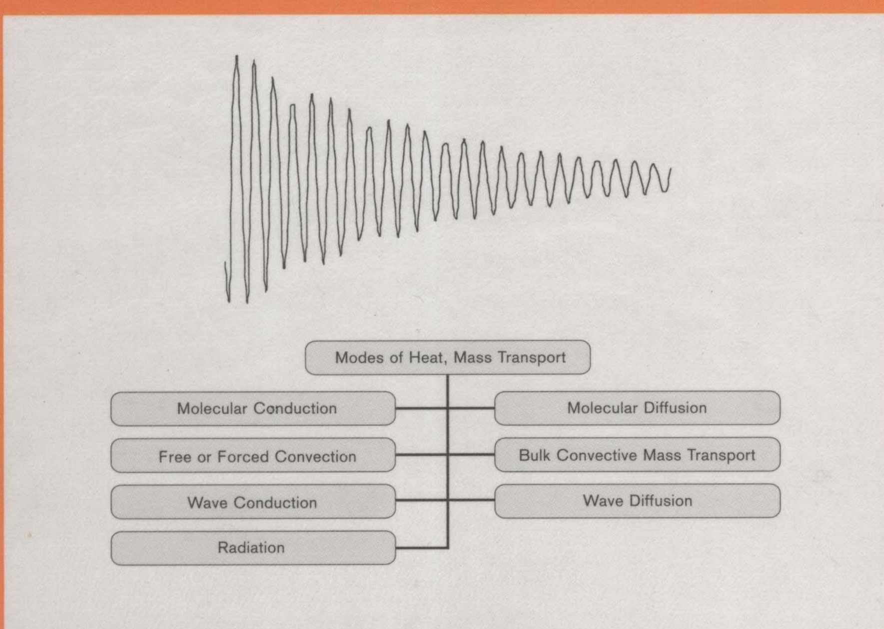
ELSEVIER

Damped Wave Transport and Relaxation

Kal Renganathan Sharma



Damped Wave Transport and Relaxation

Professor Kal Renganathan Sharma

School of Chemical and Biotechnology
Shanmugha Arts, Science, Technology & Research Academy
SASTRA Deemed University, Thanjavur, India

2005

ELSEVIER

Amsterdam – Boston – Heidelberg – London – New York – Oxford
Paris – San Diego – San Francisco – Singapore – Sydney – Tokyo

ELSEVIER B.V.
Radarweg 29
P.O. Box 211, 1000 AE Amsterdam
The Netherlands

ELSEVIER Inc.
525 B Street, Suite 1900
San Diego, CA 92101-4495
USA

ELSEVIER Ltd.
The Boulevard, Langford Lane
Kidlington, Oxford OX5 1GB
UK

ELSEVIER Ltd.
84 Theobalds Road
London WC1X 8RR
UK

First edition 2005

Library of Congress Cataloging in Publication Data
A catalog record is available from the Library of Congress.

British Library Cataloguing in Publication Data
A catalogue record is available from the British Library.

ISBN: 0 444 51943 2

♾ The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper).
Printed in The Netherlands.

Damped Wave Transport and Relaxation

Dedication

This book is dedicated to my son Chi. R. Hari Subrahmanyan Sharma (born August 13th 2001)

Preface

The mid 17th century saw the introduction of Newton's law of viscosity and the publication of his *Philosophiae Naturalis Principia Mathematica;*. in 1822 Fourier unveiled his theory, including his law of heat conduction; and in 1855 Fick proposed the first law of diffusion. Since then, numerous developments in fundamental physics have come about and a whole gamut of elucidations has become popular with many physicists and scientists, such as Einstein's theory of relativity with light having the highest velocity, the characterization of Brownian dynamics by Chandrashekar and von Kampen, and Schroedinger's wave equation to describe the movement of molecules in a box. Incorporating this understanding into the universal laws of engineering has, however, yet to happen.

Transient problems in transport phenomena have a variety of applications encompassing drug delivery systems for chemotherapy in bioengineering, heat transfer to surfaces in FBC, fluidized bed combustion boilers in mechanical engineering, simultaneous reaction and diffusion problems in the Zeigler-Natta gas phase, polymerization of polypropylene in chemical engineering, and polyacrylamide gel electrophoresis in bioinformatics. The attention given to transient problems in the leading textbooks currently in vogue represents only a small proportion of the broader heat, mass and momentum transfer discipline - often only 7% of the entire text, and not commensurate with their importance in industry. Often, the problems treated provide a Fourier series solution of a parabolic partial differential equation (PDE) and imply a certain weariness of the student.

In general, the Fourier series does not fully describe all the transient events of significance, for example: the short contact time singularity in heat flux in the widely used surface renewal theories, and the loss of universality when the heat transfer through a small film is considered. In one research problem, i.e., in the heat transfer in fluidized beds to immersed surfaces, for over 50 years, investigators have developed models for overprediction of the surface renewal theory to experiment at short contact times. New resistances were introduced, adding empiricism models that were otherwise derived from first principle models.

They seldom achieve a level of scrutiny higher than the continuum and empirical linear laws that describe forces with flows. Often, the premise of steady state is used. With increased computer resources, more fundamental phenomena can be accounted for and solved. The evaluation of the damped wave equation and the relaxation equation of heat, mass and momentum to represent transient events is one example of such an endeavor. The Euler equation and Navier-Stokes equations can be extended to include the relaxational transport term. At a molecular level, when the heat flux is defined as the energy leaving the surface minus the energy of the molecules entering the surface, it can be modified to include an accumulation of energy term. This may manifest only during transient problems where the accumulation of heat flux or temperature becomes important. In a similar fashion, the mass flux can be modified to include the accumulation of mass, and the shear stress or momentum flux can be modified to include the accumulation of momentum. The happenings in time are as important as those in space, especially in transient problems.

As discussed by Newton, when the apple falls from the tree, the net acceleration decreases to zero at the terminal settling velocity of the apple, due to the changing drag force as a function of velocity. As the velocity increases from zero at rest, the drag force increases proportional to the velocity, changing the resultant force from the difference of gravity and the Archimedes buoyancy force to the resultant gravity minus buoyancy minus drag force. So the rate of acceleration, which can be calculated as the ratio of the resultant force to the mass of the apple, is a pronounced phenomenon during transient events in fluid flow, heat transfer and mass transfer, which is not incorporated in the current theoretical depiction of transient events in the industry.

The myth of a Clausius inequality violation clouded early attempts in the literature to account for the accumulation effects using the equation that came originally from Maxwell and during the mid 20th century from Cattaneo and Vernotte in France. The mere introduction of three terms in the governing equation can lead to the "theoretical possibility" of temperature gradient and heat flux being of the same sign and thus effecting a heat flow from low to high temperature. The second law of thermodynamics is not violated by transient phenomena. Sometimes an improper perspective of the interpretation of model solutions leads to the impression of an inherent flaw in the wave equation with a damping term. At steady state, using Fourier's law and a temperature-dependent heat source, negative temperatures can arise in the solution which need to be interpreted as zero temperature and not a violation of the third law of thermodynamics.

Our primary goal is to encourage the depiction of transient phenomena with a higher level of scrutiny than Fourier's, Fick's and Newton's laws and to seek a connection with molecular phenomena. A case in point is the use of damped wave transport and relaxation equations of heat, mass and momentum. The solution methodologies used to obtain meaningful solutions are: relativistic transformation of coordinates, method of separation of variables, Laplace transforms, and method of complex temperatures. Bounded solutions without any violation of the second law of thermodynamics can be seen. Physical insight is sometimes preferred to mathematical rigor.

The conditions under which subcritical damped oscillations can be found are derived for a finite slab, a cylinder and a sphere and the results depicted in figures. For the evaluation of wave equation effects, the damping term is first removed from the hyperbolic PDE. The solution exhibits symmetry in space and sometimes in time. A zone of zero transfer can be detected in a Zeigler-Natta catalyst during simultaneous reaction and diffusion. The storage coefficient is defined to evaluate the relative contributions of thermal mass and thermal relaxation. New dimensionless groups have been introduced, such as the momentum number, accumulation number, oscillation number, modified Peclet number, heat, mass and momentum, modified Biot number, Fourier modulus, Fick modulus, permeability number, storage number, dimensionless pressure, temperature, concentration, force, stress, heat flux, mass flux and velocity, penetration length, penetration time, velocity of heat, velocity of mass and the velocity of momentum. The thermal lag time associated with realizing a heat disturbance in the interior of a slab, the exterior of a cylinder and a sphere is calculated and expressions provided.

Bessel equations are used extensively in the text and a summary of the relations used, including the generalized Bessel equation, is given as Appendix A. The commonly found inversions of Laplace transforms are available as Appendix B and the reader is referred to numerical inversions of Laplace transforms for expressions not found in Appendix B. Appendix C contains the extended Navier-Stokes equation of motion with the accumulation term included. Experimental evidence for the relaxation time in heat transfer has fallen in the range of a few seconds in the case of dispersed biological materials. This is much higher than the few nanoseconds projected by early investigators of the phenomenon. Chapter 1 provides an introduction to the damped wave transport and relaxation equation. Heat, mass and momentum transfer problems are dealt with separately in Chapters, 2, 3, and 4.

Case studies and applications are discussed in Chapter 5.

Acknowledgements

In early 1987, after the funeral of my paternal grandmother Sankari patti, I met Richard Turton, the last Ph.D student of Emeritus Professor Octave Levenspiel, who introduced me to the problem of overprediction of theory to experiment in fluidized bed to surface heat transfer. I revisited the problem of the incomplete description by Fourier to represent transient heat transfer, with some encouragement from R. Sethuraman (Vice Chancellor of SASTRA Deemed University, Thanjavur), S. Swaminathan (Dean, Students), S. Vaidya Subramaniam (Dean Planning and Development), K.N. Somasekharan (Dean, School of Chemical and Biotechnology).

Special mention is made of Victoria Franchetti Haynes Ph.D, director at Monsanto Plastics. My thoughts and prayers go to Najma Dalal MD. My maternal grandmother, Bagyalakshmi patti, will always remain in my memory. Many thanks to my parents, Sri. S. Kalyanaraman and Mrs. Shyamala Kalyanaraman, for their unfailing support and to Dr. Vidya Krishnan.

Funds for overseas travel to international conferences obtained from several sources are acknowledged, with special mention made of John W. Zondlo, West Virginia University, Morgantown, WV, USA (for travel to Maastricht, the Netherlands to present a paper at the 1987 Conference on Coal Science) and T. R. Rajagopalan Research Cell, SASTRA Deemed University, Thanjavur, India. Funds were received from Nason Pritchard to travel to the World Congress in Chemical Engineering at San Diego, CA in 1996 with some encouragement by Nithiam T. Sivaneri, Associate Chair of Mechanical & Aerospace Engineering at West Virginia University, Morgantown, WV. I was sent to Germany and Italy in 1995 to discuss the construction of the microgravity transport cell from Clarkson University, Pottsdam, NY, USA. Special thanks to Prof. Edward Wegmann and the faculty at the Physics Department at George Mason University for seeing me through 62 conference presentations in 1999, including 17 at the Dallas AIChE meeting. The encouragement of R. Srinivasan and Dr. V. S. Balameenakshi enabled me to present nearly 100 papers at 20 meetings between 1996 and 2000.

Special thanks are due to: Sri. Rangarajan, Chairman and Correspondent, Vel Institutions, Avadi, Chennai; V. Punnusami, the intranet system administrator at the computer laboratory in Vignana Vihar; and Elsevier for working with me on the proofs during the preparation of the manuscript. The blessings of his Holiness Sri. Jayendra Saraswati swamigal and His Holiness Pujyasri Sankara Vijayendra Saraswati swamigal of the Kancheepuram Sankara Mutt through the years are deeply valued.

About the Author

Kal Renganathan Sharma has received three degrees in chemical engineering: a B.Tech from the Indian Institute of Technology, Madras, India, MS and Ph.D from West Virginia University Morgantown, WV, USA. He received unsurpassed marks in mathematics in the X std CBSE examination in 1979. He has held a professional engineer's license from the state of New Hampshire since 1995. His post-doctoral training was with: Monsanto Plastics, R. Shankar Subramanian, former chair and professor at Clarkson University, Potsdam, NY; and Ramanna Reddy, Professor and Director, Concurrent Engineering and Research Center, West Virginia University, Morgantown, WV. He has authored 370 conference papers, eight journal articles, and 54 preprints on the Chemical Preprint Server. This is his third book. Positions he has held include: Adjunct Assistant Professor, Mechanical & Aerospace Engineering, West Virginia University, Morgantown, WV; Visiting Research Assistant Professor, George Mason University, Fairfax, VA; President & Chief Technical Officer, Independent Institute of Technology, Hanover, NH; Principal, Sakthi Engineering College, Chennai; Professor & HOD, Computer Science and then Chemical, Vellore Engineering College, Vellore. Honors received include the Guruvayurappan Award for the most number of papers, "Who's Who" in Science and Engineering, 2004-2005, New York Academy of Sciences, Phi Kappa Phi, Sigma Xi. He is currently a Professor at SASTRA Deemed University, Thanjavur, TN, India.

Table of Contents

1.0 The Damped Wave Conduction and Relaxation Equation

Nomenclature

a	half-width of slab (m)
A	cross-sectional area of the slab (m^2)
C_p	heat capacity (J/kg/K)
d	diameter of molecule (m)
D_{AB}	binary diffusivity (m^2/s)
E	energy coefficient (J/m^2/K)
E'	energy coefficient (J/m/K)
F_j	jth force
G	phonon electron coupling factor
h	heat transfer coefficient (W/m^2/K)
J_k	kth flow
k	thermal conductivity (W/m/K)
L_{kj}	phenomenological coefficients
l	penetration length (m)
m	mass of molecule (kg)
n'	number of molecules per unit volume
P	arbitrary distribution
P_b	ballistic part
P_m	diffusive part
q	heat flux (W/m^2)
t	time (s)
T	temperature (K)
t*	characteristic time
<u>	mean molecular speed (m/s)
u	dimensionless temperature for finite medium $(T - T_s)/(T_0 - T_s)$
u'	dimensionless temperature for semi-infinite medium $(T - T_0)/(T_s - T)$
u"	dimensionless temperature at zero initial temperature (T/T_s)
U_y	fluid velocity in the y direction (m/s)
v_h	velocity of heat sqrt(α/τ_r)
x	space (m)

Greek

α	thermal diffusivity (m^2/s)
β	characteristic length on the microscale, (m) ($\beta = E/\rho C_p$)
κ	Boltzmann constant
μ	viscosity (kg/ms)
ρ	density (kg/m^3)
τ	dimensionless time (t/τ_r)
τ_r	relaxation time (s), heat
τ_{mom}	relaxation time (s), momentum