



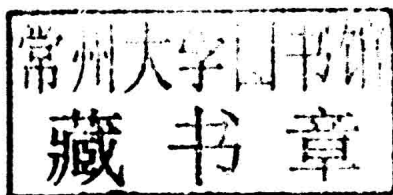
# Modeling and Simulation of Reactive Flows

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# 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

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# 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
$dx$	Infinitesimal element in $x$ -direction
$dy$	Infinitesimal element in $y$ -direction
$dz$	Infinitesimal element in $z$ -direction
$dV$	Control volume
$e$	Specific energy
$e^-$	Electron
$e_{\text{int}}$	Internal energy
$E$	Energy, error
$E_a$	Activation energy
$E_h$	Electric potential
$E_o(V)$	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

$\alpha$	Thermal diffusivity, angle, coefficient
$\beta$	Coefficient of thermal expansion, coefficient
$\delta_{i,j}$	Kronecker delta
$\Delta$	Variation, Laplacian, filter size

$\epsilon$	Viscous dissipation, error
$\eta$	Kolmogorov length, similarity variable, generalized coordinate
$\gamma$	Parameter
$\gamma_i$	Activity coefficient
$\Gamma_i$	Gamma function
$\kappa$	Thermal conductivity, von Kármán constant
$\lambda$	Eigenvalue
$\Lambda$	Matrix of eigenvalues
$\mu$	Chemical potential, dynamic viscosity, mean
$\nu', \nu_i$	Stoichiometric coefficient
$\nu_T$	Turbulent viscosity
$\xi$	Ratio by length relation, generalized coordinate
$\rho$	Density
$\sigma$	Standard deviation
$\sigma_{ij}$	Stress tensor
$\tau$	Time, tortuosity
$\tau_{ij}$	Viscous stress tensor
$\tau_w$	Wall shear stress
$\phi, \Phi$	Variable
$\Phi$	Viscous dissipation
$\chi$	Scalar dissipation rate
$\psi$	Variable
$\Omega$	Element of volume
$\partial$	Partial derivative
$\vec{\nabla}$	Gradient operator
$\vec{\nabla} \cdot$	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
$\eta$	Refers to Kolmogorov
$\mu$	Constant
$\tau$	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
+, -, ++, ...	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



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