ELSEVIER

Modeling and Simulation of Reactive Flows

A.L. De Bortoli
G.S.L. Andreis
F.N. Pereira

Modeling and Simulation of Reactive Flows

Álvaro L. De Bortoli
Greice S. L. Andreis
Felipe N. Pereira

ELSEVIER

AMSTERDAM • BOSTON • HEIDELBERG • LONDON • NEW YORK • OXFORD
PARIS • SAN DIEGO • SAN FRANCISCO • SINGAPORE • SYDNEY • TOKYO

Elsevier
Radarweg 29, PO Box 211, 1000 AE Amsterdam, Netherlands
The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, UK
225 Wyman Street, Waltham, MA 02451, USA

Notices
Knowledge and best practice in this field are constantly changing. As new research and experience broaden our understanding, changes in research methods, professional practices, or medical treatment may become necessary.

Practitioners and researchers must always rely on their own experience and knowledge in evaluating and using any information, methods, compounds, or experiments described herein. In using such information or methods they should be mindful of their own safety and the safety of others, including parties for whom they have a professional responsibility.

To the fullest extent of the law, neither the Publisher nor the authors, contributors, or editors, assume any liability for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions, or ideas contained in the material herein.

Library of Congress Cataloging-in-Publication Data
A catalog record for this book is available from the Library of Congress

British Library Cataloguing-in-Publication Data
A catalogue record for this book is available from the British Library

ISBN: 978-0-12-802974-9

For information on all Elsevier publications
visit our website at http://store.elsevier.com/

Typeset by SPi Global, India

Printed and bound in the USA

Acquisition Editor: Lisa Reading
Editorial Project Manager: Natasha Welford
Production Project Manager: Lisa Jones
Designer: Victoria Pearson

Modeling and Simulation of Reactive Flows

Preface

Numerical methods have evolved in recent decades, more intensely from the 1980s. However, this development cannot be compared with the development that occurred with computers. Virtually every 3 years, a new computer becomes obsolete.

While the solution of incompressible flows has been more frequent, both numerically and analytically, the compressible flow solution is usually obtained through numerical methods. The compressibility adds nonlinearities to the system equations, which makes it hard to obtain analytical solutions. In this context, the solution of reactive streams becomes even more complex.

Reactive flows are complex, both at low or high temperature, because the formulation typically adds to the Navier-Stokes equations a significant number of nonlinear equations due to reactions.

The combustion of hydrogen, for example, includes about 20 elementary chemical reactions and 8 species. So, eight equations, one for each species, would be added to the equations of nonreactive flow. Even for such a simple mechanism, the numerical solution is complex.

For methane combustion, one has about 300 elementary reactions among some tens of chemical species. Biofuels such as methanol and ethanol involve a similar number of elementary reactions as for methane. Complex fuels such as n-heptane and iso-octane involve hundreds of chemical species and thousands of elementary chemical reactions. For diesel and biodiesel there are thousands of chemical species and tens of thousands of elementary reactions.

Reactions that occur in aqueous media involve numerous minerals in the subsoil, about 4000, and tens of solutes. Of these, about 30 minerals and 15 solutes are the most important. Because the reactions in aqueous media are much faster than those occurring with the minerals, aqueous reactions are considered to be in equilibrium (occurring faster) in the subsoil.

Simplifications of chemical kinetics generally become an alternative. Small mechanisms of a low number of species are often reduced using the assumptions of steady-state and partial equilibrium. Large mechanisms are reduced using a combination of techniques such as direct relation graph (DRG), to obtain a skeleton mechanism and techniques based on the sensitivity analysis of the eigenvalues and eigenvectors of the Jacobian matrix of the chemical system to obtain a reduced mechanism.

Thus, reactive flow is complex and compounded by the set of equations of flow and chemical kinetics, which are solved by numerical methods frequently of semi-implicit type.

This book contains seven chapters and two appendices that were organized sequentially. However, readers, based on their experience, can read each chapter independently.

Chapter 1 deals with the chemical equilibrium, both in aqueous solution and in gaseous phase. Chapter 2 discusses chemical kinetics, starting with a description of the reaction rates. Based on steady-state assumptions and partial equilibrium, some reduced kinetic mechanisms are obtained. In the next chapter are deducted equations for reactive flows based on the balance (conservation) of the properties in the control volume. In Chapter 4, a formulation for mixing fluids and the turbulence models based on characteristics of the flow scales are discussed. The Reynolds and Favre averages are discussed. In Chapter 5, models for reactive flows are presented. Initially, techniques for obtaining reduced kinetic mechanisms, such as DRG, sensitivity analysis, ILDM, REDIM, and flamelet are presented. Then models for premixed flames, diffusion flames, and reactive flows in porous media are shown. In Chapter 6, some of principal methods used for the solution of reactive and nonreactive flows are introduced. Also noteworthy are obtaining the generalized coordinates and the application of the boundary conditions. The formulation at low Mach, very useful in the solution of reactive flows, and some techniques for the acceleration of convergence are presented. Finally, Chapter 7 discusses some solutions to diffusion flames, the flow in porous media and the premixed combustion in porous media.

During the preparation of this book, we tried to use relatively simple ways to model complex situations. Understanding the essence of a physical situation may lead researchers to improve the technique, which then will take them to a more detailed analysis.

The topics are described in a basic and objective way. Among the many existing techniques, those that are more direct and frequently used are discussed. In summary, this book aims to share with the readers some experiences gained by the authors in the solution of reactive flows. It is hoped that the readers, relatively quickly, can gain knowledge that can assist them in the modeling and simulation of reactive flows of technical interest.

Acknowledgments

This book refers to research being developed in the group Modeling and Simulation in Reactive Fluid Dynamics at UFRGS-Brazil, coordinated by Prof. Alvaro Luiz de Bortoli. Prof. De Bortoli is grateful to the collaborators from Brazil and other countries, and gratefully acknowledges the sponsor CNPq, National Counsel of Technological and Scientific Development, under the process 304798/2012-6. He also gratefully acknowledges the sponsor of CAPES, Coordination for the Improvement of Higher Education Personnel, under the process 007515/2011-70.

List of Symbols

a_i	Activity of a species
A	Area
B_j	Sensitivity matrix
c_D	Constant of Prandtl model
c_P	Specific heat at constant pressure
C_s	Smagorinsky constant
C	Concentration, Chapman-Rubesin parameter
d, D	Material derivative
D_i	Mass diffusivity, thermal diffusivity
$\mathrm{d}x$	Infinitesimal element in x-direction
$\mathrm{d}y$	Infinitesimal element in y-direction
$\mathrm{d}z$	Infinitesimal element in z-direction
$\mathrm{d}V$	Control volume
e	Specific energy
e^-	Electron
e_{int}	Internal energy
E	Energy, error
Ea	Activation energy
Eh	Electric potential
Eo(V)	Reduction potential
f_i	Surface force
f, F	Functions
F	Faraday's constant
$\vec{F}$	Vector force
$\vec{g}, g_i$	Gravitational acceleration
G	Gibbs free energy, flame front position
h	Specific enthalpy, time-step
H	Enthalpy
I	Ionic strength, identity matrix
I_{AB}	Index of importance
j_i	Diffusive flux
$\dot{m}_i$	Mass flow
n	Number of moles, number of species, exponent of temperature
$\vec{n}$	Normal vector
N	Number of nodes, number of time-steps

$O()$	Order of ()
p	Pressure
pe	Electrochemical potential
pH	Potential of hydrogen
P	Product, probability
$\dot{q}_j$	Heat flow by conduction
$\dot{q}_v$	Volumetric source of heat (internal, chemical)
q_r	Heat transfer due to radiation
Q	Heat of combustion
Q_e	Activity product
$\dot{Q}$	Potential energy
r	Radius
R	Gas constant
$\vec{R}$	Residuum vector
$\vec{S}$	Surface vector
$\vec{S}_i$	Source term
s_L	Laminar flame velocity
s_T	Turbulent flame velocity
S	Entropy, area, stiffness measure
t	Time
T	Temperature, period of time
U_c	Axial velocity
$v_j, \vec{v}$	Velocity vector
(v_x, v_y, v_z)	Velocity vector
V	Volume
$x_j, (x, y, z)$	Cartesian coordinate system
X_i	Molar fraction of a species
y_0	Distance from the wall
Y_i	Mass fraction
w	Vorticity, velocity component in z-direction
$\dot{w}$	Reaction rate
$\vec{W}$	Vector of flow variables
$\dot{W}$	Rate of work crossing the boundaries
W_i	Molecular weight
z_i	Ionic charge of a species
Z	Mixture fraction

SPECIAL SYMBOLS

α	Thermal diffusivity, angle, coefficient
β	Coefficient of thermal expansion, coefficient
$\delta_{i,j}$	Kronecker delta
Δ	Variation, Laplacian, filter size

ϵ	Viscous dissipation, error
η	Kolmogorov length, similarity variable, generalized coordinate
γ	Parameter
γ_i	Activity coefficient
Γ_i	Gamma function
κ	Thermal conductivity, von Kárman constant
λ	Eigenvalue
Λ	Matrix of eigenvalues
μ	Chemical potential, dynamic viscosity, mean
ν', ν_i	Stoichiometric coefficient
ν_T	Turbulent viscosity
ξ	Radio by length relation, generalized coordinate
ρ	Density
σ	Standard deviation
$\sigma_{i,j}$	Stress tensor
τ	Time, tortuosity
$\tau_{i,j}$	Viscous stress tensor
τ_w	Wall shear stress
ϕ, Φ	Variable
Φ	Viscous dissipation
χ	Scalar dissipation rate
ψ	Variable
Ω	Element of volume
∂	Partial derivative
$\vec{\nabla}$	Gradient operator
$\vec{\nabla}.$	Divergence operator
$\vec{\nabla}\times$	Curl operator

SUBSCRIPTS AND SUPERSCRIPTS

SUBSCRIPTS

b	Burned
c	Chemical
cl	Center line
d	Droplet
D	Diffusivity
f	Fluid
F	Fuel
i, j, k	Species, coordinate directions
ig	Ignition
int	Internal

m	Constant
n	Normal, constant
N	Numerical solution
O_2	Oxidizer
r	Radius
ref	Reference
s	Surface
st	Stoichiometric
t, T	Turbulent, true solution
u	Unburned
η	Refers to Kolmogorov
μ	Constant
τ	Refers to friction
0	Reference
$1, 2, \infty$	Refers to free condition

SUPERSCRIPTS

$k, k+1$	Refers to time-step
$n, n+1$	Refers to time-step
i, j, k	Refers to direction
0	Initial
$+, -, ++, \dots$	Ions charge

List of Abbreviations

BM	Mass transfer number
CM	Conservation of momentum
CV	Control volume
CFL	Courant-Friedrich-Lewy
CHEM	Chemical number
Da	Damköhler number
erf	Error function
Ec	Eckert number
DFS	Depth first search
DNS	Direct numerical simulation
DRG	Direct relation graph
FO	Fourier number
GCI	Grid convergence index
IAP	Ion activity product
ILDM	Intrinsic low dimensional manifold
Ka	Karlovitz number
Le	Lewis number
LES	Large eddy simulation
NOX	Number of oxidation
Nu	Nusselt number
PDF	Probability density function
Pr	Prandtl number
RANS	Reynolds averaged Navier-Stokes
Re	Reynolds number
REDIM	Reaction diffusion manifolds
Sc	Schmidt number
Sh	Sherwood number
SI	Saturation index

Contents