

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 The Chemistry and Technology of Petroleum) 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

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 disciplines, 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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Part I

COAL PROPERTIES

I. INTRODUCTION

Coal was formed from partially decayed plant and other organic material, mostly plant debris which had collected in swamps where it was buried in swampy conditions of peat bogs. These materials, however, were not the debris as it is understood but a variety of plant remains known as peat.

In general terms, the debris is made up of leaves, stems, roots, twigs, pods, and several thousand plant species that have been identified in coal beds. But it appears that some of the species that are identified in many different coals originated in brackish-water swamps. Similar types of plant remains may be found in all types (rank) 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 begins. Part of the debris is identified as coal but it is, nevertheless, "dead" in the sense that it is formed as the material is in the process of being transformed into coal. The transformation process is, in essence, the degradation of plant debris as it becomes transformed from peat to lignite to then through the higher ranks of coal to anthracite. The degree of transformation generally determines the rank (see page 35) 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 taken into the identified as peat, it is subjected to a series of chemical and physical processes that occur as part of the metamorphism. The major influences are believed to be the

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

resulting heat and pressure developed because of the overlying sedimentary cover (overburden). This leads to changes in the constituents of the debris such as an increase in the carbon content, alteration of the functional groups, alteration of the various molecular structures ultimately resulting in the loss of water, oxygen, and hydrogen with the increased resistance to solvents, heat, and oxidation.

All theories about the formation of coal require that the original plant debris eliminate oxygen and hydrogen continuously under the prevailing conditions, ultimately leading to a product containing approximately 90% w/w carbon, i.e., anthracite. In order for this maturation to proceed, chemical principles require that oxidation reactions be completely inhibited. However, in the early stages of coalification, microorganisms may play an important role and, somewhat paradoxically, they may interact with the plant material under aerobic conditions as well as under anaerobic conditions. The formation of coal under the slow conditions generally referred to as geological time may, nevertheless, be regarded as occurring in the absence of oxygen, thereby promoting the formation of highly carbonaceous molecules through losses of oxygen and hydrogen from the original organic molecules (Fig. 1-1).

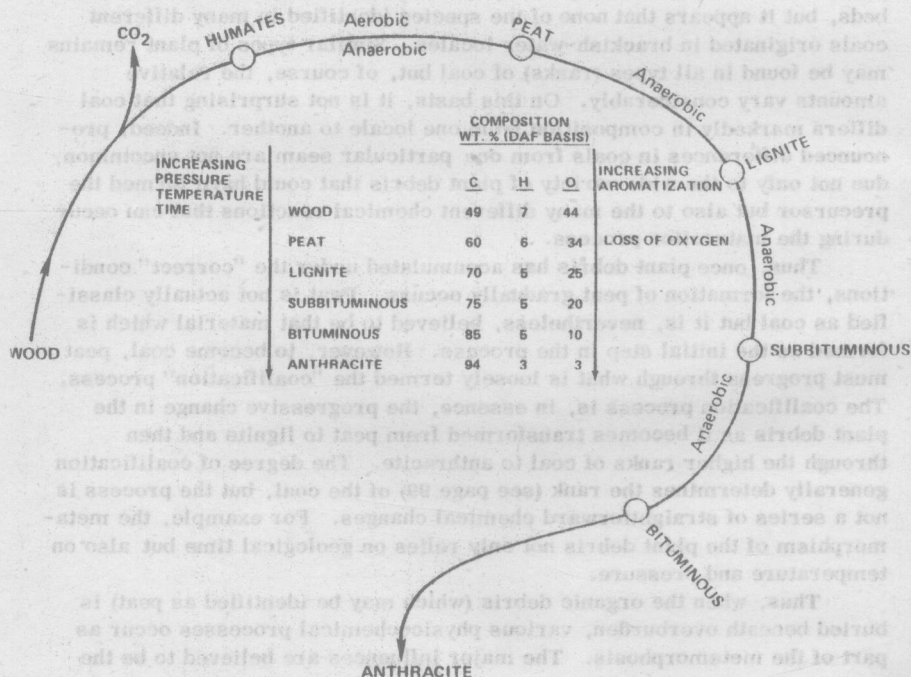


FIG. 1-1 Schematic representation of the coalification process.