COMBUSTION THERMODYNAMICS AND DYNAMICS

Combustion Thermodynamics and Dynamics builds on a foundation of thermal science, chemistry, and applied mathematics that will be familiar to most undergraduate aerospace, mechanical, and chemical engineers to give a first-year graduate level exposition of the thermodynamics, physical chemistry, and dynamics of advection-reaction-diffusion. Special effort is made to link notions of time-independent classical thermodynamics with time-dependent reactive fluid dynamics. In particular, concepts of classical thermochemical equilibrium and stability are discussed in the context of modern nonlinear dynamical systems theory. The first half emphasizes time-dependent spatially homogeneous reaction, while the second half considers effects of spatially inhomogeneous advection and diffusion on the reaction dynamics. Attention is focused on systems with realistic detailed chemical kinetics as well as simplified kinetics. Many mathematical details are presented, and several quantitative examples given. Topics include foundations of thermochemistry, reduced kinetics, reactive Navier-Stokes equations, reaction-diffusion systems, laminar flame, oscillatory combustion, and detonation.

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Contents

Preface

Part I Reactive Systems

1 Introduction to Chemical Kinetics
   1.1 A Gas Phase Kinetic Model
   1.2 Isothermal, Isochoric Kinetics
      1.2.1 O-O_2 Dissociation
      1.2.2 Zel'dovich Mechanism of NO Production
   1.3 Adiabatic, Isochoric Kinetics
      1.3.1 Thermal Explosion Theory
      1.3.2 Detailed H_2-Air Kinetics

Exercises
References

2 Gas Mixtures
   2.1 Some General Issues
   2.2 Ideal and Nonideal Mixtures
   2.3 Ideal Mixtures of Ideal Gases
      2.3.1 Dalton Model
      2.3.2 Thermodynamics of the Dalton Model
      2.3.3 Summary of Properties of the Dalton Mixture Model

Exercises
References

3 Mathematical Foundations of Thermodynamics
   3.1 Exact Differentials and State Properties
   3.2 Two Independent Variables
   3.3 Legendre Transformations
   3.4 Heat Capacity
   3.5 Mixtures with Variable Composition
   3.6 Partial Molar Properties
      3.6.1 Homogeneous Functions

Exercises
References
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6.2 Gibbs Free Energy</td>
<td>102</td>
</tr>
<tr>
<td>3.6.3 Other Properties</td>
<td>103</td>
</tr>
<tr>
<td>3.6.4 Relation between Mixture and Partial Molar Properties</td>
<td>105</td>
</tr>
<tr>
<td>3.7 Frozen Sound Speed</td>
<td>106</td>
</tr>
<tr>
<td>3.8 Irreversible Entropy Production</td>
<td>108</td>
</tr>
<tr>
<td>3.9 Equilibrium in a Two-Component System</td>
<td>111</td>
</tr>
<tr>
<td>3.9.1 Phase Equilibrium</td>
<td>111</td>
</tr>
<tr>
<td>3.9.2 Chemical Equilibrium: Introduction</td>
<td>113</td>
</tr>
<tr>
<td>Exercises</td>
<td>122</td>
</tr>
<tr>
<td>References</td>
<td>122</td>
</tr>
<tr>
<td>4 Thermochemistry of a Single Reaction</td>
<td>124</td>
</tr>
<tr>
<td>4.1 Molecular Mass</td>
<td>124</td>
</tr>
<tr>
<td>4.2 Stoichiometry</td>
<td>126</td>
</tr>
<tr>
<td>4.2.1 General Development</td>
<td>126</td>
</tr>
<tr>
<td>4.2.2 Fuel-Air Mixtures</td>
<td>133</td>
</tr>
<tr>
<td>4.3 First Law Analysis of Reacting Systems</td>
<td>135</td>
</tr>
<tr>
<td>4.3.1 Enthalpy of Formation</td>
<td>135</td>
</tr>
<tr>
<td>4.3.2 Enthalpy and Internal Energy of Combustion</td>
<td>138</td>
</tr>
<tr>
<td>4.3.3 Adiabatic Flame Temperature</td>
<td>138</td>
</tr>
<tr>
<td>4.4 Chemical Equilibrium</td>
<td>144</td>
</tr>
<tr>
<td>4.5 Chemical Kinetics of a Single Isothermal Reaction</td>
<td>148</td>
</tr>
<tr>
<td>4.5.1 Isochoric Systems</td>
<td>149</td>
</tr>
<tr>
<td>4.5.2 Isobaric Systems</td>
<td>156</td>
</tr>
<tr>
<td>4.6 Some Conservation and Evolution Equations</td>
<td>160</td>
</tr>
<tr>
<td>4.6.1 Total Mass Conservation: Isochoric Reaction</td>
<td>160</td>
</tr>
<tr>
<td>4.6.2 Element Mass Conservation: Isochoric Reaction</td>
<td>161</td>
</tr>
<tr>
<td>4.6.3 Energy Conservation: Adiabatic, Isochoric Reaction</td>
<td>162</td>
</tr>
<tr>
<td>4.6.4 Energy Conservation: Adiabatic, Isobaric Reaction</td>
<td>163</td>
</tr>
<tr>
<td>4.6.5 Irreversible Entropy Production: Clausius-Duhem Inequality</td>
<td>166</td>
</tr>
<tr>
<td>4.7 Simple One-Step Kinetics</td>
<td>169</td>
</tr>
<tr>
<td>Exercises</td>
<td>171</td>
</tr>
<tr>
<td>References</td>
<td>172</td>
</tr>
<tr>
<td>5 Thermochemistry of Multiple Reactions</td>
<td>174</td>
</tr>
<tr>
<td>5.1 Summary of Multiple Reaction Extensions</td>
<td>174</td>
</tr>
<tr>
<td>5.2 Equilibrium Conditions</td>
<td>181</td>
</tr>
<tr>
<td>5.2.1 Minimization of $G$ via Lagrange Multipliers</td>
<td>181</td>
</tr>
<tr>
<td>5.2.2 Equilibration of All Reactions</td>
<td>187</td>
</tr>
<tr>
<td>5.2.3 Zel’dovich’s Uniqueness Proof</td>
<td>188</td>
</tr>
<tr>
<td>5.3 Simple Three-Step Kinetics</td>
<td>203</td>
</tr>
<tr>
<td>5.3.1 Reversible Kinetics</td>
<td>203</td>
</tr>
<tr>
<td>5.3.2 Irreversible Kinetics</td>
<td>206</td>
</tr>
<tr>
<td>5.4 Concise Reaction Rate Law Formulations</td>
<td>209</td>
</tr>
<tr>
<td>5.4.1 Reactions Dominant over Species</td>
<td>209</td>
</tr>
<tr>
<td>5.4.2 Species Dominant over Reactions</td>
<td>210</td>
</tr>
<tr>
<td>5.4.3 Linear Mapping Features</td>
<td>211</td>
</tr>
</tbody>
</table>
5.5 Irreversible Entropy Production 213
  5.5.1 Onsager Reciprocity 213
  5.5.2 Eigenvalues at Equilibrium 222
  5.5.3 Zel’dovich Mechanism Example 226
  5.5.4 Extended Zel’dovich Mechanism Example 231
  5.5.5 On Potentials, Entropy, and Dynamics 234
Exercises 236
References 236

6 Nonlinear Dynamics of Reduced Kinetics .......................... 239
  6.1 Mathematical Background 242
    6.1.1 Nonlinear Problem 242
    6.1.2 Local Linear Analysis 244
    6.1.3 Diagnostics in the Normal Plane 247
    6.1.4 Algorithmic Diagnostic Procedure 249
  6.2 Reduction of Model Systems 250
    6.2.1 Two-Dimensional Phase Space 250
    6.2.2 Three-Dimensional Phase Space 255
  6.3 Reduction of Combustion Systems 259
    6.3.1 Zel’dovich Mechanism 259
    6.3.2 H₂-Air Combustion 263
  6.4 Diffusion Effects 270
    6.4.1 Galerkin Procedure 270
    6.4.2 Linear Example 274
Exercises 277
References 277

Part II Advective-Reactive-Diffusive Systems

7 Reactive Navier-Stokes Equations ................................. 281
  7.1 Evolution Axioms 281
    7.1.1 Conservative Form 281
    7.1.2 Nonconservative Form 285
  7.2 Mixture Rules 287
  7.3 Constitutive Models 287
  7.4 Temperature Evolution 290
  7.5 Shvab-Zel’dovich Formulation 292
Exercises 294
References 295

8 Simple Linear Combustion ............................................ 297
  8.1 Single Reaction 297
    8.1.1 Spatially Homogeneous Solution 298
    8.1.2 Steady Solution 298
  8.2 Multiple Reactions 304
    8.2.1 Spatially Homogeneous Solution 304
    8.2.2 Steady Solution 306
8.2.3 Spatiotemporal Solution 309
8.3 H₂-Air Near Equilibrium 311
Exercises 312
References 312

9 Idealized Solid Combustion ................................. 314
  9.1 Simple Planar Model 314
    9.1.1 Model Equations 315
    9.1.2 Simple Planar Derivation 315
    9.1.3 Ad Hoc Approximation 317
  9.2 Nondimensionalization 318
    9.2.1 Final Form 319
    9.2.2 Integral Form 319
    9.2.3 Infinite Damköhler Limit 320
  9.3 Steady Solutions 320
    9.3.1 High-Activation-Energy Asymptotics 321
    9.3.2 Method of Weighted Residuals 325
    9.3.3 Steady Solution with Reactant Depletion 329
  9.4 Unsteady Solutions 331
    9.4.1 Linear Stability 331
    9.4.2 Full Transient Solution 337
Exercises 338
References 338

10 Premixed Laminar Flame ................................. 340
  10.1 Governing Equations 341
    10.1.1 Evolution Equations 341
    10.1.2 Constitutive Models 343
    10.1.3 Alternate Forms 344
    10.1.4 Equilibrium Conditions 347
  10.2 Steady Burner-Stabilized Flames 348
    10.2.1 Formulation 349
    10.2.2 Solution Procedure 351
    10.2.3 Detailed H₂-Air Kinetics 359
Exercises 360
References 361

11 Oscillatory Combustion .............................. 362
  11.1 Gray-Scott Mechanism 363
    11.1.1 Spatially Homogeneous 365
    11.1.2 Spatial Variations and Pattern Formation 369
  11.2 H₂-Air Mechanism 369
Exercises 372
References 373

12 Detonation ............................... 375
  12.1 Reactive Euler Equations 376
    12.1.1 One-Step Irreversible Kinetics 376
## Contents

12.1.2 Sound Speed and Thermicity 377  
12.1.3 Parameters for H₂-Air 377  
12.1.4 Conservative Form 378  
12.1.5 Nonconservative Form 379  
12.1.6 One-Dimensional Form 381  
12.1.7 Characteristic Form 383  
12.1.8 Rankine-Hugoniot Jump Conditions 387  
12.1.9 Galilean Transformation 389  

12.2 One-Dimensional, Steady Solutions 391  
12.2.1 Steady Shock Jumps 392  
12.2.2 Ordinary Differential Equations of Motion 392  
12.2.3 Rankine-Hugoniot Analysis 395  
12.2.4 Shock Solutions 400  
12.2.5 Equilibrium Solutions 401  
12.2.6 ZND Solutions: One-Step Irreversible Kinetics 404  
12.2.7 Detonation Structure: Two-Step Irreversible Kinetics 409  
12.2.8 Detonation Structure: Detailed H₂-Air Kinetics 420  

12.3 Nonlinear Dynamics and Transition to Chaos 422  
12.3.1 One-Step Kinetics, With and Without Diffusion 423  
12.3.2 Detailed Kinetics, With and Without Diffusion 433  

12.4 Closing Comments 448  
Exercises 448  
References 448  

Author Index 453  
Subject Index 456
Preface

This book considers mathematical modeling of combustion, in particular, its time-independent thermodynamics and its relation to time-dependent dynamics. A major goal is to more fully incorporate the methods and language of nonlinear dynamical systems analysis (e.g., equilibria, phase space, sources, sinks, saddles, and limit cycles) into the pedagogy of traditional combustion theory. A second major goal is to consider problems that show how the mechanisms of advection, reaction, and diffusion influence the multiscale features of combustion systems’ evolution in space and time. The largest fraction of the book is an exposition of some standard material of combustion science. This is accompanied by original work of the author that has been a part of his graduate course lectures and some of the specialized work of the author, his students, and colleagues on relevant topics, especially model reduction, thermodynamics of irreversible processes, identification of length and time scales of one-dimensional unsteady systems, multiscale dynamics, and detonation theory, which has been adapted from studies that have appeared in the archival combustion literature.

The focus is on deterministic continuum models of gas phase combustion, solution methods, detailed development of analytical results, and physical interpretations. As computational methods and hardware expand in their capability, it is useful to take stock of what deterministic modeling can offer, and some of our examples are to this end. Indeed, practical combustion problems abound that do not yield to deterministic continuum methods. Nevertheless, the rapid insights for causality they afford will long render such models as playing a leading role in combustion science.

This book arose from lecture notes for AME 60636, Fundamentals of Combustion, a graduate course taught since 1994 in the Department of Aerospace and Mechanical Engineering of the University of Notre Dame. Many undergraduates with standard preparation in thermodynamics, fluid dynamics, linear algebra, and differential equations have successfully completed the course. The book can guide a semester-long course, although some topics may need to be omitted.

Part I is devoted to time-independent thermodynamics of reactive mixtures and time-dependent systems that are restricted to spatially homogeneous reaction, thus avoiding the significant complications that come with advection and diffusion. Chapter 1 gives a discussion of the reaction dynamics of some simple but realistic time-dependent gas phase chemistry. These examples bring to the fore many of the important topics of the book: posing of combustion problems as nonlinear dynamical
systems, identification of equilibria, time stability of equilibria via local linear analysis, phase space analysis, and full nonlinear dynamics. Next, in the spirit of physical chemistry, the thermodynamics of reacting gas mixtures is presented. Chapter 2 considers Dalton’s mixture theory. Chapter 3 presents the thermodynamics of reacting mixtures, including equilibrium thermochemistry. Chapter 4 considers the time dynamics of a single reaction, followed by its multistep equivalent in Chapter 5. Special attention is given to the topic of irreversible entropy production and its interplay with combustion dynamics. A small discussion of the large topic of model reduction is given in Chapter 6, focusing mainly on dynamical systems aspects; a brief consideration of the significantly complicating effects of diffusion closes the chapter and serves as a bridge to Part II.

Part II considers various combinations of advection and diffusion within reactive systems. Chapter 7 presents the reactive Navier-Stokes equations with detailed kinetics and multicomponent diffusion. Chapter 8 presents an idealized linear model of advection-reaction-diffusion with a simplicity that allows many features of multiscale dynamics to be exposed. Chapter 9 returns to nonlinear dynamics of systems with reaction and diffusion. Chapter 10 considers the well-studied field of premixed one-dimensional laminar flames in the context of a simple advection-reaction-diffusion model that admits a compact presentation as a dynamical system. Chapter 11 briefly considers systems that do not relax to a stationary equilibrium but rather to a long time limit cycle. We close in Chapter 12 with an extended discussion of one-dimensional detonation theory as it is connected with nonlinear dynamics. Each chapter is concluded with a few exercises appropriate for homework. The problems are either self-contained or may need standard information from a thermodynamics text. Instructors with access to software for detailed chemical kinetics can and should be able to develop problems harnessing these tools that enable consideration of a broader range of mixtures important for engineering applications. Because these software tools rapidly change and rely on specific computing systems, we have included no detailed descriptions.

Quantitative predictions are presented in detail to enable the reader to reproduce most results. Often more significant digits than are justified by experiment are presented to this end. Typically, ideal gases are considered with either modestly sized models of detailed kinetics (e.g., H₂-air, oxygen dissociation, or nitrous oxide formation) or one-step kinetics. The book is more general than a monograph and more focused than a comprehensive text. Instructors with access to software for detailed chemical kinetics can and should be able to develop problems harnessing these tools that enable consideration of a broader range of mixtures important for engineering applications. Because these software tools rapidly change and rely on specific computing systems, we have included no detailed descriptions.

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Many of the chapters reflect the significant interaction of the author with his students, colleagues, and teachers, with support from the U.S. National Science Foundation, NASA, and the U.S. Department of Energy. The author is grateful to the long years of dedicated, patient scholarship shown by his PhD students in combustion over the years: M. J. Grismer, K. A. Gonthier, S. Singh, A. K. Henrick, A. N. Al-Khateeb, J. D. Mengers, and C. M. Romick. Their work infuses this book, as does that of colleagues S. Paolucci and T. D. Aslam. And it is hoped that the guidance and wisdom of advisers H. Krier and D. S. Stewart, teacher J. D. Buckmaster, colleague P. B. Butler, and dozens of friends in the broader combustion community are reflected in the text.