*Modeling and Simulation in Science, Engineering and Technology*

# Multicomponent Flow Modeling

*Vincent Giovangigli*

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Birkhäuser
Boston • Basel • Berlin

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**Library of Congress Cataloging-in-Publication Data**
Giovangigli, Vincent, 1957–
Multicomponent flow modeling / Vincent Giovangigli.
p. cm.—(Modeling and simulation in science, engineering and technology)
Includes bibliographical references and index.
ISBN 0-8176-4048-7
1. Multiphase flow—Mathematical models. I. Title. II. Series: Modeling and simulation in science, engineering & technology.
QA922.G56 1999
532′.051—dc21

99-27050
CIP

AMS Subject Classifications: 76A, 80A, 82B, 35B, 35Q

Printed on acid-free paper.


*Birkhäuser*



ISBN 0-8176-4048-7
ISBN 3-7643-4048-7 SPIN 19901762

Typeset by the author in TEX.
Printed and bound by Maple-Vail Book Manufacturing Group, York, PA.
Printed in the United States of America.

9 8 7 6 5 4 3 2 1

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# Preface

The goal of this is book to give a detailed presentation of multicomponent flow models and to investigate the mathematical structure and properties of the resulting system of partial differential equations. These developments are also illustrated by simulating numerically a typical laminar flame. Our aim in the chapters is to treat the general situation of multicomponent flows, taking into account complex chemistry and detailed transport phenomena.

In this book, we have adopted an interdisciplinary approach that encompasses a physical, mathematical, and numerical point of view. In particular, the links between molecular models, macroscopic models, mathematical structure, and mathematical properties are emphasized. We also often mention flame models since combustion is an excellent prototype of multicomponent flow.

This book still does not pretend to be a complete survey of existing models and related mathematical results. In particular, many subjects like multiphase–flows, turbulence modeling, specific applications, porous media, biological models, or magneto–hydrodynamics are not covered. We rather emphasize the fundamental modeling of multicomponent gaseous flows and the qualitative properties of the resulting systems of partial differential equations.

Part of this book was taught at the post-graduate level at the University of Paris, the University of Versailles, and at École Polytechnique in 1998–1999 to students of applied mathematics.

The author wishes to thank many of his colleagues for stimulating discussions, especially to Professor Alexandre Ern of École Nationale des Ponts et Chaussées, Doctor Marc Massot of Laboratoire d'Analyse Numérique de l'Université de Lyon, and Professor Mitchell D. Smooke of Yale University

Mechanical Engineering Department.

The author wishes to thank the series editor, Professor Nicola Bellomo, for his encouragement and interest, the executive editor Wayne Yuhasz, and the senior production editor Louise Farkas for their precious help in editing the book.

I also wish to thank my wife Professor Hélène Dumontet of Université de Cergy, and my children Laure, Antoine, and Marine for their love and support.

Paris, France
July 1999

Vincent Giovangigli

# Contents

# 1

# Introduction

Multicomponent reactive flows arise in various engineering applications, such as combustion, crystal growth, atmospheric reentry, or chemical reactors. Modeling pollutant formation, chemical vapor deposition reactors, laminar flame extinction limits, or gas dissociation behind bow shocks around space vehicles, for instance, requires us to take into account complex chemistry mechanisms and detailed transport phenomena. There is, thus, a strong motivation for investigating the equations governing multicomponent flows and analyzing their mathematical structure and properties. The present book is an attempt to fill this need.

In Chapters 2 to 5 we first give a detailed presentation of multicomponent flow models, and, in Chapters 6 to 11, we then analyze some of their mathematical structures and properties. These developments are also illustrated by simulating numerically a typical laminar flame in Chapter 12. Our aim, in these chapters, will always be to take into account multicomponent aspects, such as complex chemistry and detailed transport.

In Chapter 2 we give a detailed presentation of the governing equations for multicomponent reactive flows, as obtained from the kinetic theory of gases. We present the fundamental conservation equations for mass, momentum, and energy and discuss various alternative formulations. We investigate thermodynamic properties, chemical production rates, as well as transport fluxes and several possible extensions of the model. We also present the entropy governing equation, which will play a fundamental role.

In Chapter 3 we discuss various ideas that can be used to simplify the general equations in special situations. These simplifications can be in the chemistry aspects, fluid aspects, or coupling between them. This chapter is devoted to filling the gap between the complete equations presented in the previous chapter and the simplified models often used in the literature. We specifically discuss the simplifications associated with one-reaction chemistry flows, small Mach number flows, strained flows, and the uncouplings resulting from the dilution limit and the incompressible limit.