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Advanced Ceramics: A Critical Assessment of Database Needs for the Natural Gas Industry

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U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
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TOPICAL REPORT

June 1986 - May 1987

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GRI Project Manager
Matthew E. Schreiner
Materials Technology and Components

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16. Abstract (Limit: 200 words)

A comprehensive survey was conducted to identify the materials properties of potential importance for inclusion in an advanced structural ceramics database. The materials of current interest for use in gas-fired heat exchangers, recuperators, radiant tubes and heat engines were determined. Existing computerized, numerical databases were surveyed and those relevant to the materials and application of interest were detailed. Analysis of the results revealed that existing databases were inadequate to fulfill the critical data needs for effective application of advanced ceramics in gas-fired, high temperature applications. Requirements for establishing a new database focussed on these materials and applications are presented.

17. Document Analysis a. Descriptors

Numerical database
Materials properties
heat exchangers
recuperators
radiant tubes
heat engines
advanced ceramics
gas-fired environments

b. Identifiers/Open-Ended Terms

c. COSATI Field/Group

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RESEARCH SUMMARY

Title	ADVANCED CERAMICS: A CRITICAL ASSESSMENT OF DATABASE NEEDS FOR THE NATURAL GAS INDUSTRY
Contractor	Center for Advanced Materials The Pennsylvania State University GRI Contract Number: 5084-238-1302
Subcontractor	Ceramics Division National Bureau of Standards CAM Contract Number: GRI-T-PSU-NBS-1302-379
Principal Investigator	C. R. Hubbard
Report Period	October 1986 - June 1987
Objectives	1.) To identify the critical data needs for effective applications of advanced ceramics in gas-fired, high temperature environments; 2.) To assess the impact of computerized access to design guidelines and critical materials property data; 3.) To review the current state-of-the-art of computerized materials databases; 4.) To determine the impact of next generation databases in terms of efficient and effective utilization of numeric data, development of materials selector codes, and applications of artificial intelligence and expert systems; and 5.) To recommend a strategy for implementing a unique computerized database to establish efficient applications of structural ceramics in gas-fired, high temperature environments.
Technical Perspective	Advanced ceramics are well known for their high temperature thermal characteristics, high corrosion resistance to severe environments, and high temperature service capability. These properties make advanced ceramics highly desirable for applications in gas-fired, high temperature environments. However, specific engineering data on ceramics often are difficult to access and use. New materials and processing technologies are being developed so rapidly that often data are incomplete in scope, widely dispersed, contained in reports to sponsors, or simply not disseminated. Further, there is no technical consensus among experts as to what material characteristics are important in specific applications. Generally, the design criteria for advanced

ceramics are very different from conventional metals. For example, the tensile strength of ceramics is only a fraction of the compressive strength. Likewise, fracture strength, often cited as a key parameter, only tells a limited story. Depending on the application environment, properties such as creep, corrosion, wear, fatigue, phase segregation, and diffusion may also be important. At the same time, the values of many of these properties are test method dependent and equipment dependent. There are very few standards available to enable direct comparison of research results. Lack of usable guidelines, coupled with confusing and sometimes contradictory information, can be a formidable barrier to the effective use of advanced ceramics in the development of high efficiency gas-fired technology. To be useful to the gas industry, specific data and design guidelines have to be developed for gas applications and environments.

The rate of progress and the diversity of technological activities pertaining to the development and the performance of ceramics has resulted in a wealth of information that suffers from a lack of communication to the design engineers who are responsible for product development. Without effective communication, the value of such data is severely limited. Computerization of selected critical data on structural ceramics would accomplish the highly effective technology transfer needed to enable the gas industry to utilize the advances in ceramics research in a timely manner. Further, advances in database technology, such as in expert systems, may achieve not only a more effective access to critical data, but also a more effective utilization of that data through intelligent processing of both the materials property data and the constraints of the intended application.

Results

A comprehensive survey identified 158 factual databases currently in operation, of which only 6 publicly available databases were found to contain a significant fraction of the documented ceramic data needs of engineers designing for gas-fired applications. None of these databases, nor any combination of them, could fulfill, even minimally, the requirements for critical design data.

Several factors were found to be inhibiting the effective use of information and data for ceramics in gas-fired applications. On one hand, the lack of existing compilations is a primary barrier, along with a lack of standards for materials specification and for property testing. There are also many thorny technical issues in computer software engineering, data system architecture, data access, data precision, data reduction, and data representation in generalized format remain 179 to be solved.

For the database to be useful, a user-friendly, step-by-step guide for the data use is required. Many people tend to underestimate the amount of effort and the degree of technical sophistication required for a numerical database. For example, a straight completion of all available data with contradiction trends and fuzzy notation is equally distressing to potential users. Therefore, heavy judgement by experts in distillation of the vast technical data into a set of simple useful numbers would be most effective in translating concepts to practice.

A strategy for establishing a computerized ceramics database for the natural gas industry is recommended to ensure the effective development of key technologies that can benefit directly from the use of ceramic materials.

Technical Approach

A comprehensive survey was conducted to identify the material properties of potential importance in an advanced ceramics database. Interviews with GRI contractors along with reviews of existing project summaries and reports provided the primary sources of information in this survey. The materials of current interest for use in gas-fired heat exchangers, recuperators, radiant tubes, and heat engines were determined by review of the literature and interviews with project leaders in the field.

Existing computerized, numerical databases were identified by review of reports prepared by the Standard Reference Data Program of NBS and other sources and by direct interviews with individuals active in the field. When a database, containing information important or relevant to the needs of GRI, was identified, details were recorded.

Results of the survey of material properties and the survey of existing databases were combined in a two dimensional matrix of properties and databases. Analysis of this matrix revealed that existing databases were inadequate to fulfill the critical data needs for effective application of advanced ceramics in gas-fired, high temperature environments. Consequently, a review of existing numerical database efforts was made to determine the requirements for establishing a new database focused on GRI applications. Contacts also were made with the ASTM committee E-49, Computerization of Materials Property Data.

The feasibility and cost effectiveness of developing a database of critical ceramics properties for gas-fired applications was assessed. Based on the potential impact and benefits, it is recommended that GRI undertake the development of a user-friendly, factual database on ceramic materials as a prototype. The success of such a database concept requires a long-term commitment from both the natural gas industry and the industrial user community which it serves.

Project Implications

The development of a user-friendly, easily accessible database for ceramic material properties will help to facilitate the transfer of vital information to design engineers working to develop advanced, gas-based technologies. The feasibility and structure of such a database effort are proposed in this assessment, and are defined relative to the needs of equipment designers working on technologies based on natural gas. The international status of database developments is described, and many of the challenges for designing a gas-industry-specific database are identified.

GRI has initiated the development of a database to function as a repository for gas-industry-specific materials data generated from the Center for Advanced Materials project as well as from related international and domestic research and development programs. It is GRI's intent to provide the initial support for establishing the structure and anatomy of such a database, with the hope that once it is successfully implemented, its existence will be sustained by federal funding agencies pursuing the development of ceramic technology as well as by its users.

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ADVANCED CERAMICS:

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programs, engineering design programs, and control and monitoring routines have been developed or refined substantially, greatly facilitating the wide scope of their application. For example, pre- and post-manufacture laboratory testing operations are being augmented by computer modeling codes, such as finite element analysis of temperature and stress distributions. The processes of designing and manufacturing products are being facilitated by a range of software packages known as computer aided design, manufacture, and engineering (CAD/CAM/CAE). The sequential steps in materials processing are increasingly monitored in real time by microsensors, and the properties and performance characteristics of finished materials are beginning to be amenable to prediction by computer modeling. Critical to such applications is the availability of accurate, reliable, and complete sets of materials data.

Computerized engineering databases, in general, are not highly developed and, in particular, are severely lacking in development for advanced materials. Consider the use of advanced ceramics. These materials are well known for their high temperature thermal characteristics, high corrosion resistance to severe environments, and high temperature service capability. These properties make advanced ceramics highly desirable for applications in gas-fired, high-temperature environments. However, specific data often are difficult to access because the field is experiencing a rapid growth in processing technology. This rapid growth has resulted in the development of new materials whose characteristics are either not known to design engineers or have not been evaluated for their suitability in specific applications.

The present rate of progress and the diversity of technological activities pertaining to the development and the performance of ceramics is generating a wealth of data and technical information. This information, however, suffers from a lack of review, condensation, and communication to the design engineers who are responsible for product development. Without review to eliminate spurious data and without effective communication, the value of such data is severely limited. Computerization of selected data on structural advanced ceramics could accomplish the highly effective and rapid technology transfer needed to enable the gas industry to utilize the advances in ceramics research in a timely manner. Further, other advances such as in expert systems, may achieve not only a more effective access to critical data, but also a more effective utilization of that data through intelligent processing of both the materials property data and the constraints of the intended application.

Currently, the primary key to the opportunities offered by computerized technical information is the development of new materials property database systems. Such development will permit a wider, more efficient access to critical data, and hence a more rapid incorporation of these data in product design. Further, the computerization of the data will result in an increase in the quality and reliability of the data because consistency, correlation, and validation tests will be more readily applied to the data. This increased reliability will result in similarly increased reliability in designs and end-products. More importantly, advances in materials research will be more rapidly and effectively translated into advances in applications.

B. <u>OBJECTIVE</u>

The goal of this project is to determine the effectiveness of using computerized materials property databases in the development of advanced applications of structural ceramics to improve the utilization of natural gas. Several objectives, as enumerated here, are required to achieve that goal.

1. Determine the data needs for developing advanced applications of structural ceramics in gas-fired, high temperature environments.

2. Assess the impact of computerized access to the full spectrum of materials property and design data.

3. Review the current status of computerized materials properties databases.

4. Investigate the potential advances and advantages that could result from the development of materials selector database codes and other applications of forefront artificial intelligence and expert systems technology.

5. Recommend a plan for developing and implementing computerized database activities to promote advances in the application of structural ceramics in gas-fired, high temperature environments.

II. TECHNICAL SECTION

A. SPECIFIC OBJECTIVES

The specific tasks to be completed as part of the database assessment study were:

- A survey of applicable materials properties database activities in the U. S. and abroad;
- A definition of the scope required of a GRI advanced ceramics database;
- A comparison of the ceramic property data needed to facilitate systems design for gas-fired applications with what is available in existing, publicly available computerized databases;
- An examination of the computer science and technology issues related to establishing a user-friendly advanced ceramics properties database;
- A review of advances in artificial intelligence and expert systems analysis to determine the feasibility of applying this technology to advance materials databases; and
- A survey of the operational characteristics of existing data activities to project the general system and facility requirements that might be expected and to estimate costs.

B. WORK PLAN

1. Materials Database Survey

A survey of existing databases was conducted using resources of the National Bureau of Standards' Standard Reference Data Program, interviews with users of engineering property data on advanced ceramics, and published summaries of existing databases. The survey covered activities through 1986 and included both domestic and international databases.

A compilation of relevant databases was prepared using appropriate selection criteria. Only those databases known to contain factual information (numeric values and related metadata) were included. Restriction was made to technical databases containing numerical property values for chemical, physical, or materials science attributes. Additional selection criteria included documentation, public availability, computer accessibility, and property values relevant to advanced ceramic applications in gas-fired systems. The resulting list is given in Table 1. Engineering databases on in-service performance, while desirable, had extremely limited availability and could not be included.

2. Definition of the Scope of Applications

The potential scope of a GRI advanced ceramics property database was assessed through extensive interactions with GRI contractors, discussions with GRI managers, and examination of the current focus of GRI research and development activities. Information gained by these efforts allowed the material properties critical to the use and performance of advanced materials in applications of interest to GRI to be identified. A comprehensive list of operating conditions, materials, design considerations, materials properties, and performance characteristics was compiled (Table 3).

3. Analysis of Critical Data and Key Design Property Requirements

The list of key design data, determined in item 2, for heat exchanger, recuperator, radiant tube, and prime mover gas-fired applications was compared to the database compilation, prepared in item 1. This comparison allowed the identification of databases containing useful data applicable to a specific gas utilization materials problem. More importantly, this analysis identified critical data requirements that were not satisfied by current computerized databases.

4. Computer Science and Technological Issues

The computer science issues in establishing a numerical database were examined by review of current literature, a series of special reports, participation in ASTM Committee E49 on Computerization of Materials Property Data, and through discussions with experts currently involved with either database management and/or networking of multiple databases. The NBS Standard Reference Data Program was of exceptional value in this task and provided extensive input based on its activities over the past ten years.

5. Expert Systems Technology

The potential for using expert systems technology in conjunction with numeric databases to enhance the utilization of the information via intelligent processing of the data was investigated by reviews of current technical computer literature and through discussions with computer scientists actively pursuing developments in expert systems.

6. Survey of Related Data Activities

The majority of publicly available, numerical materials science Data Centers were found to be at NBS. Therefore, the NBS databases were selected for a detailed examination of their structure, data flow, current and anticipated dissemination methods, and sources and size of their resources. This study was used to develop a set of recommendations on the technical structure, staffing, facilities, and operational costs for a computerized database system focused on the critical data requirements in gas-fired applications.

C. SURVEY OF EXISTING DATABASES

The number of factual databases (containing numbers, units, and other metadata*) that are publicly accessible, documented, and used is growing each year, primarily due to the reduction of computer related barriers (e.g., cost and complexity) and to the rapidly growing use of computers in materials science and engineering. The Standard Reference Data Program at NBS maintains a compendium of the characteristics and status of scientific and technical factual databases for physics, chemistry, and materials.[1] In addition to examining that summary, other sources examined included the report of the Commission on European Communities Workshop on Factual Materials Data Banks[2], the proceedings of the Fairfield Glade workshop on Computerized Materials Data Systems[3] and CODATA publications such as Nonbibliographic Data Banks in Science and Technology[4]. During the course of the study, former and current GRI contractors were interviewed to ascertain their awareness of materials property databases. No publicly accessible ceramic properties database was identified during these

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* The generic term to cover all descriptive, cross-reference, or indexed forms of data needed to identify and define a specific set of data values in a computerized database is "metadata". For example, processing method, manufacture's lot number, and percent theoretical density would be metadata in a file on flexure strength.

interviews. A few in-house databases were cited, but these databases were limited in scope and accessibility due to proprietary restrictions.

A total of 158 databases containing factual information on chemistry, physics, and materials properties were identified, a number experiencing a continuing growth rate. An example of a recently developed system is the MetSel2 set of data disks derived from the compilation Metals Handbook[5]. Of the 158 identified databases, only six publicly available, documented (mature) computerized databases had a significant focus on ceramic materials. Three developing database efforts, which are planned to contain a significant number of entries on property data on ceramics, were also identified. One that is funded by a federal-society-industry consortia, A Computerized Tribology Information System (ACTIS)[6], is expected to have the greatest overlap with GRI data needs. These nine mature and developing databases, which contain property data pertinent to design and research interests on ceramics in gas-fired environments, are listed in Table 1. Brief summaries of the six mature databases, extracted from reference 1, an NBS survey of factual databases, are given in Appendix I. Information on the producer of the data and the properties and materials are referenced in the database. Careful examination of this information has indicated that while the producers often included a wide range of materials and properties in the summary, actual computerized database contents are often far less extensive. For example, CINDAS has a computerized and publicly available bibliographic and key word file, but their property data are not available via computer systems.

Database developments abroad were also explored, with particular attention given to activities in Japan. The current understanding is that the Japanese data efforts are not intended to be internationally available. The identified efforts, excluding databases on glasses, are listed in Table 2. While generic definition of content and scope are known, definitive descriptions of content were not made available. It is probable that these Japanese database efforts are in the planning and implementation stage at this time. Their effort is intended to eliminate duplicate efforts by each company and to provide ceramic producers in Japan with a competitive advantage in the international advanced materials marketplace.

D. SUMMARY OF PROPERTIES

A summary of properties of potential importance in an advanced ceramics engineering database is given in Table 3. This table incorporated input from GRI contractors, experts at PSU and NBS, property data compilations, and GRI reports. Eight important general categories of data were identified, depending on the intended application and operating environment. These categories are (1) materials specification, (2) processing characterization, (3) structural and microstructural characterization, (4) intrinsic properties, (5) dislocation and vacancy-dependent intrinsic properties, (6) microstructural dependent properties, (7) performance properties, and (8) failure characterization. Each of the categories in Table 3 are expanded into specific properties or qualifiers.

Table 3 may be considered a first order prescription for a GRI factual database on advanced ceramics for gas-fired applications. For example, suppose a new valve for a gas-fired reciprocating engine is to be developed using a ceramic material. The material specification information would be used first to classify the candidate materials. The processing information would be examined closely since both mechanical and tribological performance characteristics may be dependent on the processing history. Detailed chemical composition and microstructural information would be required since durability and wear modes encountered in the operation of the valve may depend on the grain size distribution, the chemically active impurities, or the grain boundary characteristics. Elastic and plastic properties, yield strengths, thermal expansion coefficients, thermal conductivity, diffusivity, and shock resistance would be essential to the theoretical design of the component. The fracture modes, hardness, creep characteristics, wear properties for the desired speed, load, and temperatures, and the oxidation and corrosion effects in the presence of gas combustion products would be essential in optimizing the lifetime of the valve.

E. ADVANCED GAS APPLICATIONS

1. Materials and Properties Four applications areas were identified in which the use of advanced ceramics could increase the effective utilization of natural gas. These four areas included heat exchangers and recuperators, radiant tube heaters, prime movers, and fuel cells. The material characteristics and operating conditions for these applications were ascertained through an examination of the current literature, GRI reports, and discussions with technical experts who are active designers or users in these areas. A summary of the information obtained in this effort was prepared, as listed in Tables 4a, b, c, and d. These tables consider candidate materials, processing methods and other required characterization information, typical operating conditions, and key design properties encountered in these applications. Table 5 has been constructed to provide a better view of the range of conditions to which gas-fueled equipment may be exposed. The data in Table 5 indicate a wide range of temperatures, candidate materials, and environmental and operating conditions for gas-fueled applications. This matrix can be expanded further as in Table 6 to identify the critical materials properties needed in a focused GRI ceramics database.

2. Existing Database Coverage The background survey of existing databases summarized in Table 1 was examined to determine the utility of the available systems with respect to the gas applications analyzed in Tables 5 and 6. A further analysis of these data was focused on specific components which were deemed critical to reliable design and durable long-term application. Table 7 summarizes this matching of need and availability. Clearly shown in Table 7 is the consistent lack of the required design data in publicly accessible systems. The most comprehensive single source of data, available through CINDAS, addresses only thermodynamic properties and requires manual searching. The Phase

Diagrams for Ceramists Center will have comprehensive phase information available in computerized form in the near future. ACTIS, a new database effort in an early development stage, is intended to provide tribological data in computer accessible form, much of which will be of value to gas-fired prime mover applications.[6] The ACTIS database is intended to provide evaluated data in a form directly usable by the design community.

It may be concluded that, for the greater percentage of gas applications, little data on ceramic materials is readily available in manually accessible data collections, which could be converted to computerized form. The engineering properties of the more widely used metal alloys, particularly steels, however, have been available in manual form for some time and are now undergoing compilation and inclusion in computerized databases under the sponsorship of the American Society of Metals. The National Association of Corrosion Engineers is preparing a similar service for corrosion properties of metals.

F. COMPUTER SCIENCE AND TECHNOLOGY ISSUES

The representation and management of data on a computer generally is accomplished through a database management system (DBMS). Advanced DBMS software may be considered as providing a programming language within which a specific database may be constructed. The details of the specific database are determined by the nature of the data and the requirements of the user. It is essential, for example, that the user's options be determined prior to the design of the complete database structure. Coding for such options may involve using the DBMS language to provide the database user with the capability of searching the database to locate data meeting specified conditions, to retrieve restricted values of selected variables, to obtain tabulations of values or graphical representations, or to conduct statistical analyses or regression calculations. Further, how these options are presented to the user is of great practical importance. Menu and query formats in which the user makes selections from a list of possible choices, for example, are generally found to be superior to command formats in which the user must issue instructions to the system.

The hardware associated with the computer system, i.e. monitors, printers, and plotters, also affects the design and structure of the database program. Displays utilizing color significantly enhance the representation and understanding of the data. Color monitors, in particular, can facilitate the user's interaction with the database program.

The prescription for the database structure, in terms of the nature of the data, the software, and the hardware, must be followed by the actual development of the code, the entry of the data, and careful and intensive field testing of the system. It is highly advisable that prototype codes be developed and tested using a representative collection of data prior to synthesizing the final system.

The primary means used to disseminate factual databases include (1) centralized on-line systems, such as the widely used interactive bibliographic services, (2) packages for personal computers, and (3) the developing gateway computer concept.

The on-line approach is used when large amounts of information are to be stored and will be accessed frequently by a large number of users. Chemical Abstracts, available through several vendors, is a good example of broad use and large data volume typical of on-line systems. Generally, the on-line database vendors restrict the database contents to textual material such as encountered in bibliographic and abstract searches. However, several vendors are now beginning to offer factual databases. The Canada Institute for Scientific and Technical Information offers on-line numerical, as well as textual, search capabilities for scientific numerical databases. This system supports four crystallographic databases, the Facility for the Analysis of Chemical Thermodynamics (F*A*C*T), and an infrared spectra database. The Scientific & Technical Information Network, STN International, has announced on-line availability of its first numeric file, DIPPR, a physical property database (primarily thermochemical) on chemicals.

Use of PCs such as IBM-compatible XT and AT computers, for materials property database dissemination has recently gained momentum. The NBS - National Association of Corrosion Engineers Data Center has begun to offer computerized databases of corrosion properties of metals for use on PCs. For larger, more established databases, the storage capacity of the 5-inch floppy diskette (1.2 megabytes) has limited database dissemination via PCs. However, introduction of the 550 megabyte compact disk - read only memory (CD-ROM) storage medium permits suppliers of large databases to consider the PC dissemination option. The International Center for Diffraction Data, distributor of the most widely used numerical database, the Powder Diffraction File, announced in August, 1987, that its database would soon be available on CD-ROM for use with IBM compatible or VAX computers equipped with CD-ROM readers. Examination of a prototype version indicated that the 130 megabyte database can be searched using both textual and numeric range descriptors. The CD-ROM drive is available for less than $1000, and the CD-ROM master was produced for less than $3000. Numerous publishers, such as Oxford Press, have also announced computer searchable products based on CD-ROM technology, such as the King James Bible, encyclopedias, and unabridged dictionaries.

The gateway concept is an advanced dissemination method that is dependent on the existence of both databases and computer communications networks. The concept assumes that desirable databases may be as widely distributed, geographically, as are the users of the databases. Linking the users and the databases is a single host computer facility, which may also contain some of the desired databases. The essential feature of the gateway system is that the user interacts only with the host. While each database may be developed with its own language, rules, and protocols, the user needs to learn only one set of commands pertaining to the host facility. The host computer translates requests and replies into the appropriate languages. In an advanced version of the concept, the host computer uses an expert system to determine which one or more databases in the world-wide distributed network should be accessed to answer the user's query. The gateway concept thus has the advantage of optimizing the use of databases that individually fulfill the requirements of the user only partially. The disadvantage of the gateway method is the lack of control over the quality and reliability of the data, the methods of construction of the individual databases, the scope of the contents, and the maintenance intervals for updating the contents. The Materials Property Data Network, Inc.[7] has been established to implement this concept.

G. REQUIREMENTS FOR ESTABLISHING ADVANCED CERAMICS DATABASES

There are six critical factors that must be considered in the establishment of a computerized database of any nature. These six factors occur in an approximately hierarchial arrangement, as follows:

1. Authority
2. Funding
3. Personnel
4. Software
5. Facilities
6. Data

Within this hierarchy, items lower in the list must be given due consideration before items higher in the list can be properly addressed. Thus, the first consideration is to determine whether or not there is a need to have a database, which is the primary question addressed by the preceding sections of the present report. Given a need for a database, no progress towards computerization can be made without appropriate computer facilities. Likewise, software is necessary to operate the computer in a database format, and personnel who understand the data are required to apply the software to the computerization of the data in an intelligent manner. When these factors have been satisfied, a cost/benefit analysis can be conducted. The latter analysis would undoubtedly be utilized along with the programmatic justification that would be examined in determining the administrative authority to proceed with the implementation of the database plan.

The hierarchial list appears in a linear ordering, but it is not difficult to perceive that considerations at any level may be related or linked to considerations at other levels, either lower or higher. A schematic representation of one concept of a scientific data center[8] is shown in Figure 1, which illustrates some of the interactions. This figure emphasizes the importance of both the nature of the data and the needs of the user in determining the structure of the database. The software for the database, for example, must be capable of processing all the types of factual data to be included in the database, as well as being capable of analyzing and displaying or reporting information from the database in a manner that fulfills the requirements of the user.

There are many aspects to be examined for each of the hierarchial factors. The most involved considerations pertain to the lowest item in the hierarchy, data. Indeed, factual database management in science and engineering is highly complex, not because of the computer hardware or software, but because of the complexity of the scientific and technical data and the specialized analytical requirements of the scientist or engineer. Understanding and preparation for the development of a computerized database begins with an analysis of data-related issues, as is done in the present assessment. The full scope of the data of interest must be determined with an identification of variables and conditions. The classification of data in this early development stage may significantly influence the details of the design of the database structure. For example, the classification results may indicate that several separately addressable numeric database components might be advantageous compared to using a single, large-scale matrix of values. Careful consideration must be given to how the data will be acquired, both initially and later during the long-term operation of the system. Passive techniques, such as obtaining data as it appears in the literature, must be compared to active approaches in which experiments are deliberately designed to provide specific results for the database. The selection of the technique must be balanced against the need for controls on the data quality and the need to minimize costs. The collection of data must be followed by a careful evaluation of the data. This task involves several concerns such as: what criteria will be used to assess the data; who will appraise the data; and in what manner will confidence in the data be indicated in the database?

The latter question leads directly to the next concern, the representation of the data in the database.

The recommended procedure to be followed in establishing the details of the data component of the database system are well known[9]. The basic steps are outlined in Table 8. In computer science, the word "field" which appears in Table 8 is used to represent any variable, parameter, or piece of information that will be entered into and/or retrieved from the database. Each such quantity has a name, such as "T_a", and a technical definition, such as "ambient temperature".

Once the complete list of anticipated fields is prepared, the DBMS language must be used to specify the technical characteristics of each field. For example, T_a might be specified as a numeric field of width 6, with 2 decimal places, to be expressed in degrees Celsius, with a default value of 25 °C. This definition of T_a would permit a range of values to be entered for the ambient temperature, $-99.99\ °C \le T_a \le 999.99\ °C$, but the default value, $T_a = 25.00\ °C$, would be assumed unless the value of T_a were deliberately changed.

Fields would also be defined for metadata. Any descriptive information that is needed to specify how a number was determined may be considered as metadata. For example, the toughness of a ceramic material may depend on whether a micro-indentation test was used for the measurement or whether a macro-scale bending test was used. Thus, "METHOD" might be the name of a field containing metadata. Information gained in the present study and from other database system efforts suggests that, at a minimum, the metadata must include test methods, test conditions, and notes on data analysis procedures for each property value. Other metadata that should be included are material identification fields, units for each numerical value, data quality assessments, and specimen characterization.

During the process of entering the data into the database, "validity checks" and "error trapping" routines are necessary to ensure that all entries adhere to the defined rules and ranges of values. Provisions for "cross field validation" rules are important whenever possible to ensure the consistency and quality of the data.

After defining the fields in the database according to Table 8, attention must be given to the details of the data retrieval options. Advanced DBMS software packages that are available commercially contain standard provisions for searching, displaying, graphing, and printing. To tailor these operations or to extend them, additional code development is required. Such specialized retrieval options are highly desirable for scientific and engineering applications and would enhance the capability of a ceramics materials property database to be utilized in gas-fueled applications.

As soon as the prototype system can be used, field testing of the code must be pursued in a thorough and systematic manner. It is advisable to have both novices and knowledgeable people attempt to use the prototype system. During this test phase, the code developers must carefully observe what operations present difficulties and what features are most useful. Revision of the code must then be based on the analysis of the results of this testing. In general, two or three iterations of revisions of the features of the system should be anticipated since it is the end user to whom the system is to be suited.

The refined prototype forms the basis for the full scale system. If separately addressable database elements are used in the system, field definitions need to be changed to accommodate the individual elements. The overall features and options of the prototype would not be affected by these adaptations. The completed full scale system must be subjected to a final thorough field testing.

The final step in the establishment of a database is the dissemination of the database to the intended users. There are several possible options available to achieve the goal of disseminating a database on materials properties for use in developing or improving gas-fired applications of ceramics. The choices include printed books, on-line services, PC packages, gateway networks, or any combination of these options.

The preparation of material for printed books from a database is widely used by many data centers. The quality of the printed output depends to a great extent on the facilities and support available. Possibilities range from sophisticated computerized typesetting directly from the database, to use of high quality desktop publishing, or simply to printing formatted tables of values on dot matrix printers.

The on-line services method is used for business applications (e.g., DIALOG or COMPUSERVE) or for bibliographic data sets (e.g., ChemAbstracts). However, factual databases for scientific and technical data have recently begun to be available. The American Chemical Society and STN International have announced their first property database which provides thermochemical data for many industrial compounds. On-line services, though, tend to be rather expensive. Commercial business services charge from one to five dollars per minute of connection time. Since data transmission rates are relatively slow, the cost of conducting a single complex data retrieval could easily exceed the total cost of other options. The initial cost of loading a database into the on-line system is often very expensive and is usually absorbed by the sponsoring organization. Further, the time to complete the necessary arrangements with the host organization and to load the database into the host system is frequently as long as two years from the time the database exists. Consequently, on-line dissemination using a large commercial system may not be appropriate for a database aimed at rapid dissemination to the initial user community. The alternative of using a personal computer as the host system is a possibility worthy of consideration also. The PC host system would have the disadvantage of being accessible to a small number of people at any one time, usually only one. The hardware and maintenance costs of such a system would not be excessive for a small set of users, but user-related disadvantages might inhibit the effectiveness of this dissemination method. Users would be required to have additional hardware, a modem, and communications software, and would be required to learn their idiosyncracies before attempting to connect to the database.

The most preferable option is to supply the database and associated software in a package that could be used directly on the user's PC. This option presents the user with the greatest latitude in using the system, and encourages the user to experiment or explore applications of the system. A potential disadvantage to this dissemination method is the requirement that the user's PC be compatible with the database software. Given the wide proliferation of compatible personal computers, a PC-based database should not encounter significant difficulties. Further, PC technology has advanced far more rapidly than mainframe technology, to the extent that more sophisticated, user-friendly programming can be done with a PC-based system than would generally be found with on-line services. Implementation of a PC-based system will require establishing the optimum frequency for updating and for providing an effective update dissemination mechanism.

Finally, even for the most carefully produced database, provisions should be made for user assistance. This assistance may take the form of a user's assistance manual and/or an individual or office that could be contacted by telephone. The commitment in staff for this assistance initially would be rather small, but the amount of staff hours would grow if the number of users increases.

III. MAJOR ACHIEVEMENTS

A comprehensive survey identified 158 factual databases and available publicly currently in operation Only six of these databases provided any significant coverage of ceramic mateials properties. However, none of these databases, nor any combination of them, could fulfill the requirements for critical design data needed in advanced gas-fired applications of ceramic materials. Several factors were found to be inhibiting the establishment of a factual database for ceramics in gas-fired applications. The lack of existing compilations was a primary barrier, along with a lack of standards for materials specification and for property testing. Limited experience in building numerical databases inhibited many researchers from attempting to do so. In some cases, the lack of a clear definition of the specific needs for data prevented the needs from being fulfilled. All of these inhibiting factors could be overcome. The consequences for not aggressively pursuing the development of a factual database on ceramics, focused on gas-fired applications, were estimated to be contrary to the goal of improved utilization of natural gas. Technology transfer from parallel or related research would be significantly reduced. Advances in the utilization of ceramics would greatly lag behind the cooperative ventures of foreign competition. The prospects for achieving a ceramics database and thereby avoiding such consequences were found to be both feasible and desirable. A plan towards establishing a computerized ceramics database for the natural gas industry was developed to ensure the availability of critical data.

IV. MAJOR TECHNICAL PROBLEMS ENCOUNTERED

No major problems were encountered.

V. CONCLUSIONS

Dissemination of a ceramic property database can be an effective opportunity for technology transfer of the results of GRI sponsored materials testing and research activities. A computerized database on ceramic materials is capable of enabling more rapid utilization of new research results; faster, more efficient access to critical data, more consistent treatment of data; greater quality control and product reliability; and improved continuity of research and development programs. These benefits would begin to accrue during the development stages of the database. For example, the process of collecting data for inclusion in the database would increase communication between researchers, provide standardization of data reporting, and, thus, enhance technology transfer from research to application.

In particular, a numeric database for materials selection and design consideration is needed to develop improved or innovative applications of advanced materials for gas-fired, high temperature environments. No existing database or combination of existing databases meets the identified needs of advanced materials suppliers, equipment manufacturers, and industrial end users for a database focused directly on ceramic materials selection and critical property data. Such a database would require data that reflect the effect of the application environment on a material's performance. Hence, data from tests performed in actual or simulated environments should be emphasized. Further, emphasis should be given to property values of carefully identified and characterized materials, due to the strong dependence of properties on characteristics of the starting powders and processing parameters.

A sustained long term effort in database design, data retrieval, evaluation, and dissemination will be required to establish a materials property database focused on ceramic materials for use in gas-fired, high temperature applications. In addition to the mechanistic factors, several organizational requirements critical to the successful development and implementation of the database must be satisfied. These requirements include:

- The availability of technical expertise in computerized data compilation and retrieval,
- Ongoing detailed interactions with other materials database systems,
- Continual assessment of user and programmatic needs, and
- Maintenance of current research and engineering data through

active involvement in the materials science and engineering applications.

Based on the past and current level of GRI-sponsored efforts on tubular components for heat exchangers and recuperators in aluminum remelt applications, the first database effort would do well to focus on the key design and performance properties for this application. Other appropriate applications areas with sufficient needs for a ceramic property database include related heat exchanger/recuperator applications and structural ceramics intended for use in gas-fired prime movers.

VI. RECOMMENDATIONS

A state-of-the-art, numerical database of ceramic material property data useful to both the design engineer and the research scientist should be established. The numerical database should permit the design engineer to use it as an aid in materials selection and as a resource for qualifing property data for design purposes. Associated with the numerical database could be an additional database on GRI materials research in progress, and possibly another on materials availability. The database should be designed to permit transfer of data to design codes. With further developments in the knowledge base on structural ceramics, an expert system could be developed that would provide useful guides to the design engineer who is unfamiliar with the differences in the design requirements of ceramics and metals.

The scope of the ceramics property database should include as a starting point the properties and materials identified in this study through interviews with potential design engineers. The recommended approach is to focus on selected gas-fired application with the associated key materials and properties. Property data for materials selection and design consideration of heat exchangers, recuperators, radiant heaters and prime movers will facilitate introduction of improved or novel new gas fired systems with improved efficiency. As the development of ceramic materials for structural applications is an on-going effort, the scope must expand with time to include new materials.

The numerical database structure should be carefully planned and professionally designed to facilitate the user's access to and utilization of the data. The complexity of database design due to the need for unique identification of ceramic materials should follow the guidelines being established by national and international bodies such as ASTM. Integral to achieving this goal, a prototype system should be developed and field tested by novices and expert design engineers who are responsible for systems development. Redesign based on field testing will lead to a highly effective, efficient mode for technology transfer for GRI's sponsored research efforts. The envisioned materials property database management system should be constructed for use on PCs in order to achieve the greatest impact in a cost effective manner.

To accelerate technology transfer of GRI sponsored testing and research efforts a timely data report mechanism (i.e. computerized data report forms) should be developed collaboratively by the GRI program managers, experts in property measurement and those expert in database management. The ability to efficiently transfer the data into the database will reduce the time between property measurement and availability to the design engineer. Another benefit of a computer oriented data report mechanism is that the cost of supporting the data collection, abstraction, entry, and validation will be considerably reduced.

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VIII. TABLES AND FIGURES

TABLE 1

FACTUAL COMPUTERIZED DATABASES ON CERAMICS

<u>MATURE</u>

Wear Data (Pure Carbon Co.)

CINDAS (Purdue)

Ferroelectric Ceramic Base (Sandia)

Materials Information Databank (Sandia)

Thermal Property Bank (LLNL)

JANAF Thermochemical Tables (NBS)

<u>DEVELOPING</u>

Phase Diagrams for Ceramists (NBS/ACerS/Industry)

Fracture Mechanics Databases for Glasses and Ceramics (NBS/Rutgers)

A Tribology Computerized Information System (NBS/DOE/DOD/Industry)

TABLE 2

DEVELOPING JAPANESE CERAMIC DATABASES (excluding glasses)

Organization	Database
Japan Fine Ceramic Center	Reference data for fine ceramics
Engineering Research Association for High Performance Ceramics	Engineering data for high-performance Si_3N_4 and SiC
Japan Information Center of Science and Technology	Inorganic crystal structure data

TABLE 3

LIST OF PROPERTIES POTENTIALLY IMPORTANT IN A GRI ENGINEERING CERAMICS DATABASE

MATERIAL SPECIFICATION:

- common name
- chemical formula
- classification
- source (manufacturer, laboratory)
  - manufacturer's code
  - manufacturer's lot#
  - date of production

PROCESSING CHARACTERIZATION

- starting materials
  - chemistry
  - source
  - treatment
  - size distribution
- process
  - binder
  - dopants
  - additives
  - method (hot press, HIP, cast, extruded, CVD, ...)
- thermal history
  - sintering
  - annealing
  - crystallization cycles
- other
  - grinding
  - polishing
  - cleaning

STRUCTURAL AND MICROSTRUCTURAL CHARACTERIZATION

- chemical analysis
- grain size distribution
- grain morphology
- phase assemblages
- grain boundary characteristics
  - chemistry
  - phase
  - size
  - morphology
- porosity
- density (actual)
- density (theoretical)

TABLE 3 (cont)

LIST OF PROPERTIES POTENTIALLY IMPORTANT IN A GRI ENGINEERING CERAMIC DATABASE

INTRINSIC PROPERTIES-1 (microstructure/processing independent)

- crystal system/polymorph (Pearson symbol)
- thermal expansion coefficient - f(T)
- melting temperature
- phase transformations at T
- elastic moduli
- Young's modulus
- Shear modulus
- Poisson's Ratio

INTRINSIC PROPERTIES-2 (possibly dislocations and vacancy dependent)

- thermal conductivity
- heat capacity

PROPERTIES AND CHARACTERISTICS (microstructural dependent)

- thermal
  - diffusivity
  - shock resistivity (R' & R''')
  - emissivity as f(T)
- optical properties
  - absorptance, transmittance
  - color
- electrical properties
  - conductivity
  - resistivity
  - ionic mobility
  - dielectric constant - f(T, Hz)
  - dielectric strength (high voltage holdoff, etc)

TABLE 3 (cont)

LIST OF PROPERTIES POTENTIALLY IMPORTANT IN A GRI ENGINEERING CERAMICS DATABASE

mechanical properties
- strength -mean and range as f(T)
  - -tensile, flexure, compressive
  - -test method
  - -loading rates
- Weibull modulus
- fracture toughness
  - "R" curve
  - K_{Ic}, gamma, n
  - test method
  - environment
  - function of flaw size
- creep
- creep rupture
- fatigue (high and low cycle fatigue as f(T) and test configuration)

PERFORMANCE PROPERTIES

- hardness
- wear resistance - function of speed, load, temperature, and environment.
- coefficient of friction
- corrosion effects
- oxidation effects - f(T)

FAILURE CHARACTERIZATION

- fracture origin
- corrosion products, rates

Table 4a

APPLICATION, MATERIALS AND REQUIRED DATA

APPLICATION: Heat exchangers/recuperators

MATERIAL:

- SiC - siliconized
- SiC - alpha, sintered, water based
- SiC - alpha, sintered, plastic based
- SiC - alpha, sintered,
- SiC - nitride bonded
- SiC - reaction bonded
- Ceratherm
- Si_3N_4 - SiC refrax
- Si_3N_4

CONDITIONS:

- 1000 to 1400°C - flue gas temp
- particulate laden
- corrosive flue gas (Al remelt with fluxing; forging furnace; steel soaking)

PROCESSING DATA:

- starting materials preparation
- starting materials characterization
- consolidation technique
- thermal treatment
- chemical analysis

MICROSTRUCTURAL CHARACTERIZATION:

- density
- porosity
- grain size distribution
- grain boundary chemistry, phases
- phase assemblage

PROPERTY DATA REQUIRED:

- Chemical stability and corrosion
  flue gases, molten Al, fluxes,
  Na and Cl contamination
- Thermal expansion
- Thermal conductivity
- Thermal shock resistance
- Strength - (tensile, compressive, C-ring tests; flexure)
- Weibull modulus

Table 4b

APPLICATION, MATERIALS AND REQUIRED DATA

APPLICATION: Radiant Tubes for Indirect Heating

MATERIAL:

SiC - reaction bonded
SiC - alpha, sintered
SiC - nitride bonded
SiC - reaction sintered
SiC - CVD
Si_3N_4 - reaction bonded
composite - fibers of alumina
- matrix of alumina+silica

CONDITIONS:

1200°C - flue gas

PROCESSING DATA:

starting materials preparation
starting materials characterization
consolidation technique
thermal treatment
chemical analysis
machining

MICROSTRUCTURAL CHARACTERIZATION:

density
porosity
grain size distribution
grain boundary chemistry, phases
phase assemblage

PROPERTY DATA REQUIRED:

Chemical stability and corrosion
flue gases, molten Al, fluxes
Thermal expansion
Thermal conductivity
Thermal shock resistance
Strength - (tensile, compressive, C-ring, flexure)
Weibull modulus

Table 4c

APPLICATION, MATERIALS AND REQUIRED DATA

APPLICATION: Prime movers (internal combustion engines)

MATERIAL:

- AlN (exhaust port insulation)
- Al_2O_3-TiO_2 (exhaust port insulation)
- ZrO_2 (cylinder liners, piston caps, etc.)
- Si_3N_4 (insert components, turbocharger)
- SiC (turbocharger)
- SiC/TiB_2 (guides)
- CrC (rings)
- Al_2O_3-TiO_2 (plating on rings)

CONDITIONS: 600°C (gas turbine)

PROCESSING DATA:

- starting materials preparation
- starting materials characterization
- consolidation technique
- thermal treatment
- chemical analysis
- machining

MICROSTRUCTURAL CHARACTERIZATION:

- density
- porosity
- grain size distribution
- grain boundary chemistry, phases
- phase assemblage

PROPERTY DATA REQUIRED:

- Chemical stability and corrosion
- Thermal expansion
- Thermal conductivity
- Thermal shock resistance
- Strength
- Weibull modulus
- Fracture toughness, K_{IC}
- Hardness
- Coefficient of friction
- Wear rate

Table 4d

APPLICATION, MATERIALS AND REQUIRED DATA ǂ

APPLICATION: Fuel Cells

MATERIAL: $La_{1-x}(Ca,Sr)_xMnO_3$

CONDITIONS: 1000 C
50 mA/cm^2

PROCESSING DATA:
- starting materials preparation
- starting materials characterization
- consolidation technique
- thermal treatment
- chemical analysis

PROPERTY DATA REQUIRED:
- Chemical stability
- Thermal expansion
- Strength
- Electrical conductivity
- Ionic mobility
- Resistivity

ǂ Only a representative electrode material and property data required are shown.

Table 5

OPERATING CONDITIONS

Gas Application	Critical Component	Candidate Mat'ls	Mat'l Temp.	Atmosphere	Velocity	Particulates
<u>Heat Exchanger</u> Aℓ remelt heat recovery	Tube Header	SiC SiC	1400°C	Comb. prod. Halides	<10 ft/sec	√
Aℓ immersion heater	Tube	SiC	1000-1400°C (flue gas)	Comb. prod. Al Soot	<10 ft/sec	
Radiant heater	Tube	SiC Si_3N_4 Composites	1200°C (flue gas)			
<u>Heat Engines</u> Rotary engines	Tip Seals Bearings Exhaust System	α-SiC, Si_3N_4, SiAlON HP Si_3N_4 Al_2O_3-TiO_2, AlN	300-600°C	Comb. prod.	3600 RPM (10m/sec)	C deposits
Gas turbines	Rotors Vanes Ducting Bearings	SiC, Si_3N_4 Si_3N_4	1200°C			√ (C, ash. limestone)
Recip. engines	Turbo chargers Cylinder liners Piston head Exhaust ducting Valve cap/assembly Seats/guides	Si_3N_4, SiC ZrO_2(PSZ) PSZ $AlTiO_4$ SiC/TiB_2	600°C normal (1200°C in future low heat rejection engines)	Comb. prod. lubricants		

Table 6

CRITICAL PROPERTIES

Gas Appl.	Critical Component	Joining Components	Corrosion	Strength	Creep	Stress Rupture	Tribo	Thermal Expan.	Thermal Shock	Thermal Cond.	Stability
Heat Exchangers Al remelt heat rec	Tube Header		√	√	√	√	—	√	√	√	√
Al immersion heater	Tube		flux enhanced Na, Cl contam.	√			—	√	√	√	√
Radiant heater	Tube		√	√	√	√	—	√	√	√	√
Heat Engines Rotary	Tip Seals	√		√			√	√			√
	Bearings	—		√			√	√	√	√	
	Exhaust System	√		—			—				
Gas turbines	Rotors										
	Vanes			√	√						
	Ducting										
	Bearings										
Recip. engines	Turbo chargers	√		√	√	?	√	√	√		√
	Cylinder liners	√		√	?	?	√	√	?		√
	Piston head	√		√	?	?	√	—	?		√
	Exhaust ducting	—		—	—	—	—	√	√		√
	Valve cap/assemb.	√		√	√	√	√	√	?		
	Seats/guides	√		√	?	?	√	√	?		√

Table 7

IDENTIFIED DATABASES CONTAINING
CRITICAL PROPERTY DATA

Gas Application	Critical Component	Corrosion	Strength	Creep	Stress Rupture	Tribo	Thermal Expan.	Thermal Shock	Thermal Conduct	Stability *
Heat Exchangers Al remelt heat recovery	Tube Header									~PDFC
Al immersion heater	Tube									~PDFC
Radiant heater	Tube									~PDFC
Heat Engines Rotary	Tip Seals						?CINDAS		?CINDAS	~PDFC
	Bearings		—	—	—	~ACTIS				
	Exhaust System						?CINDAS		?CINDAS	~PDFC
Gas turbines	Rotors Vanes Ducting Bearings					~ACTIS				
Recip. engines	Turbo chargers Cylinder liners Piston head Exhaust ducting					~ACTIS				
	Valve cap/assemb. Seats/guides					~ACTIS				

~ACTIS = future coverage by A Computerized Tribology Information System
~PDFC = future coverage by Phase Diagrams for Ceramist Data Center
?CINDAS - data only available through manual search
*Thermodynamic parameter databases, such as F*A*C*T, could be used if all reactants/products are represented in calculation of equilibrium and that equilibrium conditions are expected.

TABLE 8

STEPS TO CREATE A NUMERIC DATABASE

1. List Each Valid Field

   A. Name
   B: Technical Definition

2. Define Each Field

   A. Data type (character, numeric, logical)
   B. Single value, multi value or range
   C. Units to be used
   D. Default values
   E. Validty checks
      1) List of valid values
      2) Range of valid values
      3) Other (character type, number representation)

3. Establish cross field validation rules

4. Specify which fields will be used for retrieval

5. Specify required and optional fields

6. Include essential metadata
   A. Test methods
   B. Test conditions
   C. Data analysis procedures
   D. Reliability

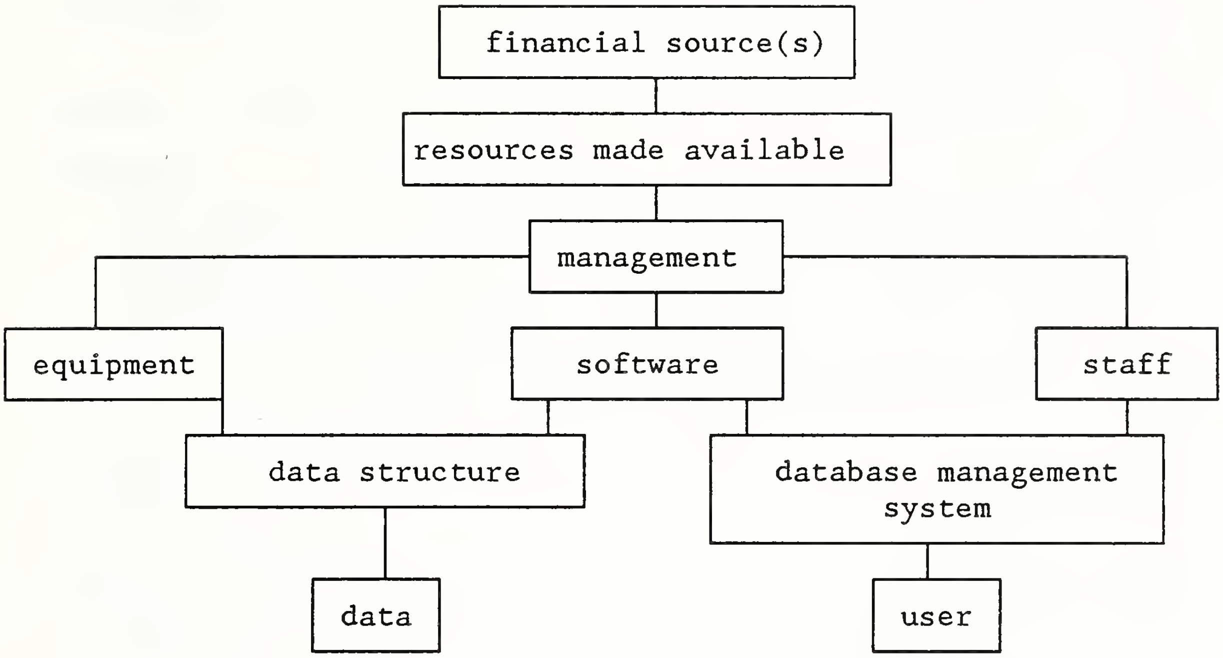

FIGURE 1. Interrelationships of Components of Scientific Data Centers

IX. APPENDIX

Appendix Ia

CHARACTERISTICS AND STATUS OF PUBLIC FACTUAL DATABASES CONTAINING CERAMIC PROPERTIES

FULL NAME
Pure Carbon Wear Data

ACRONYM: PUREWEAR

PRODUCER
Pure Carbon Company
Pure Industries Division
441 Hall Avenue
St. Marys PA 15857 USA

CONTACT: Stanley Chinowsky PHONE: (914)

VENDOR:
Pure Carbon

GENERAL PROPERTIES:
wear; friction

SPECIFIC PROPERTIES:
coefficient of friction; wear ratio

GENERAL MATERIALS:
carbons; plastics; ceramics; metals

SPECIFIC MATERIALS:

KEYWORDS:
friction coefficient; wear rate; self-lubricating bearing; metals; lubrication engineering

ABSTRACT:
Friction and wear data obtained during 18 years of testing were placed in a database. Two basic files, one for radial bearing tests and one for thrust bearing tests were set up. These files now contain data from over 6,500 tests on over 400 bearing materials. The data span loads from 0.06 to 26 MPa, speeds from 0.0002 to 5.3 m/s & bearing body temperatures from 75 to 500 degrees C.

Appendix Ib

CHARACTERISTICS AND STATUS OF PUBLIC FACTUAL DATABASES CONTAINING CERAMIC PROPERTIES

FULL NAME
Ctr. for Information & Numerical Data Analysis & Synthesis

ACRONYM: CINDAS

PRODUCER
Ctr. for Info. & Numerical Data Analysis & Synthesis
(CINDAS)
Purdue University
West Lafayette IN 47906 USA

CONTACT: C. Y. Ho PHONE: (317) 494-6300

VENDOR:
CINDAS

GENERAL PROPERTIES:
magnetic; dielectric; thermophysical; thermoradiative; electronic; optical

SPECIFIC PROPERTIES:
viscosity; specific heat; Prantl number; thermal absorption; thermal conductivity; energy bands

GENERAL MATERIALS:
metals; non-metallics

SPECIFIC MATERIALS:
inorganic; organic; ferrous alloys; non-ferrous alloys; glasses; ceramics; polymers; mixtures

KEYWORDS:
magnetic; electrical; thermophysical; optical; electronic; metal

ABSTRACT:
CINDAS cover 36 thermophysical, thermoradiative electronic, electrical, dielectric, optical and magnetic properties of all technologically important materials.

Appendix Ic

CHARACTERISTICS AND STATUS OF PUBLIC
FACTUAL DATABASES CONTAINING CERAMIC PROPERTIES

FULL NAME
Ferroelectric Ceramic Base

ACRONYM: CERAMICS

PRODUCER
Sandia National Laboratory
Division 2532
P.O. Box 5800
Albuquerque, NM 87185 USA

CONTACT: C. Gebert PHONE: (505) 844-0963

GENERAL PROPERTIES:
composition

SPECIFIC PROPERTIES:

GENERAL MATERIALS:
ceramics

SPECIFIC MATERIALS:
PZT; PSZT

KEYWORDS:
ceramics; ferroelectrics; composition

ABSTRACT:
This database contains composition and testing results with 100,000 records managed by INGRES on a VAX 750 computer.

Appendix Id

CHARACTERISTICS AND STATUS OF PUBLIC FACTUAL DATABASES CONTAINING CERAMIC PROPERTIES

FULL NAME
Materials Information Databank

ACRONYM: MCIS

PRODUCER
Sandia National Laboratory
Division 1811
P.O. Box 5800
Albuquerque NM 87185 USA

CONTACT: Keith E. Mead PHONE: (505) 844-2200

GENERAL PROPERTIES:
physical; mechanical; corrosion

SPECIFIC PROPERTIES:

GENERAL MATERIALS:
metals; plastics; polymers

SPECIFIC MATERIALS:
coatings; solders; foams; fluxes; alloys; glasses; ceramics

KEYWORDS:
materials compatibility; metals; plastics; corrosion

ABSTRACT:
This database has data on the strength, corrosion and composition properties of 1,500 materials in order to analyze compatibility.

Appendix Ie

CHARACTERISTICS AND STATUS OF PUBLIC
FACTUAL DATABASES CONTAINING CERAMIC PROPERTIES

FULL NAME
Thermal Property Bank

ACRONYM: Thermal

PRODUCER
Lawrence Livermore National Laboratory
Theoretical Physics Division
P.O. Box 808 L-71
Livermore CA 94550 USA

CONTACT: A. L. Edwards PHONE: (415) 422-4123

GENERAL PROPERTIES:
thermophysical; thermochemical

SPECIFIC PROPERTIES:
specific heat; density; thermal conductivity

GENERAL MATERIALS:
metals; plastics

SPECIFIC MATERIALS:
alloys; glasses; ceramics

KEYWORDS:
thermophysical; specific heat; density

ABSTRACT:
This database contains thermal analysis data on approximately 1,000 materials.

Appendix If

CHARACTERISTICS AND STATUS OF PUBLIC
FACTUAL DATABASES CONTAINING CERAMIC PROPERTIES

FULL NAME
JANAF Thermochemical Tables

ACRONYM: JANAF

PRODUCER
National Bureau of Standards
Office of Standard Reference Data
A323 Physics Bldg.
Gaithersburg MD 20899 USA

CONTACT: Joan Sauerwein PHONE: (301) 921-2228

GENERAL PROPERTIES:
thermochemical; thermophysical

SPECIFIC PROPERTIES:
enthalpy; heat capacity; entropy; Gibbs free energy;
phase equilibrium

GENERAL MATERIALS:

SPECIFIC MATERIALS:
inorganic

KEYWORDS:
thermochemical; temperature-dependent; inorganic

ABSTRACT:
The JANAF database contains temperature dependent
thermochemical data on inorganic compounds.

FORM NBS-114A (REV. 11-84)

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4. TITLE AND SUBTITLE

Advanced Ceramics: A Critical Assessment of Database Needs for the Natural Gas Industry

5. AUTHOR(S)

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6. PERFORMING ORGANIZATION (If joint or other than NBS, see instructions)	7. Contract/Grant No.
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Center for Advanced Materials
The Pennsylvania State University
410 Walker Building
University Park, PA 16802

10. SUPPLEMENTARY NOTES

This work was performed under contract to Gas Research Institute, 8600 West Bryn Mawr Avenue, Chicago, IL 60631, Matthew E. Schreiner, GRI Project Manager, contract number 5084-23.

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

A comprehensive survey was conducted to identify the materials properties of potential importance for inclusion in an advanced structural ceramics database. The materials of current interest for use in gas-fired heat exchangers, recuperators, radiant tubes and heat engines were determined. Existing computerized, numerical databases were surveyed and those relevant to the materials and application of interest were detailed. Analysis of the results revealed that existing databases were inadequate to fulfill the critical data needs for effective applications of advanced ceramics in gas-fired, high temperature applications. Requirements for establishing a new database focussed on these materials and applications are presented.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

advanced ceramics; gas-fired environments; heat engines; heat exchangers; numerical database; materials properties; radiant tubes; recuperators.

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