# THE CHEMISTRY AND TECHNOLOGY OF COAL

## The Chemistry and Technology of Coal

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### The Chemistry and Technology of Coal

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#### Preface

There are no documented records of when or how mankind first discovered that a certain 'black rock' would burn. However, it is known that coal was employed as a fuel in China about 1100 B.C. and that Welsh Bronze Age cultures had used coal for funeral pyres. There are many other instances where coal receives some mention in the historical literature, but the consistent use of coal seems to have evolved in England in the Middle Ages, later becoming the prime force behind the Industrial Revolution. From that point until the early decades of this century, coal had emerged as a major energy source.

However, the subsequent emergence of petroleum as a plentiful and cheap source of energy led to the "demotion" of coal to a "mere" source of combustible energy (into which the use of petroleum was steadily making inroads). Nevertheless, recent energy crises have served to emphasize that petroleum would no longer remain the cheap commodity to which mankind had grown accustomed. Indeed, assessments of the availability of petroleum have indicated that supplies of the more conventional crude oils could be virtually exhausted within the foreseeable future. This, coupled with the drastic increases in the price of the available petroleum, has caused a major shift in the emphasis of energy policies.

As a result, there has been an "outburst" of serious attempts to produce liquid fuels from the so-called "unconventional" sources such as coal, oil sands (often referred to as tar sands or bituminous sands), and oil shale. Indeed, this reemphasis of the value of these unconventional liquid fuel sources has helped reinstate coal to its once-enjoyed popularity and, perhaps, to a leading (even unique) position of being a major source of energy. In fact, power generation — once the sole domain of coal but since intruded upon by the shift to oil-fired generating plants — may also be returned to coal as the predominant combustible energy source.

As a result of this renewed interest in coal, there is a virtual vacuum in the availability of qualified personnel. This is being relieved in part by the initiation of research into the nature and properties of coal by a variety of universities, and formal training in this important area of science and engineering is essential if the use of this important natural resource is to be maximized.

Thus, it came about during the winter of 1976 - 1977 that the author was instrumental in initiating (with a colleague — John F. Fryer) a teaching course relating to The Chemistry and Technology of Coal that ran parallel with the course relating to The Chemistry and Technology of Petroleum which was offered through the Faculty of Extension at the University of Alberta. Both courses ran for several years and were also offered in the shortened multiday format through the Faculty of Continuing Education at the University of Calgary.

This book is the result of the copious notes collected and employed for the course and is intended to be a companion volume to The Chemistry and Technology of Petroleum (James G. Speight, Marcel Dekker, Inc., 1980). The text introduces the reader to the science of coal, beginning with the formation of coal in the ground and progresses through the various chemical and analytical aspects of coal science to the established and proposed processes for the production of a variety of gaseous and liquid fuels.

These latter aspects of coal technology are actually quite complex insofar as the technology is still evolving. Thus, processes that were of major interest at, say, manuscript preparation may, at the time of manuscript publication, no longer be in contention as a serious process option. There is no satisfactory method by which such changes in technology and process planning can be satisfied, and the only way to inform the reader of the various process options is to present them in outline with the cautious corollary "here today — gone tomorrow."

In more general terms, the book is written (like <u>The Chemistry and Technology of Petroleum</u>) as a teaching text from which the reader can gain a broad overview (with some degree of detail) of the concepts involved in coal science and technology. The text will, therefore, satisfy those who are just entering into this fascinating aspect of science and engineering as well as those (scientists and engineers) who are already working with coal but whose work is so specific that they also require a general overview. It will also be of assistance to petroleum refinery personnel who may, one day, be called upon to handle large supplies of liquid fuels from coal as a feedstock for the refinery system.

For those readers who may require more detail in certain of the subject areas, bibliographies have been appended to each chapter. These will either directly provide the reader with the desired detail or will provide a compilation of literature references for further consultation.

The nature of the subject virtually dictates that any text on coal must include some chemistry (and the present text is not delinquent in this respect), but attempts have been made for the benefit of those readers without any formal post-high school training in chemistry (and who may, therefore, find chemistry lacking in any form of inspiration) to maintain the chemical sections in the simplest possible form. Wherever possible, simple chemical formulas have been employed to illustrate the text. However, for the reader

Preface

with an in-depth knowledge of organic chemistry, a chapter has been included which describes in detail the organic structures found in coal.

For the benefit of those readers who have had formal training in one (or more) of the engineering diciplines, the text contains both the metric and nonmetric measures of temperature (Celsius and Fahrenheit). However, it should be noted that exact conversion of the two scales is not often possible and, accordingly, the two temperature scales are interconverted to the nearest 5°. At the high temperatures often quoted in the process sections, serious error will not arise from such a conversion. With regard to the remaining metric/nonmetric scales of measurement, there are also attempts to indicate the alternate scales.

For the sake of simplicity and clarity, simple illustrations (often line drawings) are employed for the various process options, remembering, of course, that a line between two reactors may not only be a transfer pipe but

also a myriad of valves and control equipment.

James G. Speight

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This work was completed while the author was a staff member of the Alberta Research Council (Edmonton, Alberta, Canada) prior to his move to the Corporate Research Science Laboratories of Exxon Research and Engineering Company (Linden, New Jersey). Thus, the author wishes to acknowledge the valuable assistance of Mrs. Tara Emter and Mrs. Joan MacDonald during the preparation of the manuscript. The author is also indebted to Drs. B. Nandi and J. Jorgensen (Canada Centre for Mineral and Energy Technology), to his colleague Dr. Sat Parkash (Alberta Research Council) for photographs of coal macerals, and to Mr. A. Bosman (Alberta Research Council) for the photographs in Figures 2-7, 2-8, 2-9, and 2-15.

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#### Contents

Acknowledg	gments	iii vii
PART I.	COAL PROPERTIES	
	softenore the apt	
Chapter 1.	Coal as an Organic Sediment	3
I.	Origins	3
II.	Precursors of coal	5
III.	Coal-forming processes	34
	Bibliography	39
Chapter 2.	Geology and Recovery of Coal	41
I.	The geology of coal	41
II.	Geological factors affecting seam structure	43
III.	Exploratory drilling equipment and techniques	48
IV.	Coal mining	53
v.	Coal preparation	65
VI.	Coal drying	67
VII.	Coal transportation	68
	Bibliography	69
Chapter 3.	Coal as an Organic Rock	71
I.	Physical structure of coal	71
П.	Coal petrography	72
III.	Coal petrography and utilization	89
	Bibliography	91
Chapter 4.	Terminology and Classification of Coal	93
I.	Nomenclature and terminology	93
II.	Classification of coal	94
	Bibliography	113

ix

A		Contents
Chapter 5.	Mineral Matter in Coal	115
I.	General concepts	115
II.	Origin of mineral matter in coal	116
III.	Occurrence	117
IV.	Mineral types	123
v.	Evaluation of mineral matter in coal	127
	Bibliography	133
Chapter 6.	Evaluation and Properties of Coal	135
I.	Sampling of coal for analysis	136
II.	Proximate analysis	137
III.	Ultimate (elemental) analysis	142
IV.	Calorific value	147
v.	Reporting coal analyses	149
VI.	Precision and accuracy of coal analyses	153
VII.	Interrelationships of analytical and physical data	153
VIII.	Physicochemical analyses	155
IX.	Optical properties	170
х.	Thermal properties	173
XI.	Mechanical properties	184
XII.	Electrical properties	194
	Bibliography	197
Chapter 7.	Solvent Extraction of Coal	199
I.	General concepts	199
II.	Physicochemical concepts	201
III.	Action of specific solvents	205
IV.	Influence of coal rank	206
V.	Influence of petrographic composition	209
VI.	Composition of the extracts	209
VII.	Solvolysis	212
	Bibliography	213
Chapter 8.	Chemical Reactions of Coal	215
I.	Reactions with oxygen (or air)	215
II.	Reactions with oxidants	221
ш>	Hydrogenation of coal	222
IV.	Halogenation reactions	232
V	Alkylation reactions	233
VI.	Depolymerization reactions	234
	Hydrolysis reactions	235
VIII.	Miscellaneous reactions	235
	Bibliography A	240

Contents	xi

Chapter	9.	Thermal Decomposition of Coal	241
100	I.	General concepts	241
	II.	Thermal decomposition processes	242
	III.	Physicochemical aspects	248
	IV.	Thermal decomposition products	258
		Bibliography	271
		2/10	
Chapter	10.	Organic Constituents of Coal	273
	I.	Low molecular weight constituents	274
	II.	High molecular weight constituents	279
	III.	Heteroatoms in coal	311
	IV.	Molecular weight of coal	316
	V.	Assessment of coal structure	321
		Bibliography	331
DADELI		NOAT MANTENANTANIA	
PART II	. (	COAL UTILIZATION	
		. 3.8 %.	
Chapter	11	Combustion of Coal	335
Chapter	I.	Influence of coal quality	335
	II.	Mechanism of coal combustion	336
	III.	Physicochemical aspects	338
	IV.	Combustion systems	351
	V.	Environmental aspects	364
	٧.	Bibliography	368
		Dibliography	000
Chapter	12.	Carbonization of Coal	371
	I.	Low-temperature carbonization	372
	II.	High-temperature carbonization	374
	III.	Physicochemical aspects	377
	IV.	Formed coke	380
	V.	Coal tar processing	382
		Bibliography	385
		1ªAIR	
Chapter	13.	Liquefaction of Coal	387
	I.	Physicochemical aspects	387
	II.	Reactors	393
	III.	Processes	398
	IV.	Liquid products	440
	V.	Solid products (bitumens)	446
	VI.	Refining coal liquids	452
		Bibliography	457

XII		Contents
Chapter 14.	Gasification of Coal	461
I.	Physicochemical aspects	461
II.	Processes	468
III.	Underground gasification of coal	502
IV.	Gaseous products	511
	Bibliography	515

517

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Index

#### Part I COAL PROPERTIES

Part I Coal Properties

#### Chapter 1

#### Coal as an Organic Sediment

#### I. ORIGINS

Coal was formed from partially decomposed (and subsequently metamorphosed) plant debris which had collected in regions where waterlogged or swampy conditions prevailed. These conditions prevented complete decay of the debris as it accumulated and eventually led to the material now known as coal.

In general terms, the debris consisted of trees, ferns, rushes, lycopods, and several thousand plant species that have been identified in coal beds, but it appears that none of the species identified in many different coals originated in brackish-water locales. Similar types of plant remains may be found in all types (ranks) of coal but, of course, the relative amounts vary considerably. On this basis, it is not surprising that coal differs markedly in composition from one locale to another. Indeed, pronounced differences in coals from one particular seam are not uncommon, due not only to the wide variety of plant debris that could have formed the precursor but also to the many different chemical reactions that can occur during the maturation process.

Thus, once plant debris has accumulated under the "correct" conditions, the formation of peat gradually occurs. Peat is not actually classified as coal but it is, nevertheless, believed to be that material which is formed as the initial step in the process. However, to become coal, peat must progress through what is loosely termed the "coalification" process. The coalification process is, in essence, the progressive change in the plant debris as it becomes transformed from peat to lignite and then through the higher ranks of coal to anthracite. The degree of coalification generally determines the rank (see page 99) of the coal, but the process is not a series of straightforward chemical changes. For example, the metamorphism of the plant debris not only relies on geological time but also on temperature and pressure.

Thus, when the organic debris (which may be identified as peat) is buried beneath overburden, various physicochemical processes occur as part of the metamorphosis. The major influences are believed to be the