

AN ASSESSMENT OF MATERIALS REQUIREMENTS AND RESEARCH NEEDS FOR OPEN CYCLE MAGNETOHYDRODYNAMICS (MHD) SYSTEMS

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Abstract - Major programs are underway in the United States and elsewhere to develop and demonstrate a number of advanced coal-to-electricity conversion systems. The principal efforts are centered on MHD, fuel cells, and gas turbines as these technologies hold more or less equal promise to fulfill the potpourri of needs of the utilities and industry. All, however, have equally challenging technical problems which ultimately relate to the degradation of materials under extremely hostile service conditions.

For MHD, significant progress in engineering component development has been made and no longer are "proof of concept" and commercial feasibility questioned. Acceptance of the technology by the industrial sector still requires further demonstration of the performance, reliability, and durability of many interacting parts and components. Durability and reliability of MHD materials of construction are indeed prime issues which probably can be resolved through a combination of engineering/economic trade-offs and materials development derived from directed basic and applied research.

This paper attempts to put the materials issues confronting MHD in proper perspective through a review of the development status of the overall system on a component-by-component basis. Pressing materials problems are defined and related to high temperature research needed to assist in their solution. Emphasis is placed on materials applications in the MHD generator (electrodes) and heat exchangers as these components present the most demanding service conditions.

INTRODUCTION

Under the current national energy plan the United States is pursuing a variety of strategies designed to reduce its dependence on oil imports and to provide renewable, essentially inexhaustible sources of energy needed for sustained economic growth. Within this context the U.S. Federal Government is supporting a number of fossil energy technology R&D programs, from their early developmental stage on to providing the engineering basis for commercial demonstration of those technologies which are technically, economically, and environmentally most promising. One major objective of the fossil energy program is to, "Develop systems that will use coal in a more economic, efficient, and environmentally acceptable manner for the 1990's and beyond" through consideration of:

- ° MHD electric power generation (coal based)
- ° Fuel cells based on coal-derived fuels for either urban central station or dispersed electric generation
- ° High temperature turbines for improved efficiency as well as turbines that allow combustion of heavier and dirtier fuels
- ° Other advanced thermodynamic cycles (i.e., pressurized fluidized bed and combined cycle gasifier with high temperature turbine) and heat recovery systems.

Thus, the fossil energy program strategy involves the development of several coal-to-electricity conversion systems which can satisfy the future needs of industry and the utilities. As these needs are complex and difficult to quantify it is projected that a combination of conversion systems will be required. Presently, MHD occupies a place in this combination.

The purpose, then, of this paper is to examine the potential role of MHD vis-a-vis alternate technologies, to assess its current development status, particularly in the materials area, and finally, to define high temperature research efforts needed to help alleviate some of the more pressing materials (Note a) problems.

Note a. No attempt will be made here to describe MHD principles, concepts, and systems or to elaborate in detail results and accomplishments of the various fossil energy programs or projects; it is assumed that the reader has a working knowledge of these aspects. Further, individual citations will not be given as these are far too extensive for detailed compilation. Prime literature references, however, are included in a general listing at the end of this paper.

BACKGROUND

MHD role

The utilities and industry require a wide assortment of efficient and reliable coal-to-electricity (and/or heat) conversion systems which can accommodate the very specific needs of the user. These may be generally categorized as:

<u>System</u>	<u>Principal Candidate Conversion Technology</u>
<u>Central power</u>	
Large central station plants for base, intermediate, or peaking load operation	- MHD - Gas turbine - Fuel cells (?)
<u>Dispersed power</u>	
Small-to-medium municipal or industrial plants for cogeneration (electricity and process heat), residential/commercial total energy supply and small-scale utility power	- Fuel cells (except cogeneration) - MHD (cogeneration only) - Gas turbine

Within the above classification three primary conversion technologies--MHD, fuel cells, and gas turbines--hold more or less equal promise to fulfill commercial needs. Each has their advantages and unique technical problems to overcome before they can reach the marketplace. R&D programs presently are in place in the United States, principally with Government support, to solve attendant problems. The nature of problems, however, is diverse and, therefore, it is difficult to present one-on-one comparisons. Nevertheless, some common denominators are evident and worth pursuing.

Potential applications. In the combined cycle mode, MHD, being a volume device (efficiency improves with scale), is ideally suited for central station base load applications. Gas turbines have the similar attributes. Peaking and intermediate load commercial systems needs also can be satisfied by both MHD and gas turbines. It is noteworthy that under the Soviet program MHD peaking systems will be the first commercially demonstrated. Gas turbines have been used by the utilities for years for peaking service, but these have proven to be inefficient single cycle systems. On the other hand, fuel cells, although conceptually possible, hold no real immediate potential for central power applications. Their real forte lies in dispersed systems. Gas turbines (single cycle) have equal potential in this area as waste heat can be utilized for industrial processing or space heating. MHD, except for some unexplored cogeneration possibilities, is inappropriate for dispersed systems.

The potential offered by MHD, fuel cells, and gas turbines ostensibly is attractive and comparable. This conclusion is supported by the landmark Energy Conversion Alternatives Study (ECAS) and by other studies by the Electric Power Research Institute (EPRI), at least for base load central power systems having a variety of system configurations and conditions. In the majority of cases, the costs of electricity (COE) are about equal and favorable, and the environmental impacts are projected to be in compliance with the EPA new source performance standards. The results of these studies, however, were generally based on optimum system arrangements selected to produce the best possible efficiencies and COE's without a full accounting of their technical achievability in part or in total, or of the resulting ramifications of the failure to meet necessary objectives of associated R&D programs.

Fuels. The utilities and industry require a degree of fuel flexibility. MHD is the only conversion technique which can meet this need; it can be adapted for either direct coal use (coals of all classes) or for oil or gaseous fuels, though probably not on an interchangeable basis. As gas turbines and fuel cells must operate on very clean liquid or gaseous fuels, usage of coal would require extensive pretreatment (i.e., gasification, plus hot gas cleanup).

Reliability and durability. Reliability and durability of parts and components of conversion systems are of prime consideration to the utilities, especially for base load applications. Equipment must be reliable in its operation; it must have a reasonable degree of maintainability with scheduled outages totaling no more than 500 to 1000 hours per year; and it must have a predictable endurance. In essence, the utilities wish no surprises. Endurance requirements are difficult to estimate as they depend upon specific system configurations and purpose and attendant costs of replacement or repair. For MHD, the generator is the most critical component where estimated lifetimes for continuous operation range between 2000 and 10,000 hours. A similar durability figure might be projected for gas turbines. Fuel cells (stacks) need to operate 40,000 hours to gain favorable cost competitiveness. Most tests to date for each of the conversion systems have been under less than stringent service conditions necessary for commercial acceptance. Even so, none have achieved maximum design goals. In all cases materials limitations are the prevailing problem.

R&D program objectives. Each R&D program adheres to a development philosophy of building on past experience through the testing of units/facilities of increasing complexity and more severe operating conditions. All have a definite engineering orientation; supporting

applied and fundamental research, especially in the materials area, is less than optimum for an emerging technology.

Of the three programs, only MHD has a set of goals and schedules which encompasses a complete combined cycle (MHD and steam) demonstration facility (currently targeted for the late 1990's). From what can be perceived from limited access to program planning documents it appears that gas turbines (2600 °F inlet temperature, clean fuel) might be "technically ready" by 1990. An integrated commercial scale, combined cycle, base load system will be ready at some unspecified time thereafter. For fuel cells, a 4.8 MW phosphoric acid type, hydrogen fueled demonstration facility is now in place (1980) to establish operational feasibility and system integration of an early design. Second generation, molten carbonate fuel cell systems are "being sought" by 1990 to determine their commercial feasibility (not demonstration). Third generation solid oxide types are much further downstream. Generally both the fuel cell and the gas turbine programs must develop and demonstrate the most advanced designs in order to match MHD's potential. Here the technical (materials) problems are as formidable as those confronting MHD.

Overall, MHD, gas turbine, and fuel cell technologies have a potential for fulfilling the potpourri of needs of the utilities and industry. The exact mix remains to be decided. All have challenging technical problems mostly of a materials nature. Associated R&D programs have rather optimistic development schedules and commercial fruition of advanced systems might come at a later date than now projected (i.e., > year 2000). At present all three must be viewed as companion, not competing technologies.

Historical perspective

Electric power generation by MHD had its embryonic beginnings in 1831 with the work of Michael Faraday on the principles of electromagnetic induction. Although the first patents on MHD devices were generated as early as 1911, specific development did not begin until 1942 when Westinghouse attempted (unsuccessfully) to demonstrate a combustion driven MHD generator. In 1959-60 MHD became a laboratory reality with the the operation, though of short duration, of sizeable generators at AVCO and Westinghouse. These successes, coupled with advances in plasma physics and superconducting magnet technology promoted private and Government interest in MHD technology for both utility power and military applications. Research programs of varying sizes were established in the mid 1960's in the United States, Soviet Union, England, West Germany, France, Japan, and Poland, primarily under Government sponsorship although there was some private investment. In the late 1960's enthusiasm of the western governments began to diminish primarily because of the optimistic expectations regarding the development of nuclear energy. The English, French, and German efforts were terminated, while the Japanese and United States programs were held at minimum levels pending review. The Soviet Union, on the other hand, accelerated its program to commercialize MHD.

In the United States the review of MHD was conducted under the auspices of the Office of Science and Technology. The OST panel, in its 1969 report, confirmed the potential of MHD for electric power applications, especially for coal fired systems, and recommended further development at a level of about \$4 million yearly with equal support to be provided by Government and industry. Based on the OST review the Office of Coal Research in 1971 commissioned the Massachusetts Institute of Technology to further define the technical issues facing MHD and to propose a systematic program for its development. The resulting MIT plan called for a nine-year, three-phase program which included the construction and operation of a 300 MW_T pilot plant. If successful, a fourth phase, a five and one-half year effort, would follow to demonstrate commercial readiness (1500 MW_T base load facility).

Although the initial elements of the MIT plan were started with Government support, financial backing by industry never materialized to any great extent. Thus, MHD technology development languished in the United States until the mid-1970's when, prompted by the realization of an impending energy shortfall, a host of advanced energy conversion programs (MHD, gas turbines, fuel cells, etc.) were revitalized or started through the newly-formed organizations--Energy Research and Development Administration (ERDA) and Electric Power Research Institute (EPRI).

MHD program plans

In 1975 EPRI developed a program strategy (An Overall Program for the Development of Open Cycle MHD Power Generation), modeled in part after the MIT plan. Although EPRI itself never proceeded to the implementation stage, its plan was essentially adopted (with variants) by ERDA and the Department of Energy (DOE), ERDA's successor. The DOE program plan (Note b) revolves about a three-phase approach to commercialization as outlined below.

Note b. A companion "Environment Development Plan" was formulated by DOE in 1977. This plan basically calls for environmental, health, and safety issues to be keyed to and addressed as the technology development progresses.

<u>Phase</u>	<u>Approximate Time Span</u>
Phase I	
<ul style="list-style-type: none"> ◦ Demonstrate engineering and performance of major components including combustor, generator preheaters, superconducting magnet, and heat/seed recovery systems ◦ Design and construct CDIF, CFFF, and AEDC facilities ◦ Test components and subsystems in CDIF, AEDC, and CFFF ◦ Establish commercial plant base-line design ◦ Complete ETF conceptual design 	FY 75 → 86
Phase II	
<ul style="list-style-type: none"> ◦ Design and construct the ETF ◦ Demonstrate ETF system performance ◦ Optimize components and subsystems ◦ Complete preliminary design of commercial scale plant 	FY 84 → 90 (and beyond)
Phase III	
<ul style="list-style-type: none"> ◦ Design, construct, and operate full scale plant to demonstrate commercial feasibility 	FY 89 → 97 (and beyond)
<p>Notes: CDIF - Component Development Integration Facility, Butte, Montana CFFF - Coal Fired Flow Facility, Tullahoma, Tennessee ETF - Engineering Test Facility (Pilot Plant) AEDC - Arnold Engineering Development Center Facility, Tullahoma, Tennessee</p>	

In an effort to accelerate the commercialization process, DOE in December 1979, proposed a two-phase alternate strategy. In this, Phase III (above) would be eliminated and Phase II modified to include an expansion in size of facilities (CDIF--from 50 to 100 MW_T and ETF--from 250 to 500 MW_T). DOE believed that this alternate plan would demonstrate commercial feasibility and result in time and dollar savings.

In 1981, with the change in Administration in the United States, the DOE MHD effort underwent a complete re-evaluation. As of this writing (July 1981), the future direction of the U.S. Federally-supported MHD program is not known.

ASSESSMENT

General Status

The efficacy of open cycle, coal burning MHD system for utility and industrial applications depends on the performance, durability, and reliability of many interacting components. Durability and reliability are prime issues and a number of significant technical questions must be resolved to demonstrate that the technology will be commercially acceptable. These questions are reviewed below with respect to each major MHD component/subsystem.

Combustor. The development of coal-fired MHD combustors lags somewhat behind that for clean fuel MHD systems because the technology is relatively new and far more complex. Powdered coal fuel (~ 65 kg/s) must be burned with high efficiency at significant pressures (0.5 to 1.0 MPa) to generate a stable, uniform, high temperature conductive plasma (2700 to 3100 K) with a velocity near Mach 1. Additionally, with minimum heat loss, the combustor must effectively ionize a seed feedstock, accommodate a preheated flow of oxidizer, and tolerate the erosion/corrosion effects of molten and vaporized slag derived from the coal. Combustor design and development depend on the resolution of long-standing technical issues concerning how best to manage the corrosive slag. It is clear that construction materials will include cooled metals with partly solidified slag and, probably, sacrificial ceramic oxides as linings. More importantly, two distinct operating approaches are under consideration which include: (1) use relatively simple engineering designs to combust coal but allow a large portion of the slag to "carryover" to downstream components, and (2) use more complex designs so that a large portion of the slag (e.g., > 85 percent) is rejected at the combustor. Single stage combustors will handle the first approach and limited short duration experience for small units has been obtained. The large slag carryover (> 50 percent) option, however, transfers technical problems to other downstream components. Possible penalties include accelerated corrosion/erosion of downstream construction materials by large quantities of slag and severe difficulties in separating the slag from the seed at lower temperature regions in the system.

In principle, multistage combustors can be used for the second approach but testing experience is limited. Conceptually, nearly 90 percent of the slag is rejected at these complex units but the real thermodynamic and kinetic limitations have not been quantified for larger operations. For example, vaporized slag plus liquid entrainment may account for amounts far greater than the goal of a maximum 10 to 15 percent carryover. In this context, multistaged combustion may not differ substantially from the single stage approach. Presently, because of the lack of thermodynamic (and kinetic) information on slags, it is impossible to effectively model and predict slag transport in chemically complex, multiphase streams. Additionally, methods to maintain low solubility of seed in slag (an important economic consideration) by inexpensive oxide additions to the coal at the combustor remain laboratory curiosities and are not intended for serious testing. Resolution of these debatable, but not insurmountable, issues demonstrates the need for a perhaps accelerated effort to test these concepts. Realistic testing, however, cannot come about without effective modeling which factors in the fundamentals of slag chemical and physical characteristics. The "basics" of slags are so important that this aspect of the research efforts should be strengthened, even though the MHD effort has an engineering orientation.

Generator. The heart of the MHD system is the generator or channel which extracts the electrical energy from the conductive plasma moving through a magnetic field. Theory and experimentation with many small units throughout the world have proven the MHD concept. The critical design limitations for linear generators are well established so that a commercial scale device is technically feasible. However, channel construction materials (electrodes/insulators) are subject to excessive deterioration by the combined effects of large thermal/electrical/mechanical stresses and electrochemical corrosion/erosion. These degrading processes are present in varying degrees regardless of what fuel is used (even natural gas or gasified coal). Presently it has not been demonstrated conclusively that any combination of materials will function for greater than about 500 hours under continuous power generation. These tests were conducted in relatively sulfur-free environments. (A modest sulfur partial pressure in the plasma could be expected to alter (reduce) lifetimes drastically.) Other issues involving such factors as optimum heat losses, fine-tuning of electrode designs, interfacing, etc., appear solvable with time and are less important than the durability question. In this context, there may be ways to mitigate against the degradative processes; for instance, limited efforts are underway to develop "super-hot" wall generators. Conceptually, the generator would operate at high enough temperature (> 1800 °C) to avoid condensation of slag. Proponents believe that corrosion and other electrochemical problems associated with condensed slag will be avoided as the environment approaches that for clean fuel combustion. This approach, combined with a repairability concept (i.e., patching with cements having electrode compositions), is attractive and warrants greater attention.

Magnet and inverter. The superconducting magnet, and probably the inverter system, are the best developed components in MHD technology. Large magnets (4-6T) have been constructed in the United States and elsewhere. Given additional time for R&D, a commercial size magnet (nearly 6T, over a volume of ~ 100 m³), more than likely can be developed. Similarly, the technology to adapt existing inverter systems to MHD is available and only engineering questions related to methodology need be addressed.

Downstream components. The remaining but by no means trivial segment of an open-cycle MHD system consists of numerous components designed to increase overall efficiency. Although normally alluded to as the heat-seed recovery and bottoming plant systems, major functions include: (1) diminish velocity of the plasma exiting the channel while maintaining a high enough pressure to prevent pressure losses further downstream (a diffuser section, 2300 to 2400 K inlet); (2) slag/seed management (separation, removal, reprocessing, disposal), (3) residence chamber for NO_x control, if necessary; (4) secondary combustion, if necessary; (5) steam plant to generate ac power, and (6) preheat of oxidizer and, possibly, coal for the combustor.

Except, perhaps, for the first and last functions outlined, programs addressing the other subsystems are just now getting underway. Thus, although functional requirements are known only limited experimental and testing data are available. Problems associated with possible construction materials, therefore, are not quantified or thoroughly evaluated. Interfacing problems, including valving systems and ductwork, are largely unexplored. For example, the performance of a diffuser can be evaluated only after interfacing with several downstream subsystems.

Heating of the oxidizer for the combustor is possible by direct or indirect methods. Presently, no preheaters exist that are directly fired by the MHD gas stream. Several relatively small test beds, designed to evaluate construction materials and seed/slag flow characteristics, however, are operational. In contrast, the technology to develop indirectly fired or lower temperature directly fired, regenerative preheaters is available because of less stringent materials requirements. Preheat temperatures to 1675 K and, possibly, to 1975 K are within the state-of-the-art. At present, it appears that preheaters, indirectly fired by clean fuel or gasified coal, are realistic choices for first generation MHD systems. In addition, preheat temperatures could be decreased if heated air

is benefited with "impure" oxygen. Efficiency/cost penalties apparently are not too significant. Apart from the indirectly fired or low temperature directly fired regenerative preheater alternatives, major technical issues are not evident although interfacing within the MHD loop and further testing are necessary.

None of the essential components for the slag/seed management and seed reprocessing systems exist (except perhaps for injection of seed to the combustor). Slag/seed management will be dictated largely by the method proven best to operate the combustor (see above). For large scale carryover, slag must be extracted beyond the diffuser prior to the steam plant. The risk here is that the slag will have captured so much seed that separation at lower temperatures within the cycle is not technically possible. Separation of seed from solidified slag after extraction is a significant technical problem. Indeed, the philosophy of slag rejection at the combustor is traceable, in part, to these possible difficulties. External factors such as fuel, seed, and processing costs will define the seed losses that can be tolerated for fixed seeding levels.

During combustion with sulfur-bearing coal, seed, initially introduced in carbonate form, scavenges the sulfur within the cycle by forming potassium sulfate. This is beneficial from the standpoint of minimizing emission of sulfur oxides to the environment. However, at least part of this sulfate ultimately must be reprocessed for conversion to the carbonate. The thermodynamics of several reaction paths are well-established to perform this regeneration but kinetic limitations are unknown and engineering aspects and containment materials have not been developed. Seed management also should not ignore the tendency for highly corrosive trace elements (e.g., vanadium, halogens, heavy metals, etc.) to concentrate within the seed fraction during recycling.

Slag/seed management and processing is a complex, controversial subject which has produced conflicting results from laboratory studies and small scale tests. Technical issues and approaches appear manageable given testing experience with realistic components.

The steam generating portion of an MHD system is frequently cited as being similar to a conventional, coal-fired plant. Obviously, this technology can be utilized realizing that for current practice nearly 80 percent of conventional failures are due to corrosion, erosion, and fouling of metal tubing. The MHD exhaust, however, contains alkali seed which is expected to accelerate the corrosion of all heat exchange surfaces beyond the diffuser including the metal tubing of the steam plant. Laboratory testing suggests that super-alloys, protective metal claddings, and, possibly oxide coatings may solve the corrosion problem for the steam plant. High costs (i.e., very expensive materials) and technical issues related to design, fabrication, and actual operation of a plant (e.g., interfacing, seed removal, emergency combustors, etc.) will become important considerations.

Effective system control and safeguards for the environment and plant personnel are important for an integral MHD loop. Modeling of the system is demonstrating that computer control is possible using diagnostic process parameters. Reliable sensors for critical measurements are being developed currently but actual interfacing with control hardware is not well developed. Emissions detrimental to the environment are expected to be minimal. Particulates probably can be handled by modified conventional methods. Oxides of sulfur are scavenged by seed (see above) while NO_x can be controlled by appropriate operation of primary and/or secondary combustion. Conversion to nitric acid or use of catalytic secondary combustors are alternative procedures. The potential effects of large magnetic fields on workers remains undefined and should be investigated.

Materials

From the above discussion it is apparent that the development of power generation by MHD involves many technical questions some of which are of an engineering nature, others more basic. Most issues involve competitive procedural philosophies derived from limited laboratory and testing data. Further research and testing should resolve most of these conflicts. By far, a prime critical technical problem confronting MHD is the selection, design, and fabrication of construction materials for every component. Their durability and reliability must be qualified for in excess of thousands of hours before user (e.g., utility and metal/chemical processing industries) interest is justified.

The status of MHD materials is, however, a controversial subject in which a definitive, clear cut assessment cannot be made with unanimity. Nevertheless, in the authors' view, the general state of materials development might be summarized in a subjective way, as illustrated by Table 1. The table identifies major MHD components and gives a corresponding "materials rating," A through D, defined as:

- A (established): Data base sufficient; firm selections from commercial materials in required forms can be made; only minimal, routine engineering application required.
- B (near-term): Data base incomplete; a number of candidates can be identified from commercial or near commercial materials; short extra extrapolations from data base required through confirmatory testing and minimal R&D.

- C (developmental): A number of candidates are identifiable from developmental materials; data base incomplete and important gaps exist requiring large extrapolations; considerable R&D required.
- D (speculative): Only small number of candidates can be suggested; data base sparse or absent; extensive R&D required.

It is evident from the table that materials for MHD are still a significant technical issue basically because the MHD environment is so aggressive. The high temperatures and large thermal stresses coupled together with the presence of corrosive/erosive seed and slag media provide damaging processes which are most pronounced within the heat exchanger sections and in particular, in the critical generator area where destructive electrochemical effects are present. If materials and pertinent design were not major problems, MHD would be closer to commercial success despite other technical and cost factors.

TABLE 1. Materials status

Component	Rating [*]
Combustor	
- Metal Walls	A-B
- Ceramic Lining	C-D
Generator (Electrodes/Insulators)	
- Super Hot (> 1700 °C)	D
- Hot (1000 °C - 1700 °C)	D
- Cold (< 1000 °C)	C (low sulfur coals) D (high sulfur coals)
Magnet	B
Heat Exchangers	
- Ceramic Regenerator	
> 1500 °C	C
1200 °C	A-B
- Metal Recuperator	
600 °C	D
< 600 °C	A-B
Valves	C
Seed/Slag Management	C

^{*} See text for explanation of rating.

RESEARCH NEEDS

The development of materials for MHD is a fruitful field for theoretical and experimental research. Considering the urgency of progress toward commercially viable, coal based systems many of the problems are being approached in a pragmatic way. The emphasis has been, and still is, on the design of increasingly larger facilities and the testing of components and system performance. Little time and effort has been available for a systematic, scientific study of the physical and chemical processes that take place in a MHD system. This is particularly true for the area of materials investigation. It might be appropriate to innumerate for materials scientists some of the exciting problems where more fundamental to applied understanding is badly needed, not only for MHD but also for other advanced coal based technologies.

Coal characterization

There is no doubt that a major deficiency in the development of all coal conversion processes is our lack of knowledge of the composition, structure, and properties of coal. The three most important aspects of the feedstock in coal utilization are coal handling (which involves many physical properties of coal), the chemistry of coal reactions, and pollutants from coal. In all three areas the problems are complex, involving molecular structure of the coal, mineral constituents, and such properties as porosity and moisture content. During the last ten to fifteen years a number of new or refined methods have become available, offering means to provide much previously unobtainable information.

Although coal is a very reactive solid, very little is known about the relative abundance of various groups and their "organization" within the coal molecule. There is still considerable uncertainty about the fractions of aromatic and aliphatic groups. It should

be possible by application of high resolution NMR techniques (using ^{13}C as the nuclear probe) to learn more about the nature of the carbon bond and the hydrogenation process. The resolution of the NMR technique can be increased by using ultrahigh magnetic field, pulse sequencing, and "magic angle" spinning of the sample. It is important that this spectroscopy be applied to samples at high temperature.

After carbon and hydrogen, the elements oxygen, sulfur, and nitrogen are also important atoms present in coal. It is necessary to know not only the exact concentration of each of these elements but also how they are bonded. Usually oxygen is determined by subtraction after C, H, N, S, and the flyash component have been measured. Furthermore, one would like to find out how the oxygen is distributed over the various functional groups: hydroxyl, ether, carbonyl, carbonate, etc. A number of novel techniques and modified, older methods may be able to provide the answer: energy dispersive x-ray analysis (EDX), ESCA, NMR, IR, UV, and Raman spectroscopy all show promise. In some cases, the solution will depend on the development of entirely new experimental approaches.

Sulfur is often present as a compound with iron (pyrite). In that case the Mössbauer technique can be very helpful. Much information can be derived from the use of the isotopes ^{17}O , ^{33}S , and ^{15}N in NMR spectroscopy.

Most coals contain quite a number of trace elements in the mineral matter, but some of these elements are bound in organometallic groups. Often it is critical to determine the amount of these trace metals; a number of them are very toxic like As, Hg, Pb, and Cd, especially in the form of metallo-organic compounds. Many techniques can be used to detect these small impurities including neutron activation analysis (NAA) and proton-induced x-ray emission (PIXE).

In addition, coals contain about 10 percent inorganic material mainly in the form of oxides. The most abundant are SiO_2 and Al_2O_3 , ranging from 30 to 65 percent for the former and 25 to 55 percent for the latter. During combustion or gasification this mineral content forms a combination of gas, liquid, and solid phases which are carried downstream to other sections of the system. The specific nature of the vaporization and condensation process is relatively unknown and presently cannot be modeled with any certainty. Here knowledge of vaporization characteristics under reactive conditions is essential; a technique such as high temperature-high pressure mass spectrometry is an important tool. Further, additional information is needed on the characteristics of the liquid phase constituents of the gas stream. This includes not only the chemical and phase composition but also physical properties like viscosity. Presently we can measure viscosity as a function of specific composition and temperature but cannot predict it on the basis of liquid structure or other generalized models.

Another different, but important aspect of the mineral matter is the particle size and composition of the flyash (solid phase constituent) in the gas stream. The simple presence of these particles is detrimental from a corrosion/erosion standpoint. From the emission point of view the flyash is a health hazard if it consists of glassy particles of submicron size. Consequently, it is essential to determine the fraction of the concentration of flyash particulates and to measure their size, size distribution, and composition on samples collected under a wide variety of conditions.

Erosion/Corrosion

The need for research in this area is obvious: degradation of materials affects practically all aspects of fossil energy technologies, not the least the capability of measuring the essential process parameters. Studies of erosion and corrosion should cover the entire spectrum: basic studies, engineering applications, and testing, with close interaction between these three stages.

Erosion can be caused both by particles in a liquid and by particles in a gas. Attention should be paid to several classes of materials: metals and alloys, ceramics and glass. Surface degradation should be investigated as a function of particle concentration and composition, particle size, shape, and distribution, velocity, and angle of incidence of the particle-laden flow (laminar or turbulent). As far as the impacted material is concerned, the following aspects are of prime importance: hardness, surface roughness, and composition, its crystallinity or lack thereof, as well as the temperature of the surface. Both short- and long-term experiments are in order.

This kind of basic approach should be coupled with a systematic study of erosion effects in various applications both solid/liquid and solid/gas: erosion in straight, constricted and bent tubes, in cylindrical or rectangular reactors, erosive effects on nozzles, films, and blades, erosion of materials covered by protective coatings, etc.

Much of the above applies also to corrosion research. More work should be directed toward a fundamental understanding of what happens at the surface in contact with either liquid or gas. When protective oxide films are being formed, what is the nature of these films? How well do they adhere? What are the essential parameters for formation? Is it possible to produce these layers not only by metal diffusion to the surface from the inside (followed by oxidation), but also by deposition of appropriate coatings onto the surface?

What are the mechanisms of general and of localized corrosion considering that corrosion involves a host of chemical phenomena, not only oxidation and reduction, but also the effects of hydrogen, sulfur, alkali, and several other elements and compounds. The pH of the environment as well as the presence of electric fields play important roles and should be investigated more fully.

Finally, for MHD in particular the corrosion caused by electrochemical effects is of utmost importance. The relative roles of ionic and electronic transport in the electrical conduction mechanism of solids and liquids must be ascertained and related to the mobilities and diffusion of ions and atoms in the presence of large thermal gradients and electromagnetic fields.

Thermal and mechanical properties

The reliability and efficiency of coal conversion plants depends directly on the proper selection of construction materials. Considering the very severe conditions, both physically (temperature, pressure, etc.) and chemically (corrosive atmosphere), that one finds in most segments of such plants, the choice of metals, alloys, and ceramics is very limited. Aggravating the problem is the fact that reliable, accurate data on material properties in these extreme environments is rather scarce. Nevertheless, design and materials performance data are needed and include mechanical property information on elastic constants, creep, fracture, strength (tensile-, compressive-, yield-) and hardness not only under ambient conditions, but also as a function of temperature and pressure. That means for metals and alloys, temperatures up to 1000 °C, and for ceramics 1600 to 2000 °C. High and low pressure data are also needed as well as information on behavior under cyclic conditions.

Further these data should be coupled with fracture mechanics models since the mechanisms that govern the elastic and inelastic behavior of solids are not well known. Strength and fracture measurements should be accompanied by detailed microstructural studies and nondestructive evaluation methods. Similar gaps in our knowledge apply to thermal properties. The major thermal characteristics needed for construction materials and process liquids or solids are thermal conductivity (or diffusivity), thermal expansion, and heat capacity. However, the measurement of these parameters is not routine although a host of such data is required under the conditions of high temperature, high pressure, and highly reactive environments.

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