The Dirty Face of Coal

The chemical makeup of coal, a surprisingly complicated material, is still poorly understood despite centuries of study and use

By IVARS PETERSON

"Coal is a beautiful material," says Herbert L. Retcofsky. "Cut a thin section, look at it under a microscope, and you'll see brilliant reds and yellows." Sometimes visible, imprinted in the rock, are the delicate traceries of prehistoric plants.

Coal also presents a frustrating, yet fascinating, puzzle. Although it has been mined, studied and analyzed for centuries, researchers are still debating the origins and chemical structure of coal.

The problem is that one lump of coal is chemically unlike another. The term "coal" covers a wide range of organic materials with vastly different compositions and properties. Perhaps the only general statement possible about coal is that coal is a dirty, combustible rock.

Retcofsky, analytical chemistry chief at the U.S. Department of Energy's Pittsburgh Energy Technology Center, deals with both the beautiful and the dirty aspects of coal. His laboratory has analyzed coal samples from shipwrecks to determine their origin and studied the chemical reactions that occur while coal burns.

The great variability of coal allowed the laboratory to determine for National Park Service historians the origin of a small lump of coal recovered from a California coast shipwreck. The sample came from the paddlewheel steamship *Winfield Scott,* which ran aground and sank 130 years ago off Anacapa Island in the Santa Barbara Channel. The lab was able to tell the historians, interested in U.S. trade practices during the California gold rush, that the coal had come from Wales.

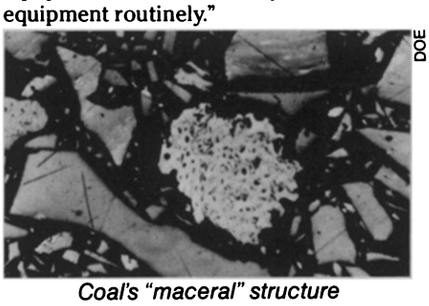
The same variability that allows coal analysts to pinpoint a sample's origin provides headaches for users of coal. Many processes are sensitive to coal composition. Coal liquefaction, for instance, involves breaking the complex molecular networks that compose coal into smaller pieces. Retcofsky says, "You can burn almost any organic material and get carbon dioxide and water, but when you're going only part of the way, the composition and structure are important."

Even the burning of coal is no longer a simple matter. Trace elements and minerals present in coal can poison pollution control devices and keep them from operating effectively. Systems designed for coal from one mine may not work as efficiently for coal mined elsewhere. At times, coal taken from different places in the same seam has caused problems.

At last month's International Conference on Coal Science, held in Pittsburgh, more than 600 coal scientists discussed their progress toward unraveling the structure of coal. Many of the papers described the effects of various coal properties on processes like liquefaction and combustion.

In his keynote speech, Irving Wender of the University of Pittsburgh quoted another coal researcher, "When I am asked what particular research on coal would be of most practical value to those who have to sell it, equally with those who have to use it, I have no hesitation in saying: research on the composition of coal."

During the last two decades, as improved analytical techniques became available, a new model of coal's structure emerged. George R. Hill of the University of Utah in Salt Lake City commented on the advances. "In the 1950s and 60s, it was almost impossible to induce a proud possessor of a new mass spectrometer ... or a sophisticated infrared absorption spectrometer to put 'dirty' coal into his equipment," he said. "Today, we use such equipment routinely."



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Coal's "maceral" structure

Hill contrasted the present picture of coal to earlier chemical models. Coal was once thought to consist of sheets of carbon atoms arranged in a pattern of six-sided rings, laid out neatly like tiles on a floor. Hydrogen, nitrogen and oxygen atoms were randomly scattered throughout this graphite-like structure.

The newly emerging molecular picture of many coals is of a three-dimensional network of units, each consisting of several carbon rings. These units are linked by methylene (CH_2) chains or oxygen, sulfur, nitrogen and hydrogen atoms. In fact, coals typically contain a mixture of these gigantic "molecules," with one molecule sometimes caught in the web of another. Although some researchers have described coal's structure as polymeric, it lacks the uniformity and regularity common to polymers like polyethylene and nylon.

In addition, coal may trap clays and microscopic mineral crystals (including compounds of heavy metals). K.C. Hsieh of the University of Illinois at Urbana-Champaign commented, "It is very likely that [with enough persistence] almost any mineral existing in nature might ultimately be found in coal."

Coal's variety is not limited to the molecular level. Although to the naked eye, coal usually appears to have a uniformly black face, a light microscope reveals complex patterns. Just as rocks consist of mixtures of minerals, coals contain mixtures of "macerals." In contrast to minerals, however, macerals do not have a well-defined chemical composition. Instead, these distinct components appear to reflect different plant origins.

The maceral vitrinite, for example, is the most common ingredient in coal and is derived from wood. The presence of exinite, which contains resin droplets and plant remains like pollen and spores, may account for the tendency of some coals to ignite spontaneously (SN: 8/27/83, p. 133). Fusinite, largely responsible for the dirtiness of coal, consists of the charred remains from forest fires. Like a chunk of charcoal, a fusinite-containing coal lump leaves a black mark on a piece of paper.

Some researchers argue that coal's widely varying composition may make it impossible to develop a coal chemistry that adequately accounts for all of the variation. One scientist noted, "What we call 'coal' may be a whole series of only tenuously related families of organic materials."

James J. Reuther of Pennsylvania State University in University Park introduced his paper with a similar remark. "Various coal combustion phenomena have been scientifically investigated for several decades now and remain very complex, inadequately understood and controversial," he said. "This dilemma is the result, in part, of the simple fact that there is actually no such material as coal, but there are only coals, ranked according to various ... criteria."

In spite of these pessimistic views, investigating the inner arrangement of coal is the kind of challenge that coal scientists relish. Retcofsky is optimisic that refinements in analytical techniques will allow a steadily deeper understanding of coal's quirks. Particularly promising are nuclear magnetic resonance methods that may pinpoint the location of hydrogen atoms within coal molecules. When coal is heated up, it should also be possible to watch what happens to the molecules, Retcofsky says. "I would like to see physicists pay a little more attention to coal," he adds, to help develop other methods for peering into coal.

In the meantime, however, even coal analysis suffers its share of mysteries. William McKinstry, who analyzed the *Winfield Scott* sample, says, "Because it is so sample-dependent, I often refer to coal analysis as black magic." □