

# Fundamentals of the Physical-Chemistry of Pulverized Coal Combustion

Edited by

J. Lahaye and G. Prado

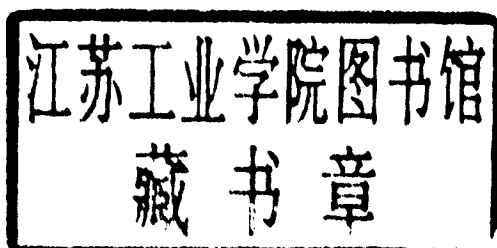
NATO ASI Series

# Fundamentals of the Physical-Chemistry of Pulverized Coal Combustion

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**J. Lahaye and G. Prado**

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## PREFACE

The study of coal for the production of energy is certainly not a new area of research. Many research works were carried out to improve the efficiency of industrial and domestic facilities. In the sixties, however, because of the availability and low cost of petroleum, coal consumption decreased and the research effort in this area was minimum.

Meanwhile, the situation has totally changed. Considering the reserves of oil and the instability of regions where they are located, it is becoming absolutely necessary to develop other sources of energy. The major alternative to oil appears to be coal, at least for the near future. Indeed, the reserves known today represent several centuries of energy consumption. It is therefore becoming urgent to develop efficient and non polluting technologies to produce energy from coal. The main possibilities are :

- . liquefaction
- . gasification
- . directed combustion.

Research and development efforts on liquefaction have been considerably reduced because of high cost of technologies involved and poor prospects for the next two decades. Research works on gasification are progressing; it is a promising approach.

However, direct combustion either in pulverized coal furnaces or in fluidized beds is the more promising way of expanding rapidly the utilization of coal. These techniques are already used in some facilities but many environmental problems remain, slowing down their development.

It is of primary importance to be able to achieve a proper physical description with accurate models of the different processes occurring in industrial facilities, in order to develop efficient and non polluting equipments.

Beginning in the early eighties, many laboratories have been involved in coal sciences. Several computer codes have been developed, describing flow aerodynamics with some coupling with chemical reactions. In order to avoid the manipulation of empirical parameters which make these models inappropriate for solving practical problems, it is necessary to introduce data relative to the fundamental mechanisms of the combustion of a coal particle. It is also important to take into account the different types of coal and for a given coal the heterogeneity of maceral composition and size of the particles.

At the Twentieth Symposium (International) on combustion held at Ann Arbor (Michigan) in 1984, a fairly large number of papers were concerned with the combustion of coal. We noticed that, unfortunately, it was difficult to do an acceptable synthesis of the results published by the different laboratories. We decided at that time, encouraged by our colleagues from M.I.T. involved in coal combustion science, to organize a workshop to put together for a week the specialists of the domain in order to establish the state of the art and formulate recommendations for future work.

The final programme was divided into six sessions. Eight main lectures were completed by twelve communications.

In the first session a review of coal properties known to be important to coal combustion behaviour was presented.

When coal is subjected to high temperature in oxidative or not oxidative atmosphere, devolatilization occurs. In the second session, three main lectures were devoted to the kinetics of devolatilization, the role of volatiles in coal combustion and the morphological transformation of coal during pyrolysis.

Heterogeneous combustion of the char obtained by devolatilization of coal was reviewed in the third session.

The largest obstacle to the public acceptance of increased coal use is the perception that coal combustion is polluting. The fourth session addressed this key problem.

Much of the recent progress in the understanding of coal combustion is attributable to new advanced diagnostics. The fifth session reviewed the techniques for in situ measurements of coal flames.

The sixth session was concerned with the transfer of fundamental results to the modeling of burners and boilers.

The last part of the meeting was devoted to a synthesis of the workshop by three sub-committees.

The question, comments, and answers submitted in a written form have been edited in the present volume.

Special thanks are addressed to the Scientific Committee, Profs. J.B. Howard, H. Jüntgen and F.E. Lockwood, Dr R.E. Mitchell, Profs. A.F. Sarofim and T.F. Wall, for their efficient collaboration in the preparation of the meeting.

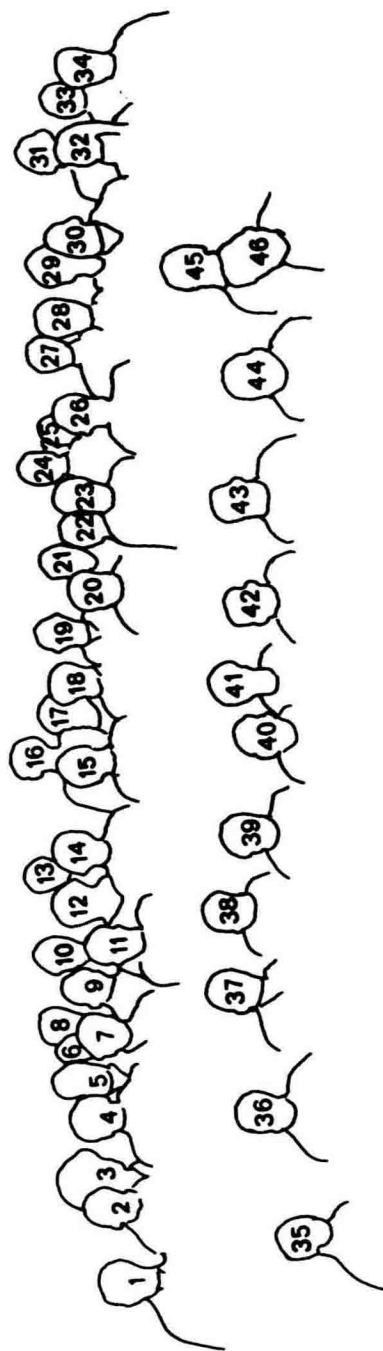
We are grateful to C. Denninger, F. Muller, P. and S. Wagner for their technical assistance before and during the workshop.

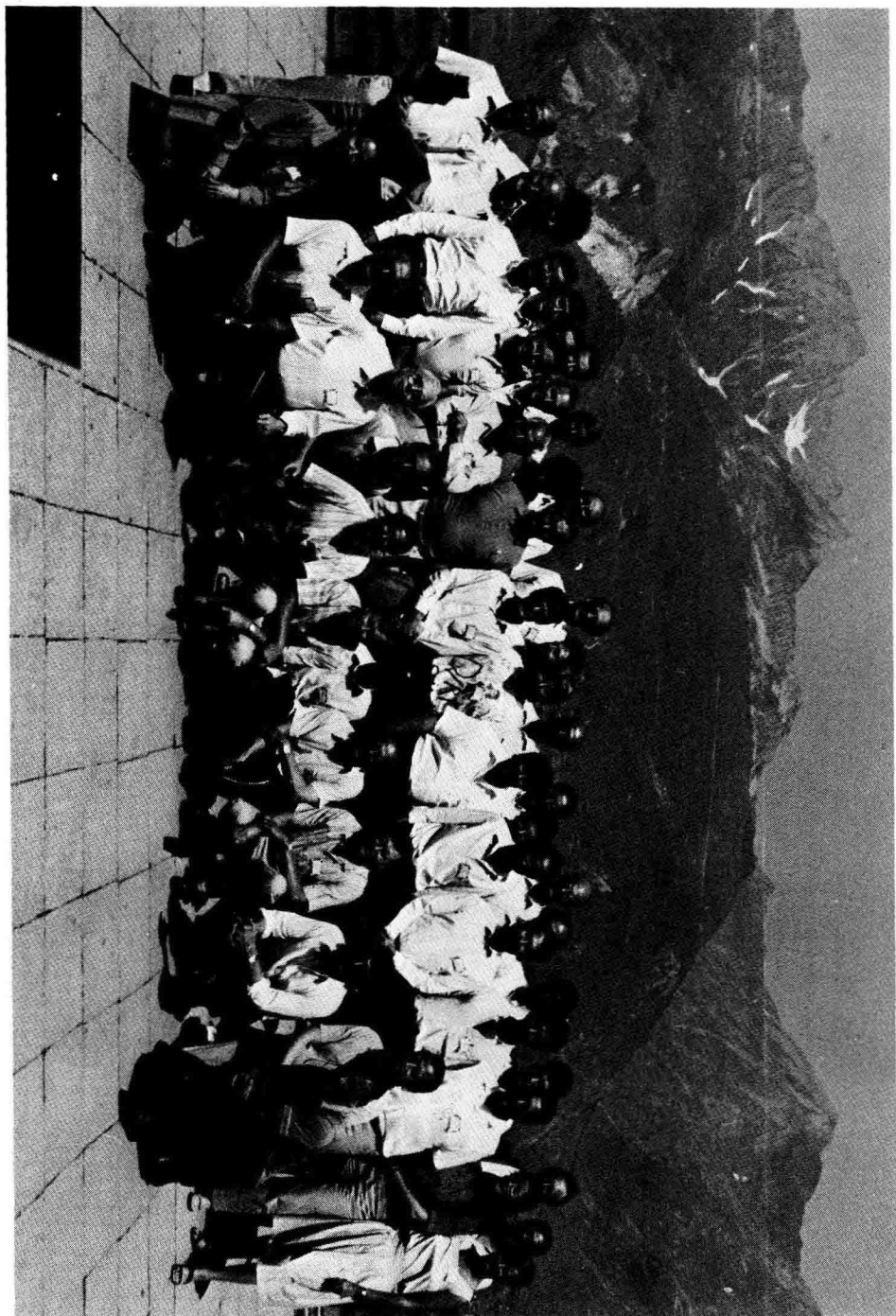
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# NATO ASI Series

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## INTRODUCTION SESSION

## COAL CHARACTERIZATION IN RELATION TO COAL COMBUSTION

Harald Jüntgen  
Professor Dr.rer.nat.

# 1. INTRODUCTION

Most coals are used worldwide for combustion today. Generally all kinds of coals are applicable for combustion. The major methods of burning are fixed bed firing, fluidized bed firing and suspension firing. The last technique is used in big industrial plants for electric power generation. In fixed bed firing heating rate is slow (a few K/s), and combustion time ranges from minutes to hours, depending on particle size. In fluidized bed combustion heating rates can be estimated at  $10^3$  to  $10^4$  K/s, burning temperatures are between 800 and 900° C, and burning times are in the order of minutes. In suspension firing heating rates also are high, temperatures are more than 1500° C, and burning times are in the order of seconds. In these firing systems characteristic and very different particle sizes are used: Lump coal in a range from 5 to 50 mm in fixed bed firing, crushed coal in a size range from 1 to 5 mm in fluidized bed firing, and pulverized coal with sizes of below 100  $\mu$  in suspension firing.

It is generally agreed that particle size of coal is the most defining parameter with respect to the dominant reaction mechanism of combustion /1/. Beyond that coal properties also influence the combustion behaviour. As combustion of coal is a complex process consisting of several parallel or consecutive reactions, which are partly governed by heat and mass transfer phenomena, it can not be expected that there are simple correlations between parameters of physical and chemical coal structure on the one hand and overall characterization parameters of coal combustion on the other hand. There is the fundamental need to have a clear picture of the influence of coal properties on combustion behaviour, because coal properties are very significant for practical questions of design and operation of combustion technology. There is the need to design boilers for a much wider range of coals, for equipment both smaller and larger than previously used, and for more exact operation conditions /2/.

The relationship between coal properties and combustion behaviour can be considered under various aspects. First of all it has to be taken into account that coal properties systematically change with coal rank. Some chemical, physical and calorific properties of coal are needed for achieving the heat and mass balance for boiler design.

As previously shown the particle size is a fundamental question of using different burning technologies, and hence it follows that design of crushing equipment is a precondition of boiler performance. Therefore mechanical properties of coal are important for the characterization of crushing behaviour and grain size distribution.

An especially important task is the prediction of the combustion behaviour. That is only possible, if the mechanism of the basic steps of combustion is identified, and if a relationship between the characteristic coal properties and important parameters of each basic step has been established. Then there is the hope that the modelling of single steps of combustion and their coaction can also be performed.

To meet the demand for minimizing the discharge of sulfur, nitrogen oxides, and particulates the correlation between the occurrence of nitrogen and sulfur in coal and the formation of correspondent gaseous compounds during combustion must be understood better. Also coal properties by which boiler slagging and fouling are affected are of great interest.

The aim of this paper is mainly to discuss the relationships between coal properties and performance of basic steps of combustion like pyrolysis, ignition and combustion of pyrolysis products, and of ignition and combustion of residual char. Another important point is the description of coal nitrogen in respect to  $\text{NO}_x$  formation.

## 2. CLASSIFICATION OF COAL ACCORDING TO RANK

Coal is a chemically and physically heterogeneous rock, mainly containing organic matter. It principally consists of carbon, hydrogen and oxygen and on less amounts of sulfur and nitrogen. Coal also contains ash forming inorganic components distributed as discrete particles of mineral matter throughout the coal substance.

Coals originated through the accumulation of plant debris that were later covered, compacted and changed into the organic rock we find today. The conversion - called "coalification" - is based on biological reactions in the first stage, followed by a second phase in which geochemical reactions take place. This phase can be described by a very slow pyrolysis reaction under specially low rates of heating /3/4/. This transformation successively leads to peat (in the case of humic coals) lignite, bituminous coal and anthracite. The progress in this coalification scale (figure 1) is called the rank of coal and is suitable for coal classification. Coal properties determining rank like moisture content, carbon content, content of volatile matter and mean reflectance of vitrinite are listed in table 1. There the relationship to the rank is also shown.



Typical ultimate analysis of coals of different rank are given in figure 2. From there it can be seen, that with increasing rank the H/C ratio and the O/C ratio are decreasing. That can be interpreted - as will be shown in the following - by a loss of functional oxygen containing groups and by an increase of the aromaticity of the coal-macromolecule.

The properties of coal are not only influenced by their rank but also in a certain extent by the kind of precursor material and the kind of the environments during the coalification process. So humic coals are developed in mostly oxidative environments and pass through a peat stage in which the so called huminification takes place. Sapropelic coals which are relatively rare are formed in more reductive environments and do not pass a peat stage.

The petrographic components of coals are defined as macerals and can be characterized by microscopy. They are derived from different precursor materials. Single maceral are summarized in maceral groups, those precursor materials, H/C ratio and aromaticity values are listed in figure 3. The most frequent maceral group in humic coals is that of vitrinites. Therefore the determination of the rank is based on the mean reflectance of the vitrinite.

The development of the different macerals can be best demonstrated in the H/C versus O/C diagram shown in figure 4. D.W. van Krevelen has given an extensive explanation in his book /5/.

A diagram of more practical purpose is that of figure 5 in which experimentally derived relationships between volatile matter, carbon content, hydrogen content, H/C ratio and mean reflectance are shown /6/. A correlation between the maximum vitrinite reflectance and the content of vitrinite on C, S, H and N is given in figure 6 /7/.

### 3. COAL PROPERTIES NEEDED FOR ESTABLISHING HEAT AND MASS BALANCE FOR COAL COMBUSTION

The standard coal data needed for setting up the mass balance, their relationship to coal rank and to other parameters are listed in figure 7 /8/. Most data, with the exception of ash content, mineral matter, S-content, N-content and specific heat of coke are related to rank parameters as volatiles, mean reflectance or ultimate analysis.

In the next figures some examples of correlations of these data are given for special coal basins. Figure 8 shows the C-, H-, and O-content of coals from the Ruhr district as a function of volatiles /9/. In figure 9 the correlation between volatiles and C-content is presented for lignites