Our technical message is clear: dwindling mineral resources in the aggregate, with the exception of reduced carbon and hydrogen, are per se unlikely to cause Malthusian catastrophe. But the exception is critically important; man must develop an alternative energy source. Moreover, the incentive to keep the price of prime energy as low as possible is immense. In the Age of Substitutability energy is the ultimate raw material. The living standard will almost surely depend primarily on the cost of prime energy. We therefore urge moving as vigorously as possible, not only to develop satisfactory inexhaustible energy sources—the breeder, fusion, solar and geothermal power—but to keep the program sufficiently broad so that we can determine, perhaps within 50 years, the cheapest inexhaustible energy source.

Our social message is less clear and certainly less optimistic. Although we see during the Age of Substitutability no insuperable technical bars to living a decent rather than a brutish life (assuming, of course, a stable population), whether in fact this will happen is far from certain. As Heilbroner (*19*) has pointed out, local shortages, which in the course of history are destined to be viewed as transitory, can and do cause large social and political instability. Heilbroner's "wars of redistribution," pitting the overpopulated have-nots against the underpopulated haves, could collapse society long before our carbon runs out. That the Age of Substitutability will, in principle, be autarkic, since mankind will no longer depend on reduced carbon (which is located in a few places), is little solace for governments or peoples today who look upon shortages of coming decades as threatening our entire social structure. We do not argue that the Age of Substitutability will be an easily achieved technological heaven-on-earth. Rather we urge attention to those institutional deficiencies that now prevent us from passing through stage 2 of our human voyage without causing the boat to capsize. The landfall, if we arrive at stage 3, should be surprisingly better than the catastrophists have predicted.

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11. A convenient small battery that does not use scarce materials and lasts a long time is an obvious target for research. However, if such a battery were never developed, we could revert to standard miniaturized dry cells (based on zinc and manganese) with only slight inconvenience. It must be remembered that in a 25-g cell used to power a portable computer, there are only 10 g of mercury. Even if the price of mercury rises 100-fold, the overall cost of the computer would rise by $12 if we elected to stay with the mercury battery instead of converting to shorter-lived, cheaper Zn-Mn dry cells. In the longer term, a substitute for the lead battery also may be needed.
12. Other examples of elements with finite resources that may have very high leverage are silver, which is used in photography; tungsten, in tool-making; lead and antimony, in storage batteries; beryllium, in beryllium-copper alloys; and perhaps manganese, in steel-making. More study is needed to identify other such critical situations.
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15. Even if copper is replaced by aluminum, the energy per ton of avalloy changes by less than 10 percent.
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20. We wish to thank E. R. VanArtsdalen and G. Marland for their help in preparing the manuscript. Oak Ridge National Laboratory is operated by Union Carbide Corporation for the Energy Research and Development Administration. The Institute for Energy Analysis is operated by Oak Ridge Associated Universities for the Energy Research and Development Administration.

Chemicals from Coal

By-products of conversion of coal to clean fuels will offer new options to the maker of chemicals.

Arthur M. Squires

Coal maintained its historic role in the chemical industry until the close of World War II (*1*). By 1950, however, new procedures and new products were firmly established as prime opportunities for growth: to give examples, ammonia from methane, synthetic rubbers, polyethylene, and aromatic feedstocks from petroleum. The United States abandoned ammonia and methanol from coal in the mid-1950's. By now, the shift to petrochemicals is almost complete. The role of by-product coke ovens is greatly diminished: they supply only 10 percent of the U.S. benzene market and 2 percent of the phenol. Petrochemicals now take 10 percent of the U.S. oil and gas supply, and have expanded at 7 percent per year in recent years.

When and where will petrochemicals give way, as they eventually must, to a revival of chemicals from coal?

A return to coal will be slow. The historic shift to petrochemicals was fast not only because oil and especially gas (*2*) were often cheaper than coal but also because processing equipment for the cleaner, fluid fuels is far cheaper. The equipment can conveniently reach large rates of production from individual processing units (*3*). Historic coal conversions did not develop beyond unit sizes that are far too small to be congenial now. Much development effort lies before the question, When and where? A better question might be, What among many R & D opportunities can pay off soonest?

Chemicals as By-products

Coal chemicals were mostly by-products of two carbonization procedures, one to supply town gas (*4*), and another, coke for steelmaking. Even ammonia synthesis depended upon gasification of the coke by-product of town gas manufacture (*5*). Viewed broadly, petrochemicals are by-products of the production and delivery of gas and oil for use as fuels.

One factor conducive to preeminence of

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petrochemicals has been the steady advance in throughputs of petroleum in refineries. Quantities of oil treated are now so large that even a constituent present in a minor amount can be plucked out and provided for chemical use at a cost no competition could meet.

Even after world production of oil flags, as it eventually must, flows of hydrocarbons that undergo some sort of processing will continue to increase. Most U.S. refineries convert well beyond 90 percent of domestic crude oil to products of high economic value, such as fuels for transport and home heating, lubricants, and chemical feedstocks. Refineries elsewhere, in general, convert much less of the crude oil to such materials, often only about 50 percent. The remainder is provided as heavy fuel oil to industry, including industry of the United States, which imports fuel oil. Revamping of refineries for further treatment of heavy oils will reinforce, for some time to come, the petroleum processor's advantage as a supplier of many chemical feedstock species.

Another factor that will extend the role of petrochemicals on the world scene is the impending development of gas resources of countries far from industrial populations. Such resources now provide tempting investment opportunities. Iran will ship gas to Europe via pipeline. Much gas will reach the United States in liquefied form (LNG). The United States is willing to import gas at around \$3 per million British thermal units (1 Btu = 1.055×10^3 joules). This puts the value of gas almost anywhere in the world at around \$1 per million Btu's as soon as someone provides the large capital needed to build LNG plants and tankers.

Development of the gas resources of Venezuela, Nigeria, Indonesia, Saudi Arabia, Qatar, Abu Dhabi, Kuwait, and expecially Iran will enable these countries to dominate the world's supply of ammonia and methanol for decades. Ammonia already moves in world commerce in 50,000-ton tankers, and a 70,000-ton vessel is on the way. Venezuela is shipping ammonia, and Arab commitments in petrochemicals exceed \$20 billion, with more than \$30 billion in projects under study (*6*). Proved reserves of natural gas in the Middle East are about 20 to 30 percent of the world's total (*6*). Iran is the giant: its proved reserves are already comparable to those of the United States, and probable resources are far greater, yet present production is but 5 percent that of the United States.

Existing technology for converting coal to ammonia or methanol cannot compete in much of the United States with conversion of natural gas to these chemicals in Venezuela, for example. Gas now being flared in that country could be converted to ammonia for sale in the United States at a price well below the cost of ammonia from coal (*7*). The Venezuelan ammonia would still be competitive if gas in Venezuela were valued at about \$1.50 per million Btu's. This comparison takes into account a shipping cost of about \$45 per ton. Gas in Venezuela could be valued at about \$2 per million Btu's for conversion to methanol for the United States, taking into account a shipping cost of about \$25 per ton.

No doubt it will be good policy to have some domestic ammonia and methanol synthesis to establish a domestic price and to ensure at least a partial supply. Some production from subbituminous coals of the West may even be economically competitive in local markets because of high costs to ship the imported chemicals over land.

By-products of Clean Fuels

These considerations lead to the view that early opportunities for chemicals from coal must be sought where coal is processed in very large amounts for other needs.

The projection of world oil production shown in Fig. 1 (*8*) suggests that the world market for heavy fuel oil may dry up soon. Indeed, the major oil companies of the world already have in hand the design studies for revamping refineries to convert heavy oil to lighter, more valuable products. Only specialists in methods of technological change can fully appreciate how alarmingly short the time is that remains before the world must make a major shift from oil to coal for its industrial energy needs (*10*).

It goes without saying that a return to coal must not recreate the "smoky Pittsburghs" of the past. The urgent R & D goals are processes for clean combustion of coal and its conversion to clean industrial fuels.

Such processes can provide the earliest R & D payoffs: they will be simpler and cheaper to develop and build, as well as higher in coal conversion efficiency, than processes for synthetic methane or gasoline. This is not to say the latter are not important, but as I pointed out before (*4*), the quickest way to capture significant supplies of "new" gas and oil is to convert existing boilers and furnaces to clean fuels from coal.

Which processes for clean fuels from coal can be realized the soonest? What chemical by-products might they yield?

Gasification with Steam and Oxygen

I do not see much play, at least soon, for complete gasification of coal by steam and oxygen. Costs are high, especially for gas cleaning. The Lurgi gravitating-bed gasifier (*4*), for example, makes a gas difficult to clean because of tars. Gas from the Koppers-Totzek system (*4*) contains much extremely fine dust. The latter system also faces a heavy cost for gas compression if the gas is required at pressure.

Complete gasification yields primarily H_2 and CO. The latter can be converted to hydrogen by the reaction

$$CO + H_2O = CO_2 + H_2$$

and scrubbing out CO_2. Partial conversion of CO to H_2 yields a synthesis gas for methanol

$$CO + 2H_2 = CH_3OH$$

Complete conversion to H_2 and addition of nitrogen yields a synthesis gas for ammonia

$$N_2 + 3\,H_2 = 2\,NH_3$$

The Office of Energy R & D Policy of NSF engaged Chem Systems, Inc. (*7*), to study chemicals from coal and identify R & D objectives worth pursuing. Chem Systems recommended work on systems for complete gasification that yield synthesis gas at high pressure. The gas should contain the least possible amount of methane, hence also, zero tar.

Chem Systems endorsed work in progress at the Pittsburgh Energy Research Center of ERDA on homologation of methanol by its reaction with synthesis gas to yield ethanol (*11*)

$$CH_3OH + CO + 2\,H_2 = C_2H_5OH + H_2O$$

The latter can be dehydrated readily to supply ethylene.

The Electric Power Research Institute is looking at the interface between systems for coal-based synthetic alcohols and electricity generation. An urgent need of the electricity industry is a clean liquid fuel to fire gas turbines used to meet peaks in demand for electricity. In past screenings of catalyst formulations for methanol synthesis, those that gave higher alcohols were passed over. Tailoring a catalyst for large yields of higher alcohols could give a gas turbine fuel while allowing some "creaming off" of methanol for sale as a chemical.

By Fischer-Tropsch synthesis and related syntheses, CO and H_2 can be converted to an astonishing variety of products (*12*): liquid fuels, lubricants, waxes, soaps, detergents, alcohols, aldehydes, and acids, and even fats reported to be similar in taste and nutritive value to natural butter (*13*). Many of the products were made on what was a large scale for the German economy of 1944.

South Africa has operated a Fischer-Tropsch plant for nearly 20 years, and has recently announced a nearly tenfold expansion from the present daily output of 4000 barrels of gasoline and a variety of chemicals. Australia has announced a plant of comparable size.

The thermal efficiency of Fischer-Tropsch synthesis, in practice, is below 50 percent; capital cost is high; and its development in South Africa and Australia is attractive because coals are available there at unusually low costs. Chem Systems (*7*) concluded that liquids from the synthesis, when conducted in gas- or liquid-fluidized beds of catalyst, are expensive feedstocks for cracking to ethylene in the United States. Ruhrchemie AG of West Germany, however, has worked to modify the synthesis in its fixed-bed reactor to afford increased yields of C_2 to C_4 olefins. On laboratory evidence Schnur (*14*) projects a product running as high as 50 to 55 percent ethylene and propylene. Schnur believes that this product might represent an economic proposition at coal costs appreciably higher than those for the South African and Australian enterprises. The Ruhrchemie reactor, as it appears in the South African installation, is so small in scale as to be uncongenial to U.S. engineering thought, but it ought to be remembered that reactors contribute but a minor part of the total capital cost of a Fischer-Tropsch installation. Ruhrchemie is developing a larger fixed-bed reactor.

As improvements are made in coal gasification techniques, recurring reevaluation of Fischer-Tropsch synthesis would appear in order. The best opportunities may lie in approaches that yield a variety of products, including synthetic methane for sale to pipeline gas companies. Laboratory work on Fischer-Tropsch catalysts can be expected to increase yields of specific chemical products. In the long run, large supplies of synthesis gas are certain to appear in plants for converting coal to gasoline or synthetic natural gas. At the least, it may be anticipated that parasitic syntheses of chemicals will follow.

Partial Conversion of Coal

The need suggested by Fig. 1 is so urgent that development opportunities must be sought that offer the fewest hurdles. Proposals for advanced systems for complete gasification or liquefaction of coal face difficulties that could take much time. It is sensible to look closely at proposals for partial conversion of coal that ought to be easier and quicker to develop.

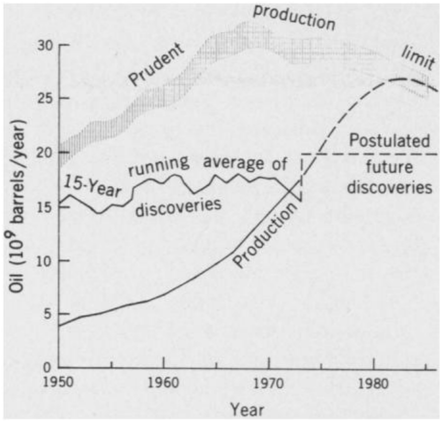

Fig. 1. Projection of oil production in non-Communist countries made by Warman (*8*) just before the Yom Kippur War. He reckoned annual discoveries of oil on basis of present knowledge of their size. Since production should not prudently exceed about 1/15 of reserves, collision between growing demand and declining production capability became inevitable when production topped the 15-year running average of discoveries, unless oil geologists could promptly step up discovery. The projection assumed future annual discovery at 20 billion barrels. Warman (*9*) estimates the current discovery rate at about 10 billion barrels. An offsetting factor is reduced growth in demand, caused by OPEC's increase in price as well as by economic recession.

Such proposals, of course, face the problem of marketing a by-product coke or char. This should not be too difficult, once everyone understands in his bones, as well as in his head, the difficult spot the world is in. There is sure to be a great expansion in combustion of coal. It might as well be coke or char. Burning these solid fuels in pulverized form presents no great problem if a fuel gas is furnished in relatively small amount to stabilize the flame. Availability of these fuels, however, will give the advantage to the new fluidized bed combustion systems (*15*).

Other things being equal, there will be an advantage for proposals that yield coke or char in form of relatively large particles, rather than as a fine dust. Special advantage will accrue to proposals that yield a coke low in sulfur. Availability of such coke in lump form could stimulate the production of fuel gas on a small scale in air-blown gas producers (*4, 5*).

Some interesting possibilities would not yield a coke of sufficiently low sulfur content if practiced on the high-sulfur coals more common in the eastern part of the United States, but would yield such a coke from the low-sulfur coals typical of the West. These possibilities should be studied because bringing western coal East may be the best way to put many boilers and furnaces into compliance with sulfur dioxide emission standards. Commonwealth Edision Co. of Chicago is already burning about 9 million tons of Montana subbituminous coal per year, and eastward shipments of such coal are certain to increase. Their interception in plants to cream off a clean fuel gas or liquid could make good sense.

With a few exceptions, recent U.S. efforts have dealt with complete conversion of coal to a single product, and therefore multiproduct proposals have received less attention. There is room yet for invention. I offer the following discussion of several such proposals, some still in the laboratory, as much to illustrate as to direct attention to specific ideas.

Flash Pyrolysis

Occidental Development Company, Inc., is developing a process for flash pyrolysis of coal at atmospheric pressure (*16*). The coal would be heated almost instantaneously to about 925°C, and the residence time of vapor product at this temperature would be about 2 seconds. Working on a typical subbituminous coal of the West, the process could convert about 30 percent of the coal to a gas having a higher heating value, when dried, of about 630 Btu per cubic foot (1 standard cubic foot at 60°F and 1 atmosphere = 0.0268 normal cubic meter at 0°C and 1 atmosphere). The process yields about 10 percent tar, but Occidental proposes to recycle the tar, cracking it to extinction. The raw gas is rich in ethylene, and the process, if exploited on a large scale, could supply a significant fraction of U.S. demand for ethylene.

Char of 0.6 percent sulfur content would result from a typical Western subbituminous coal containing 0.83 percent sulfur. The char would meet the current legal requirement for fuel in the United States. An electric utility operating both coal-fired and gas- or oil-fired boilers might adopt flash pyrolysis to supply char to the former and gas to the latter, especially if the latter are expected to operate at a high load factor for a number of years.

Partial Gasification by Steam

A surprise of the Synthane development of the Pittsburgh Energy Research Center of ERDA was appearance of methane in gas at elevated pressure from steam-fluidized beds in amounts leading to calculation of equilibrium ratios near the top line of Fig. 2, which I published in 1961 (*17*). Lines A, B, and C in Fig. 2 had shown a downward trend in equilibrium ratio for steam-fluidized gasification of anthracite, cokes, and chars as pressure increased. I had supposed a similar downward trend would appear for gasification of raw coals of bituminous and lower rank. The new Synthane data (*18*) were for a lightly pretreated bituminous coal.

I hypothesized (*17*) that the equilibrium ratios of Fig. 2 reflect a quasi-equilibrium between hydrogen and the active carbon present in a steam-fluidized bed. Dent (*19, 20*) had pointed out that gasification kinetics in such beds are dominated by the fact of solid mixing, which brings frequent exposure of carbon to steam at high concentration near the bottom of the bed, reactivating the carbon. Gasification reactivity of an oven coke, that has soaked for many hours at more than 1000°C, is poor in a gravitating bed, yet is comparable in a fluidized bed to reactivity of anthracite or a char made at much lower temperature (*21*). Yields of methane during early stages of gasification of a fresh char (Fig. 3) (*17, 22*) tend to support my hypothesis with respect to Fig. 2. The early yields suggest that activity develops substantially to the level for continuous gasification of a raw bituminous coal and then declines. The percentage of carbon gasified is greater for lines A, B, and C of Fig. 2 than for the top line.

The credibility of the hypothesis is enhanced by data from a U.S. Bureau of Mines experiment on the reaction of Pittsburgh seam coal in a fixed bed with steam at 400 atmospheres (*23*). The coal was heated in flowing steam to 800°C in 2 minutes, and the coke was quenched directly thereafter. If it be assumed that substantially all gas was made in the second minute of the 2-minute heat-up time, one calculates a methane equilibrium ratio of 0.32 from the gas yield data. If it be assumed that substantially all gas came off in the last one-half minute, one gets 0.55. It might be noted that the gas, water-free, contained 39 percent methane. The calculated ratios compare with 0.75 from the top line of Fig. 2. It should be emphasized, however, that I would limit the hypothesis to steam-fluidized beds. There is no reason to expect Fig. 2 to correlate equilibrium ratios from fixed beds and dilute suspensions or from reaction of coals with hydrogen (*24*).

A commercially attractive operation can be visualized with essentially no extrapolation from known large-scale experimental facts. Figure 4 is a new concept for gasification of coal in a fast fluidized bed (*25*), with the advantage that reaction of steam and raw coal is conducted in a zone that is free of products of combustion. The concept takes advantage of the fast bed's relative freedom from the massive backmixing of gas that characterizes a slow, bubbling fluidized bed (*26*). Gas from the top of the steam-reaction zone ought to have a methane content approaching that indicated in the top line of Fig. 2. For operation at an elevated pressure, this gas will be a rich fuel gas. In the upper part of the vessel, the gas mixes with products of combustion of coke with oxygen that occurs in the annular space provided around the upper part of the steam-reaction zone.

A calculated example for Illinois bituminous coal uses a vessel 3.66 meters in inside diameter and 20 meters tall working at 20 atmospheres and 900°C. The velocity of the fluidizing gas is 3.66 meters per second. Coal feed is 8509 tons per day (1 short ton = 0.907 metric ton) on a moisture-and-ash-free basis, and the coke product is 4332 tons per day on the same basis. The percentage gasification of fixed carbon is less than that for most data on the top line of Fig. 2. The fuel gas product has a higher heating value of 536 Btu per cubic foot after removal of water, sulfur species, and carbon dioxide. The product's total heat value amounts to 101,000 million Btu's per day, and so it could substitute for about 100 million cubic feet of natural gas per day or about 17,000 barrels of oil per day. Oxygen consumption is 1810 tons per day (*27*), and steam flow is 166.5 tons per hour (*28*).

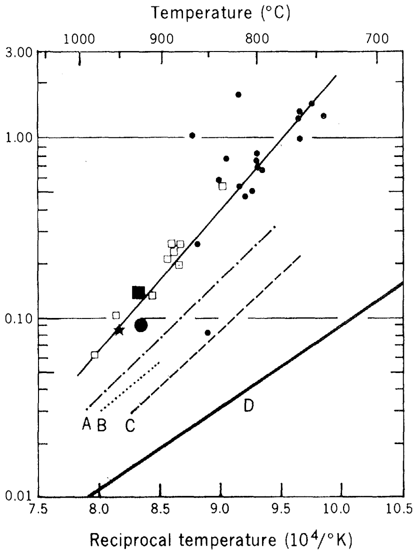

Fig. 2. Methane equilibrium ratios (*17, 18*), $y_{CH_4}/y_{H_2}{}^2P$, reckoned from composition of gases emerging from steam gasification of coals and chars in fluidized beds; y, mole fraction; P, pressure in atmospheres. ★ and □, A caking bituminous and a subbituminous coal, respectively, treated at atmospheric pressure. •, Peat at atmospheric pressure. ■ and ●, Synthane pilot units at 25.5 and 40 atmospheres, respectively (711 and 102 mm in inside diameter, respectively). The top line is based on data where all carbon in volatile matter and, typically, about one-half of the fixed carbon were gasified. Line A represents atmospheric-pressure gasification of anthracite, cokes, and chars that were previously soaked in nitrogen for many hours at gasification temperature. Line B is for a bituminous char, also soaked in nitrogen, at 9.3 atmospheres. Line C is for anthracite at 12 to 17 atmospheres. Data for lines A, B, and C in general reflect gasification of more than 80 percent of the fixed carbon. Line D is thermodynamic equilibrium for graphite.

Distributing Industrial Gas

Processes like Fig. 4 or like Occidental's flash pyrolysis could supply fuel gas attractive for distribution to industrial parks or industrialized regions extending for scores of miles. A process working at elevated pressure would have the advantage of reducing costs for gas compression. Costs for cleaning a gas at high pressure also are less, especially in the case of a process like that indicated in Fig. 4 where operating conditions may be chosen to eliminate tars.

Candela's suggestion (*29*) that a regional system for industrial fuel gas might embrace the entire northeastern portion of the United States is worth examining. The system might be put together, at least in part, by preempting a portion of the present pipe network for distributing natural gas. The system would restore lost flexibility in fuel supply. It could provide fuel gas for peaking gas turbines as well as for combined cycle systems. It could provide fuel gas to retrofit old oil- or gas-fired boilers that have only a few years of remaining life or that operate at low load factor. Gas could be added to the system wherever it passes a coal field or a large customer for coke or char by-product.

Gas from the system could be re-formed with steam at low capital cost to provide synthesis gas for ammonia or methanol. This is the best hope for domestic sources of these chemicals to compete with sources from countries like Venezuela and Iran. In the long run, the price of industrial gas from regional systems might govern the world price of these chemicals.

Flash Hydrogenation

Chem System's study for NSF (*7*) identified flash hydrogenation as an R & D objective that could lead to aromatic feedstocks of low cost as by-products of conversion of coal to synthetic natural gas. Flash hydrogenation is a variant of the Hydrane process under development for a number of years at the Pittsburgh Energy Research Center of ERDA (*30*). Coal would be heated rapidly in hydrogen at high pressure, and the vapor product of reaction would be quenched after a residence time at temperature of only seconds. The City College Clean Fuels Institute (*31*) has reported conversion of 10 percent of carbon in Illinois bituminous coal to benzene, 7 percent to ethane, and 14 percent to methane in experiments at 700°C, 100 atmospheres, and a vapor residence time of 3 seconds. Brookhaven National Laboratory (*32*) reported somewhat higher conversions of lignite to benzene. Ethane from flash hydrogenation could become an important source of ethylene.

Supercritical Gas Extraction

Well known to producers of natural gas is the phenomenon of retrograde condensation, the condensation of the heavier hydrocarbon species present in the gas when its pressure is reduced. The opposite of this phenomenon may be termed "supercritical gas extraction," the vaporization of heavy molecules by a gas above its critical pressure. The equilibrium content of the heavy molecules in the "extract" is greatest if the critical temperature of the extracting gas is close to the temperature of the experiment. Great Britain's National Coal Board (NCB) (*33, 34*) has studied supercritical gas extraction of coal for a number of years.

To understand how extractable material can be present in coal, consider the reactions that occur when coal is heated slowly. Kirov and Stephens (*35*) provided insight into these reactions by subjecting a large number of Australian coals to parallel thermogravimetric, viscosimetric, calorimetric, and chloroform extraction experiments. These authors identified two chemical reactions that occur before coal decomposes to release appreciable quantities of gas and tar vapor.

"Reaction 1" occurs between about 250° and 300°C, and is evidenced by an endotherm amounting typically to a little under 0.2 kilocalorie per gram-atom of carbon in the coal. There is a decrease in the coal's acidity, and Kirov and Stephens speculated that reaction 1 involves the breaking of hydrogen bonds, since participation of a phenolic hydroxyl group in such a bond increases its acidity.

A second endotherm, typically about the same in magnitude as the first, announces "reaction 2" between about 340° and 400°C. There is an increase in phenolic oxygen, and Kirov and Stephens speculated that reaction 2 is a splitting of ether bonds,

$$R_1OR_2 = R_1O^{\cdot} + {}^{\cdot}R_2$$

followed by transfer of nearby hydroaromatic hydrogen in the coal to satisfy the free valences and give

$$R_1OH + HR_2$$

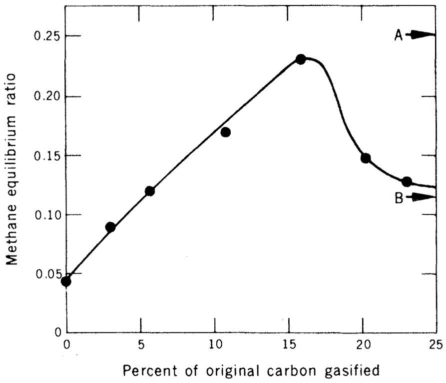

Fig. 3. Methane equilibrium ratios (*17, 22*) during early stages of gasification of a fresh bituminous char (never soaked at temperature in nitrogen) in a steam-fluidized bed at 871°C and atmospheric pressure. Arrow A points to equilibrium ratio for raw coal (top line of Fig. 2). Arrow B points to the ratio for chars previously soaked in nitrogen (dot-dash line of Fig. 2).

They speculated that the ratio of hydroaromatic hydrogen to ether oxygen may be an important parameter for characterizing coals (*36*). Kirov and Stephens emphasize that both reactions 1 and 2 are rapid and appear to involve a tiny fraction of the chemical bonds in the coal.

Australian coals of lower and higher rank (below and above, respectively, about 85 percent carbon content) display distinctive behavior with respect to chemical decomposition and development of fluidity when heated at 3°C per minute. In both types of coal, reaction 1 is accompanied by only minor release of water vapor and alkyl aromatic species. After a coal of lower rank has been heated to 350°C and then cooled, it will release a larger extract to chloroform at 100°C than will unheated coal. Reaction 1, on the other hand, liberates little additional matter extractable by chloroform from a coal of higher rank.

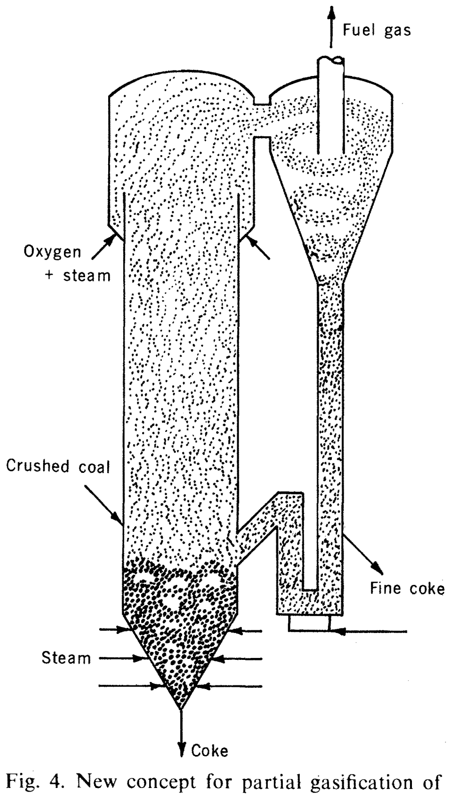

Fig. 4. New concept for partial gasification of coal by steam in a fast fluidized bed.

In a bituminous coal, reaction 2 develops plasticity (*37, 38*). A coal of lower rank begins to decompose almost at once, and remains plastic over only a relatively small temperature interval as the coal is heated further at 3°C per minute. In a coal of higher rank, on the other hand, reaction 2 precedes significant releases of gas and tar vapor. Such a coal melts over a narrow temperature range, at the same time releasing material extractable by chloroform at 100°C. Typically, the viscosity of the fluid coal is about 1×10^6 poise. This remains nearly constant over a 30° to 40°C interval during subsequent slow heating. Onset of decomposition occurs well after melting. Later on, loss of fluidity occurs over a relatively narrow temperature range, a little ahead of the temperature at which the rate of decomposition is at a maximum.

NCB (*34*) reports that supercritical toluene at 350°C extracts 17 percent of a British 802 coal (such coal contains more than 36 percent volatile matter and is very weakly caking). Another report (*33*) suggests that yields up to 33 percent are obtained at about 400°C with fractions of coal tar or petroleum naphtha as extracting gas. Yields of gas and water are small. This is consistent with Kirov and Stephens' views concerning their reactions 1 and 2, and NCB appears justified in its conclusion that supercritical gas extracts have undergone little if any chemical degradation during their extraction. It might also be remarked that recombination or polymerization reactions, such as lead to the solidification of a fluid bituminous coal as it undergoes decomposition, probably play little if indeed any role in supercritical gas extraction at temperatures up to 400°C.

The extracting gas including extract has a low density and viscosity, making separation of undissolved char residue easy. Reduction to atmospheric pressure causes the coal extract to precipitate, allowing its separation from extracting gas.

I understand the separated extract to be a solid at normal temperature, but to melt below about 100°C. The NCB's toluene extract at 350°C contained 0.1 percent sulfur, and this suggests that an extract of many U.S. coals from the West might be sufficiently low in sulfur to find use as a utility fuel, attractive for retrofitting oil- and gas-fired boilers as well as for firing gas turbines. Study of this opportunity would appear in order.

NCB (*33*) reports that the extract residue is a porous, nonagglomerating char. Extraction of high-volatile coals at 350°C should yield a char still containing a significant amount of volatile matter, an aid in pulverized fuel combustion. An incidental benefit for U.S. coals from the West would be removal of their typically high content of water.

About 20 percent of the toluene extract at 350°C was an oil soluble in petroleum ether, about 65 percent asphaltenes soluble in benzene, and the remainder "pre-asphaltenes" insoluble in benzene. The average molecular weight of the oil was about 300, that of asphaltenes, about 600 (*39*). Atom ratios of hydrogen to carbon were about 1.20 and 1.05, respectively.

Examination of the toluene extract by spectroscopic methods and gas chromatography revealed an aromatic skeleton of open chain structure. Substituted benzene units are strung together along with smaller numbers of naphthalene, dihydroanthracene, and other larger aromatic moieties. Biphenyl linkages, methylene and ether bridges, and hydroaromatic units bind the structure. Nearly all aromatic units carry methyl or higher alkyl groups.

Reduction in molecular weight could produce chemical feedstocks, especially benzene and a variety of alkyl benzenes. The NCB (*34*) pointed out that the open chain structure offers the prospect that this might be easily accomplished. Indeed, some processing of the extract might be necessary to replenish the extracting gas. If so, supercritical gas extraction of coal would almost inevitably become a supplier of by-product chemicals.

I should emphasize that supercritical gas extraction remains in the laboratory stage of its development. It awaits engineering study before its potential can be judged. I discuss it here, in part, to illustrate what may emerge if more thought is given to opportunities for partial conversion of coal to clean fuels.

Chemicals from Coal Tar

The glorious history of the coal tar industry's great service to mankind makes it sad for me to set down my belief that this industry faces a dim future. Chemicals derived from coal tar have always represented a small fraction of the total, a by-product of a by-product, as it were. I cannot conceive that new carbonization plants will be built simply to supply chemicals.

The future of coal tar depends upon the future of gas-making processes that yield tar, carbonization as a technique for providing liquid fuels, and operations to supply the steel industry with coke.

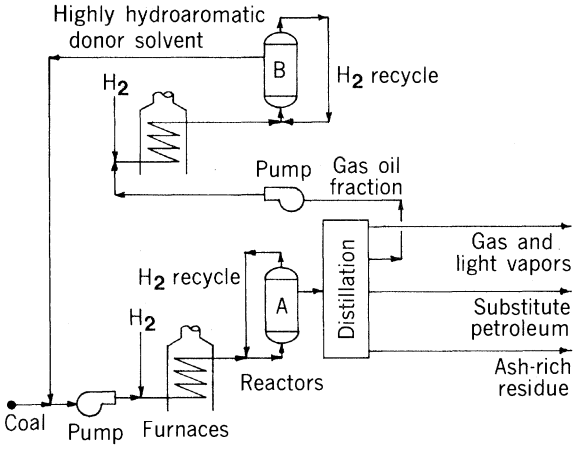

Fig. 5. Exxon's coal liquefaction process (highly schematic). Reactor A is noncatalytic. Reactor B contains catalyst and probably operates at higher pressure.

The Lurgi gravitating-bed pressure gas producer (*4*) may provide basis for a few plants to provide synthetic natural gas, although even this proposition has been thrown in doubt with realization that a Lurgi plant for 250 million cubic feet per day (about 0.4 percent of the current U.S. gas demand) will cost on the order of $1 billion. Major supplies of tar chemicals are not likely to arise from this source.

I see little future for carbonization as a technique for supplying liquid fuels. Tars are difficult and expensive to upgrade to synthetic petroleum or chemicals. They usually crack and deposit coke upon reheating for their supply to a catalytic hydrogenation; and, when a furnace cannot be used, the cold tar must be injected into a large flow of hot hydrogen just ahead of the catalyst. Conversion of tars to useful products entails large consumption of hydrogen. Attempts to develop catalysts that will convert anthracene to two molecules of toluene, for example, have not been successful (*40*). Phenanthrene has been converted catalytically to biphenyl, but only in small yield (*41*). Work toward such goals is worth continuing at the bench, but does not yet provide basis for commercial hopes.

Slot ovens for metallurgical coke are long-lived, and many ancient ovens are still in use. The steel industry for its expansion is apt to turn to new coke-making processes [for example (*42*)] more easily made acceptable environmentally and capable of processing a wider range of coals. Some new processes yield more benzene than conventional ovens, and Chem Systems (*7*) assumed that the steel industry will continue to supply about 10 percent of the benzene demand. A hazard to this assumption is the development of large shipments of steel from countries like Venezuela and Iran (*43*).

Coal Liquefaction

Direct liquefaction of coal is far from ready for use on a modern scale. A plant for 100,000 barrels of synthetic oil per day would need to process about 30,000 tons of coal per day. Germany's largest Bergius unit in World War II treated 600 tons per day, and the largest pilot unit now operating in the United States is for 50 tons per day. Most developments still work at a far smaller scale.

Most approaches liquefy coal through the agency of a donor solvent. Finely divided coal is slurried with an oil rich in polycylic species that contain both aromatic and hydroaromatic ring structures. When the slurry is heated to beyond about 400°C, the hydroaromatic rings of such species can release hydrogen. The aromatic rings that result from this release can be easily hydrogenated to restore the species' original capability of "donating" hydrogen to the coal. Tetralin (1,2,3,4-tetrahydronaphthalene) is an example of a donor solvent species. It is converted to naphthalene when it releases its four available hydrogen atoms.

Coal in the heated slurry reacts rapidly to release, in high yield, matter soluble in pyridine and benzene (pre-asphaltenes and asphaltenes, respectively) (*44*). The release of this matter occurs even if a donor solvent is not present (*45*), but in its absence, much of the matter polymerizes irreversibly to "coke" (*46*). The donor solvent's role, apparently, is to inhibit formation of coke by providing hydrogen to satisfy free valences that appear in the reacting coal substance.

With further time at temperature, the pre-asphaltenes and asphaltenes are converted by slower reactions to oils soluble in pentane.

Engineering approaches differ primarily in selection of location in the processing sequence at which the "spent," hydrogen-lean solvent is hydrogenated to restore its donor capability.

Current thinking in the United States is running against the Pott-Broche process approach, operated in Germany during World War II at the 100-ton-per-day scale. The coal-solvent slurry is pumped to a moderate pressure, 10 to 30 atmospheres, and held at about 425°C for an hour to dissolve about 75 percent of the coal. Dissolved material is separated from a solid residue, pumped to a higher pressure, and hydrogenated catalytically. A gas-oil fraction of the product is recycled to provide the donor solvent. In this approach, separation of unreacted coal and ash from reaction product is difficult.

Most U.S. efforts are elaborations of the Uhde approach, also operated in Germany. The slurry is pumped to a high pressure, typically 100 to 200 atmospheres; hydrogen is added; and the slurry is held at 425°C or beyond in presence of hydrogen to dissolve more than 90 percent of the coal. Hydrogen's role is apparently to restore at least part of the solvent's donor capability during the coal treatment, for it appears that the coal should contain ash matter having some catalytic virtue toward hydrogenation of the solvent.

Pittsburg & Midway Coal Company, a subsidiary of Gulf Oil Company, and, more recently, Southern Services Company and the Electric Power Research Institute have used the Uhde approach to produce a "solvent refined coal" that is low in sulfur and suitable for firing utility boilers and gas turbines. Hydrocarbon Research, Inc., a subsidiary of Dynalectron, the Pittsburgh Energy Research Center of ERDA, the Gulf Oil Co., and the Lummus Co. have modified the approach by adding a catalyst to the dissolution step to promote better hydrogenation of the solvent. These modified processes can operate to make a "refined coal" suitable for utility use, or at more severe conditions, such as 200 atmospheres and 455°C, to make a substitute petroleum.

In a further elaboration of the Uhde approach, Exxon (see Fig. 5) prepares a donor solvent by hydrogenating a synthetic gas oil under severe conditions. The solvent acquires a greater content of hydroaromatic carbon than has been used hitherto. Exxon's discovery is that the greater power of this solvent to donate hydrogen can convert coal in presence of hydrogen gas to a relatively light liquid. This can be distilled to provide both the synthetic gas oil for reuse and a petroleum substitute. Ash-rich residue from distillation is sufficiently small so that it can be disposed of by combustion or gasification. Exxon's approach has the advantage of avoiding a difficult filtration of ash residue from coal liquid.

Development of a coal liquefaction industry will eventually create opportunities for pulling out light aromatics and phenols. For the purpose of cracking to make ethylene, coal liquids are at a disadvantage with respect to the more aliphatic shale oils.

The Acetylene Alternative

Acetylene is a competitor for ethylene for making materials such as vinyl acetate, vinyl chloride, and acetaldehyde. Work has been in progress for many years on rapid pyrolysis of coal in a plasma arc at temperatures beyond 1400°C to make acetylene. Yields are of the order of 30 to 35 percent by weight of the coal, with 12 to 17 percent acetylene by volume in the gas leaving the pyrolysis reactor. There is a large recycle of hydrogen to the arc, and the process requires extensive equipment for acetylene recovery and gas purification. Operation is cyclic, since carbon tends to deposit in the reaction chamber, and frequent injections of steam are needed for its removal.

Chem Systems (*7*) believes that plasma arc processes have the potential of making acetylene competitive with ethylene, but they face large and difficult development tasks. Chem Systems assigned these a relatively low priority, since acetylene can substitute for ethylene in only about 17 percent of its uses.

Conclusion

For some time yet, chemicals will remain by-products of systems that supply natural gas, natural petroleum, and clean fuels from coal. The last-mentioned presents exciting near-term opportunities, especially in connection with clean fuels for industry that are so urgently needed. In the longer run, the world will be able to choose flexibly among gas, oil, and coal for supply of almost every fuel-based chemical.

References and Notes

1. Although ammonia from natural gas first appeared early in World War II, procurers of munitions deemed it prudent to build large plants synthesizing ammonia from gas made by gasifying coke in water-gas sets.
2. After World War II, development of pipelines made natural gas the cheapest industrial fuel in many parts of the United States, and gas displaced coal as a source of chemical process heat and often even as fuel to boilers for process steam. Coal held its place only in the manufacture of electricity, steel, and cement.
3. Sometimes a new petrochemical procedure could be taken directly from the laboratory bench to a commercial scale, and therefore many petrochemical engineers came to consider the pilot plant obsolete. Engineering education tended to deemphasize synthesis of engineering art and came to emphasize the analysis that would allow piloting on an ever smaller scale. Forgotten was how developers of historic coal conversions had struggled with problems of preparing, feeding, and processing coal; of withdrawing ash or coke; of purifying the gas or liquid product that was often contaminated by matter present in an amount so small as to remain undetected until it brought trouble in pilot operation. Some recent efforts in coal engineering have remained too long under analysis, delaying truths that only large pilot operations can reveal.
4. A. M. Squires, *Science* **184**, 340 (1974).
5. Disappearance of gas coke removed a factor for flexibility in supply of clean fuel since air-blown producers (*4*) can easily convert coke to power gas.
6. D. C. Ion, *Availability of World Energy Resources* (Graham & Trotman, London, in press).
7. Chem Systems, Inc., New York City, "Chemicals from coal and shale: An R. & D. analysis for National Science Foundation," No. PB 243,393 (National Technical Information Service, Springfield, Va., 1975). Chem Systems developed costs for methanol and ammonia on the scale of 1000 tons per day and used either the Koppers-Totzek gasification system (*4*) or a hypothetical improved system yielding gas under pressure. The capital for coal-based plant is more than double that for a plant based on gas.
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25. J. Yerushalmi, D. H. Turner, A. M. Squires, *Ind. Eng. Chem. Process Des. Dev.* **15**, 47 (1976).
26. A. M. Squires, in *Future Energy Production: Heat and Mass Transfer Problems*, J. Hartnett, Ed. (Hemisphere, Washington, D.C., in press).
27. Oxygen requirement of the Koppers-Totzek system is more than 4000 tons per day for production of 101,000 million Btu's of gas per day at far lower heating value.
28. The concept of Fig. 4 is also attractive with substitution of air for steam and oxygen to the annular combustion space. A gas at a heating value approaching 225 Btu per cubic foot can be made at 20 atmospheres, a remarkable figure for an air-blown gasifier. I should note that the fast fluidized bed is also well suited for "moving burden" gasification, in which heat of reaction is supplied by circulating hot solid from a combustion zone [J. W. R. Rayner, *J. Inst. Fuel* **25**, 50 (1952); M. E. Sacks and R. T. Eddinger, in *Coal Processing Technology* (American Institute of Chemical Engineers, New York, 1975), vol. 2, p. 94]. I prefer the simpler arrangement of Fig. 4 as quicker to develop, recognizing that improvements can follow.
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39. D. S. Montgomery [Fuels Research Centre, Department of Energy, Mines and Resources, Ottawa, Canada, personal communication, 1972] cleaved ether bonds in a western Canadian Cretaceous coking coal (Balmer 10, containing 89.4 percent carbon) and subsequently octylated the material by a procedure given by Sternberg *et al.* (*38*), to obtain a substance more than 90 percent soluble in benzene. The substance had a molecular weight that reflected a molecular weight of about 300 in the material after the cleaving of ether bonds and before the octylation. It may also be noted that asphaltenes from Synthoils made at 415° and 450°C display molecular weights of 686 and 417, respectively [H. W. Sternberg, R. Raymond, F. K. Schweighardt, *Science* **188**, 49 (1975)].
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46. It is tempting to associate Kirov and Stephens' reaction 2 with the release of soluble matter; also, to associate its subsequent conversion to coke in absence of a donor solvent with the solidifcation of a fluid bituminous coal as it undergoes slow heating. Coals of lower rank are harder to liquefy, and this fact may reflect chemical disparities that also underlie differences in behavior of coals of low and high rank as they undergo pyrolysis (*37*).
47. Work on the fast fluidized bed and flash hydrogenation of coal at The City College is supported by grant AER-72-03426 A (formerly GI-34286) from the RANN Program (Research Applied to National Needs) of NSF. For informative discussions, I thank M. Sherwin of Chem Systems, Inc., L. Topper of the Office of Energy R & D Policy of the NSF, and S. B. Alpert, R. H. Wolk, and W. C. Rovesti of the Electric Power Research Institute.

World Changes and Chances: Some New Perspectives for Materials

Trends in use, world trade, and international politics define issues and research directions.

S. Victor Radcliffe

In a controversial revival or reexamination of Malthus's hypothesis, system dynamics models of the world economy have suggested that the resource constraints of a finite planet will not permit ongoing trends in population and industrial growth to continue far into the future. Shortages of materials are identified as one of the key limiting factors. Despite their uncertainties, such analyses, combined with recent world events, do affirm the significance of materials and the other natural or physical resources as part of the larger economic and social system. It is in these terms rather than solely technical ones that this article focuses attention on the role of materials over the transition period from now into the early part of the next century and beyond.

How are we to get from here to there without being more certain where *there* is? How can goals and policies involving materials be formulated to facilitate the transition, and how can science and technology assist in discerning better the most likely long-term demands on natural resources—for what and in what quantities—and the options for meeting them? In particular, how can we better assess what priorities appear appropriate for materials research? This article attempts a preliminary attack on such questions. It is based on the belief that we must better understand the present and how we got here before we are likely to be prescient as to the resource needs and opportunities of the transition period and the further future.

Materials and Natural Resources

Appropriate research for materials, if it is to be conducted in the manner now accepted for such other major resources as energy and food, should encompass the full spectrum of activities involved in the materials system, that is, the resources from which materials are derived, their processing and utilization, and the discharges and wastes to which such activities give rise. The interrelationships of materials and the other natural resources are shown in Fig. 1 in terms of the flow of resources, as means to attain given ends, through the successive production stages of "raw materials" and "processed materials" (both of which figure prominently in world trade as the "primary commodities") into industrial use and consumer use. These different types of derived resources have key common features: (i) their importance lies less in their being specific things or substances than in providing "the function or operation of attaining a given end such as satisfying a want" (*1*), and (ii) they are dynamic, in that they are created, and in some cases, destroyed, by man.

The delineation of function as a key

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