COAL COMBUSTION AND GASIFICATION

(The Plenum Chemical Engineering Series)

L. Douglas Smoot
and
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江苏工业学院图书馆
藏书章

PLENUM PRESS • NEW YORK AND LONDON

Library of Congress Cataloging in Publication Data

Smoot, L. Douglas (Leon Douglas)
Coal combustion and gasification.

(The Plenum chemical engineering series)
Bibliography: p.
Includes index.
1. Coal—Combustion. 2. Coal gasification. I. Smith, Philip J. II. Title. III. Series.
TP325.S57 1985 662.6'2 84-17937
ISBN 0-306-41750-2

© 1985 Plenum Press, New York
A Division of Plenum Publishing Corporation
233 Spring Street, New York, N.Y. 10013

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Printed in the United States of America

COAL COMBUSTION AND GASIFICATION

The Plenum Chemical Engineering Series

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ENGINEERING FLOW AND HEAT EXCHANGE
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. . . he that receiveth light, and continueth in God, receiveth more light; and that light groweth brighter and brighter. . . .
Doctrine and Covenants 50:24

DEDICATION

Recognizing its several limitations, we unpretentiously dedicate this book to our Creator, Who, through holy writ, has inspired us to seek light and understanding where darkness exists, and Who, through these same records, has taught us to place our professional pursuits in perspective with greater obligations of service to family and to society.

PREFACE

The use of coal is required to help satisfy the world's energy needs. Yet coal is a difficult fossil fuel to consume efficiently and cleanly. We believe that its clean and efficient use can be increased through improved technology based on a thorough understanding of fundamental physical and chemical processes that occur during consumption. The principal objective of this book is to provide a current summary of this technology.

The past technology for describing and analyzing coal furnaces and combustors has relied largely on empirical inputs for the complex flow and chemical reactions that occur while more formally treating the heat-transfer effects. Growing concern over control of combustion-generated air pollutants revealed a lack of understanding of the relevant fundamental physical and chemical mechanisms. Recent technical advances in computer speed and storage capacity, and in numerical prediction of recirculating turbulent flows, two-phase flows, and flows with chemical reaction have opened new opportunities for describing and modeling such complex combustion systems in greater detail. We believe that most of the requisite component models to permit a more fundamental description of coal combustion processes are available. At the same time there is worldwide interest in the use of coal, and progress in modeling of coal reaction processes has been steady.

We have been working during the past ten years on coal combustion and gasification processes. This work has included both basic measurements and development of analytical models. In our modeling work, we have attempted to develop fundamental models based upon the general equations of conservation and to use the most appropriate literature information available as sources for model components and parameters. One of the major purposes of this new book is to document our general modeling approach for pulverized-coal systems. This model emphasizes processes using finely pulverized coal which is entrained in a gaseous phase. Problems of particular interest include combustion in

pulverized-coal furnaces and power generators, entrained coal gasifiers, coal-fired MHD power generators, and flame propagation in laminar and turbulent coal dust/gas mixtures. In addition, we have reviewed work by others in modeling of combustion or gasification in entrained, fluidized, and fixed beds. We have also briefly considered other combustion problems associated with oil shale, tar sands, and other fossil fuels.

This book is the second published by the authors (with others in the first book, Plenum Publishing Co., New York, 1979) which relates to coal combustion and gasification. For the case of pulverized-coal models, the authors (with others) provided detailed fundamentals on which modeling is based in the earlier book (Smoot and Pratt, 1979). This earlier book emphasized general principles for reacting, turbulent or laminar, multiphase systems. General conservation equations were developed and summarized. The basis for computing thermochemical equilibrium in complex, heterogeneous mixtures was presented, together with techniques for rapid computation and reference to required input data. Rate processes were discussed, including pertinent aspects of turbulence, chemical kinetics, radiative heat transfer, and gas–particle convective–diffusive interactions.

This book differs from the first in several significant ways. Most of the material in this book is different from that in the first book. The scope of the new book has been expanded to include material on fixed- and fluidized-bed process characteristics. The details of interactions between turbulence and chemistry for coal-laden systems is a major new emphasis in this book, which has been prepared for use both as an advanced textbook and as a reference and source book for those who work in fossil-fuel combustion and gasification. Technical problems for solution have been included at the end of each chapter. A single nomenclature and list of references is used for the entire book.

The book is divided into five major topic areas:

1. Chapters 1 and 2 consider general characteristics of coal processes and properties.
2. Chapters 3–5 treat basic reaction processes of coal particles, including coal devolatilization, char oxidation, and volatiles combustion. Some of these topics were treated in the first book but have been updated or expanded significantly. New sections on heatup and ignition have been added.
3. Chapters 6–8 deal with practical fossil combustion flames. Processes are classified by flame type and then each is considered in some detail, with particular emphasis on pulverized-coal flames. Recent laboratory data for combustion and gasification are used to illustrate flame characteristics. A review of methods for modeling fixed, fluidized, and entrained beds is included together with a summary of data for evaluation of predictive methods.

4. Chapters 9, 10, and 14 provide the fundamental equations and background for turbulent combustion systems.
5. Chapters 11–13 and 15 document in some detail the approach and theory for the interactions between chemistry and turbulence in reacting systems encompassing gaseous flames, particle-laden systems, and pollutant formation in these systems.

This work has formed the basis for model development at our Combustion Laboratory. These fundamentals were treated generally in the first book. The treatment in this new book for governing equations and for radiation is not greatly changed. However, significant new material is added for chemically reacting, turbulent, heterogeneous systems and for formation of nitrogen oxide pollutants.

Included in several of these chapters are comparisons of measurements with predictions from a comprehensive model developed at the Combustion Laboratory. These comparisons demonstrate the state of development of the comprehensive code which, in the view of the authors, is suitable for some practical application to pulverized-coal systems. While this method has been developed principally for pulverized-coal combustion and gasification, this and similar methods have far more general applicability. The code is directly applicable to nonreactive gaseous and particle-laden flows and to reactive gaseous systems. Progress is being made for application to coal slurries and only minor work would be required for use with liquid fuel flames.

The authors recognize the several uncertainties in constructing and applying models of this nature. Coal is a very complex heterogeneous substance whose structure and behavior are highly variable and are not well known. Pyrolysis and oxidation of coal are dependent upon coal type, size, size distribution, temperature history, etc., thus making generalization difficult. In addition, the complexities of turbulent recirculating flows, turbulent reacting flows, and turbulent two-phase flows are not fully resolved. Only recently has formal computation of recirculating flows been possible. Suitable generalized parameters for the turbulence models are not well-established. The very important interactions of turbulence with chemical reaction are even less well-developed. Significant uncertainties also pertain to the effects of gas turbulence on the motion of the particles. It is known that the random gas fluctuations are a major force in dispersing particles, but treatments of this effect are in the formative stages.

Finally, there has been little previous attempt to develop models which consider several of these aspects jointly. For this reason, models of pulverized-coal systems must be validated by comparison with experimental measurements. Measurements of outlet gas or char composition or temperature alone are not suitable for this model validation. Profiles of at least time-mean, local properties from within the reactor provide a more acceptable basis for the model evaluation.

As a part of the research program being conducted by the authors and colleagues such measurements are being obtained, some of which are presented and compared with model predictions in this book. These measurements include data for laminar, premixed coal dust/air flames and methane–air flames, as well as spatially resolved measurements of gas and char composition from inside entrained gasifiers and combustors. Further, profile measurements have been and are being made for particle-laden, recirculating jet flows without chemical reaction. Comparison of these measurements and those of several other investigators with model predictions will permit evaluation of particle and gas-flow effects in the absence of chemical reaction complications.

Much of the work upon which this book is based has been supported at our laboratory by federal and industrial organizations. We especially express our appreciation to The United States Department of Energy (Morgantown Energy Technology Center and Pittsburgh Energy Technology Center), the Electric Power Research Institute (Fossil Fuels Division), the National Science Foundation, the Tennessee Valley Authority, and the Utah Power and Light Co., for contract or grant support related to measurements and model development for pulverized-coal systems. We further acknowledge the College of Engineering and Technology and Research Division of Brigham Young University for financial research support and for assistance in preparation of the manuscript. We are also grateful to Elaine Alger for typing and editorial work on the manuscript and to Mr. Daniel Gleason for preparation of the illustrations. Appreciation is also due Exxon Corporation, Los Alamos National Laboratory, and Morgantown Energy Technology Center for financial support for preparation of parts of these materials which were used in technical lectures given by the author(s) at each of these institutions. Much of the materials of Chapters 1–5 were initially prepared at the request of Exxon Corporation, who kindly gave permission for inclusion of these materials in this book. We gratefully acknowledge our faculty colleagues and graduate students at the Combustion Laboratory for significant research contributions related to much of the material in this book.

Contents

1. Introduction

1.1 Objectives 1
1.2. Scope 2
1.3. Approach 3
1.4. General References 3

2. Solid Fossil Fuels (Mostly Coal): Processes and Properties

2.1. Coal Availability and Uses 7
2.2. Coal Processes 9
2.3. Coal Slurries 10
2.4. Issues in Increasing Use of Coal 14
2.5. Coal Characteristics 16
2.5a. Formation and Variation 16
2.5b. Coal Classification 17
2.5c. Physical and Chemical Properties of Coal 17
2.5d. Structural Characteristics of Coal 20
2.5e. Mineral Matter Removal 21
2.6. Properties of Coal Slurries 28
2.7. Properties of Other Solid and Liquid Fossil Fuels 31
2.8. Illustrative Problems 33

3. Coal Particle Ignition and Devolatilization

3.1. Introduction and Scope 37
3.2. Elements of Coal Reactions 38
3.3. Ignition 41
3.3a. Background 41
3.3b. Theory of Ignition 43
3.3c. Ignition Data 44

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3.4. Particle Heatup and Temperature 47
3.4a. Heating Processes 47
3.4b. Measurements 47
3.4c. Predictions 52
3.5. Devolatilization 54
3.5a. Experimental Studies 54
3.5b. Devolatilization Models 59
3.5c. Effects of High Moisture Content 66
3.6. Volatiles Combustion 67
3.6a. Background 67
3.6b. Experimental Data 68
3.6c. Computational Approaches 70
3.6d. Volatiles Reaction Rates 72
3.7. Illustrative Problems 74

4. Heterogeneous Char Reaction Processes
4.1. Reaction Variables 77
4.2. Global Reaction Rates 80
4.2a. Char Oxidation Data 81
4.2b. Effects of Coal Moisture on Char Oxidation 88
4.2c. Effects of Mineral Matter 90
4.2d. Global Modeling of Char Oxidation 91
4.3. Intrinsic Char Reaction Rates 94
4.3a. Background 94
4.3b. Intrinsic Rate Data 95
4.3c. Conceptual (Macroscopic) Model of Intrinsic Reactivity . 99
4.3d. Extended (Microscopic) Intrinsic Reactivity Models . . 104
4.4. Other Aspects of Particle Reaction 108
4.5. Illustrative Problems 108

5. Combustion of Coal in Practical Flames
5.1. Introduction and Scope 111
5.2. Classification and Description of Practical Flames 112
5.2a. Flame Classification 112
5.2b. Classic Flame Types 114
5.3. Practical Process Flame Characteristics 117
5.4. Physical and Chemical Processes in Practical Flames 121
5.4a. Flame Processes 121
5.4b. Pulverized-Coal Diffusion Flames 121
5.4c. Coal Slurry Diffusion Flames 137
5.4d. Premixed Flames 142
5.5. Illustrative Problems 149

6. Gasification of Coal in Practical Flames
6.1. Introduction and Scope 151
6.2. Basic Process Features 152
6.2a. Basic Reactions 152
6.2b. Gasification Process Types 154
6.2c. Comparison with Combustion 155
6.3. Physical and Chemical Gasification Processes 156
6.4. Gasifier Data 158
6.5. Illustrative Problems 161

7. Modelling of Coal Processes
7.1. Background and Scope 163
7.2. Basic Model Elements and Premises 164
7.3. Plug-Flow Model 168
7.3a. Model Assumptions 168
7.3b. Differential Equations 170
7.3c. Auxiliary Equations 172
7.3d. Model Predictions and Comparisons 174
7.4. Multidimensional Flame Codes 177
7.4a. Basis 177
7.4b. General Description of Subroutines 178
7.4c. Code Development 179
7.5. Other Pulverized-Coal Codes 179
7.6. Fixed-Bed Combustion Models 184
7.6a. Background 184
7.6b. One-Dimensional Fixed-Bed Models 189
7.6c. Fixed-Bed Models: Evaluation and Application 192
7.7. Fluidized-Bed Models 193
7.7a. Background 193
7.7b. One-Dimensional FBC Models 196
7.7c. Two-Dimensional FBC Models 200
7.8. Some Observations on Modeling 206
7.9. Illustrative Problems 208

8. Evaluation of Comprehensive Models
8.1. Background and Scope 211
8.2. Evaluation Methods 211
8.2a. Numerical Evaluation 212
8.2b. Sensitivity Analysis 215
8.2c. Trend Analysis 218
8.2d. Comparison with Comprehensive Data 219
8.3. Detailed Local Data for Model Evaluation 220

8.3a. Data Requirements and Categories 220
8.3b. Data Cases Considered and Selected 220
8.4. Data Needs 221
8.5. Illustrative Problems 221

9. Basic Modeling Equations
9.1. Introduction 229
9.1a. The Continuum Hypothesis 230
9.1b. Eulerian and Lagrangian Reference Frames 233
9.2. Reynolds Transport Theorem 234
9.3. Eulerian Equations 237
9.3a. Formulation 237
9.3b. General Continuum Equations 238
9.3c. Decoupled Gas and Solid Equations 239
9.4. Illustrative Problems 242

10. Turbulence
10.1. Introduction 245
10.2. The Closure Problem 247
10.3. Prandtl Mixing Length 249
10.4. One-Equation Closure Models 250
10.5. The k-ε Model (Two-Equation Closure Models) 252
10.6. Turbulent Stress Closure Models 259
10.7. Effects of Particle-Laden Jets 261
10.8. Boundary Conditions 262
10.8a. Boundary Conditions for k 262
10.8b. Boundary Conditions for ε 263
10.9. Illustrative Problems 264

11. Chemistry and Turbulence of Gaseous Fuels
11.1. Introduction 267
11.2. Mean Reaction Rate 268
11.2a. Type A: Reaction Time Scale $\gg$ Turbulent Time Scale . 270
11.2b. Type B: Reaction Time Scale $\ll$ Turbulent Time Scale . 271
11.2c. Type C: Reaction Time Scale $\simeq$ Turbulent Time Scale . 272
11.3. Mixture Fraction 273
11.4. Probability Density Function (PDF) 274
11.5. Favre Averaging 279
11.6. Mixing 281
11.7. Chemical Equilibrium 284
11.8. Nonequilibrium Chemistry for Type B Flames 288
11.9. Sample Computations 290
11.10. Illustrative Problems 296

12. Particulate and Droplet Reactions in Turbulent Flows
12.1 Introduction . . . 299
12.2. Approaches . . . 300
12.3. Lagrangian Particle Description . . . 302
12.4. Turbulent Particle Dispersion . . . 305
12.5. Particle Reactions . . . 313
12.6. Particle Source Terms . . . 318
12.7. Illustrative Problems . . . 319

13. Chemistry and Turbulence of Coal Reaction Products
13.1. Introduction . . . 321
13.2. Coal–Gas Mixture Fraction . . . 322
13.3. Mean Chemical Properties . . . 326
13.4. Probability Density Functions . . . 334
13.5. Energy Balance Considerations . . . 337
13.6. Problems and Research Needs . . . 341
13.7. Illustrative Problems . . . 348

14. Radiative Heat Transfer
14.1. Introduction . . . 349
14.2. Fundamentals . . . 351
14.2a. Intensity . . . 351
14.2b. Emissive Power . . . 353
14.2c. Absorption . . . 355
14.2d. Scattering . . . 357
14.3. General Equation . . . 359
14.4. Solution Methods . . . 360
14.4a. The Hottel Zone Method . . . 360
14.4b. The Monte Carlo Method . . . 361
14.4c. The Diffusion Method . . . 361
14.4d. Flux Methods . . . 361
14.4e. Recommended Flux Method . . . 362
14.5. Coefficients . . . 365
14.6. Illustrative Problems . . . 371

15. NO_x Pollutant Formation in Turbulent Coal Systems
15.1. Introduction . . . 373
15.2. Mechanism . . . 375
15.2a. Coal Devolatilization . . . 375
15.2b. Homogeneous Formation of NO . . . 376
15.2c. Heterogeneous Reactions of NO . . . 379
15.3. Turbulence Fluctuations . . . 380
15.3a. Species Continuity . . . 380

15.3b. Time-Mean Reaction Rate 381
15.4. Computations 384
15.5. New Measurements Needed 398
15.6. Illustrative Problems 404

Appendix 405

Nomenclature 409

References 415

Index 435

Behold, all ye that kindle a fire, that compass yourselves about with sparks: walk in the light of your fire, and in the sparks that ye have kindled.
Isaiah 50:11

1

INTRODUCTION

1.1. OBJECTIVES

This book deals with reaction processes involving coal, char, coal–water mixtures, and other solid fossil fuels. Properties and uses of these solid fossil fuels are treated; physical and reaction processes of coal particles are also considered and modeled. Then, these results are applied to the description of coal processes.

Key objectives for preparation of this book have been to:

1. Provide a review of the existing and potential uses of coal and the processes most commonly applied.
2. Identify the general chemical and physical properties of solid fossil fuels, emphasizing the complexity and variability of these natural materials.
3. Summarize major issues being addressed in the increasing uses of coal and other solid fossil fuels.
4. Characterize effects of key variables such as particle size, heating rate, temperature, pressure, and oxidizer type on coal particle reaction rates.
5. Outline useful existing methods for modeling of coal particle reactions in a turbulent environment including ignition, devolatilization, gas-phase reaction of volatiles, and heterogeneous oxidation processes.
6. Identify the nature and controlling processes of coal dust flames in various coal processes, including direct combustion and coal gasification.
7. Provide a fundamental foundation for a description of complex, reacting particle-laden systems through treatment of turbulence and its interaction with chemical reactions, radiation and related basic topics.

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