THE THERMOPHYSICAL PROPERTIES RESEARCH CENTER. AN EFFECTIVE ANSWER TO INFORMATION NEEDS ON THERMOPHYSICAL PROPERTIES OF MATTER

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Abstract—The aims, functions and operations of a specialized research center which has proven effective in meeting the needs for thermophysical properties information is discussed. The integrated aspect of this center comprises three interrelated, yet distinct, areas of activity; namely: (1) Scientific Documentation, (2) Critical Tables of Properties, (3) Experimental Research to fill in gaps and to resolve areas of discord. The scope of activity in each of these three areas is discussed, giving particular emphasis to the special procedures used and the philosophy which constitutes the basis of these operations. Specific examples are cited to illustrate the major accomplishments and contributions made during the center's first five years of operation. Finally, the author presents the steps taken for the center's expanded activities as a separate entity at Purdue University.

"THE summation of human experience is being expanded at a prodigious rate, but, the means we use for threading through the consequent maze to the momentarily important item is the same as was used in the days of square-rigged ships... the modern great library is not generally consulted; it is nibbled at by a few."

The author of these words was Vannevar Bush, who used this statement eighteen years ago as a springboard to a number of suggestions for mechanizing the library search problem. Since that time, much has been said and written on what is variously referred to as "the information explosion", "information crisis", "finding what is known", "the paper curtain", "reinventing the wheel", or simply "how to cope with information by means of automated storage and retrieval techniques." National academies of sciences. National technical and scientific societies, National governmental bodies, as well as individual scientists and engineers, have explored this problem and have come up with a variety of recommendations. However, the increasing magnitude of the problem seems to be outstripping these recommendations no sooner than they are proposed.

While this universal recognition of the seriousness of the problem concerning scientific literature has been most healthy and already some steps are being taken to ameliorate the situation, it seems that the relative importance of certain fundamental questions has been either overlooked or underestimated. Primary among such basic considerations are:

- (1) How do the needs for information between the basic sciences and engineering differ.
- (2) The distinction between storage and retrieval of sources of information (reports, documents, etc.) and the factual information itself (such as numerical data).
- (3) The distinction between raw information as found in original research literature and the synthesis of this information and its expert evaluation (such as critical data).
- (4) The behavioral characteristics of scientists and engineers, which will have to be matched in order to obtain the maximum of effectiveness from a given information system.

Without going into the details of the arguments concerning the points just raised (since these fall beyond the scope of this presentation), this writer has arrived at the following conclusions based on his firsthand experiences, both

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as a user and generator of scientific and technical information on thermophysical properties. These are:

- (1) Our technical know-how and capabilities are fully adequate to solve the document retrieval problem adequately from the machine and systems design standpoint.*
- (2) The greatest bottleneck which confronts us in the solution of scientific information problems is the lack of qualified scientific and technical people *interested* in working in this area. The primary reason for this lack of personnel is not one of the need for more extensive training, but rather the stigma associated with such an activity as a second grade activity not par with the conduct of original research.

Early in 1956, an effort was initiated at Purdue University for the establishment of a permanent center dedicated to the advancement of knowledge of the thermal properties of matter. With the financial support of a number of industrial and governmental organizations, the Thermophysical Properties Research Center (normally referred to as TPRC), was established in January 1957.

Purdue University's concept of the TPRC is unique both in scope and operational procedure with the following broad objectives:

"To become a world center for research and the collection, analysis, correlation, and dissemination of thermophysical properties information and as such, to serve education, science, and technology through a better knowledge of this area."

Operating on a broad front, TPRC's overall operations consist of three major areas of activity, namely:

- (1) Scientific Documentation.
- (2) Critical Tables of Properties.
- (3) Experimental and Theoretical Research.

Each of these areas, while distinct in itself, is interrelated to the other two. Each would be only partially effective in the absence of the other two. Indeed, the whole of TPRC's operations has capabilities beyond the sums of the capabilities of its parts. The activities in each of these areas and their end products are discussed briefly in the following paragraphs.[†]

SCIENTIFIC DOCUMENTATION

TPRC's pioneering activities in this area are becoming increasingly well known through the publication in December 1960 of Volume I of the *Retrieval Guide to Thermophysical Properties Research Literature*. This major work, consisting of a set of three books, has been recognized in international reviews for its thoroughness in coverage and its originality in presenting source information on the thermophysical properties of *all* matter.

One of the main aims of the Retrieval Guide is to reach the ultimate in comprehensiveness of coverage of thermophysical properties information. An important segment of the information reported here may never appear in abstracting journals. Comprehensiveness of coverage, coupled with efficiency and speed of information retrieval provided herein, fully justifies the high level of financial and intellectual investment made by TPRC in the search, coding, mechanization and dissemination of information on thermophysical properties.

Volume II of the Retrieval Guide (available early 1963) brings the total coverage of this work to 20 000 research papers covering the world literature contributed by approximately 19940 authors published in over 2420 journals. Nearly 30 000 substances are reported in some 81300 reference entries, covering the initial thirteen of a contemplated forty-seven thermophysical properties. The coverage includes the open literature, government reports, academic dissertations and to a limited degree reports of private and industrial organizations.

^{*} The basic argument between a centralized, all inclusive, national information center vs. the specialized and decentralized centers with capabilities of functioning in depth seems to be resolved in favor of the latter. This conclusion can be substantiated both through factual operational experience as well as the logical prognosis of the problem. (In this context, the term "decentralized" should not be interpreted as "disorganized" as some have tried to allude in their arguments in support of an all inclusive national information center.)

[†] For details of TPRC's current activities, the reader is referred to TPRC's Annual Report.

This original work, in essence, brings to the user's desk the equivalent of a digital computer, whereby a simple procedure of co-ordinated use of these three books, any query within the scope of TPRC's activities can be answered in a matter of minutes. In short, this publication represents the intermarriage of one of the oldest mediums of communication—the printed page with one of the most recent tools of cybernetics the electronic computer.

Subsequent volumes of the Retrieval Guide will be published approximately every eighteen months, each volume adding to the previous ones an additional 10 000 or more research papers on thermophysical properties. With the publication of Volume III, it is anticipated that nearly all of the world literature of the first seven groups of thirteen properties, covering all matter, will have been reported in highly organized form for all literature back to the year 1920. The properties presently covered (first seven groups listed below) and those contemplated beginning with Volume IV, are as follows:

THERMOPHYSICAL PROPERTIES COVERED BY TPRC IN RETRIEVAL GUIDE

Propetty group	Number of properties	Property names
1	2	Thermal conductivity, accommo- dation coefficient
2	1	Specific heat at constant pressure
3	2	Viscosity, fluidity
4	4	Emissivity, absorptivity, reflec- tivity, transmissivity (total and spectral)
5	2	Diffusion coefficient, permeability
6	1	Thermal diffusivity
7	1	Prandtl number
8	3	Coefficient of thermal expansion (linear, superficial, cubical)
9	1	Surface tension
10	1	Thermal diffusion coefficient
11	1	Specific heat at constant volume
12	3	Thermoelectric constants (Seebeck, Peltier, Thomson coefficient)
13	2	Electrical resistance, ionic mobility
14	2	Solubility, missibility
15	1	Velocity of sound
16	8	Temperatures and heats of sub- limation, fusion, vaporization, transition
17	1	Vapor pressure

Property group	Number of properties	Property names
18	7	Critical constants, equation of state data, virial coefficient, com- pressibility, Joule-Thomson coefficient
19 20	3 1	Enthalpy, internal energy, entropy Density

It should be pointed out here that the Retrieval Guide reports not only on numerical data but also research on the theory for these properties, and experimental techniques to observe these properties. Major reviews, compendium, books, etc. are also included in the coverage.

Since TPRC's search capability of the world literature is the key to its Scientific Documentation activities, it is quite appropriate to sketch briefly the scope of this operation and the procedures used in this connection. Research of interest comes to TPRC's attention through the following major channels: (1) abstracting journals in the areas of pure and applied sciences; (2) governmental and industrial research reports; (3) reports of private research institutions and universities, including Doctoral and Master's dissertations; (4) major research centers throughout the world with whom information exchange agreements have been established and; (5) special collections, compendia, reference works and the more obscure and fugitive sources of information.

Among the various sources of information enumerated above, abstracting journals constitute the most extensive and readily accessible source of literature references. Furthermore, since many of the major abstracting journals have been issued over a period of several years, they provide a unique source for a systematic search of the literature. However, a brief familiarization with any one of the major abstracting journals will enable one to realize that a brute force, page by page, scanning of the issues of abstracting journals is prohibitive in time and effort. Alternately, the search of abstracting journals through use of their subject indexes does not prove adequate for a comprehensive search and, therefore, it is not a generally recommended procedure for a major operation

such as that of TPRC's. Furthermore, since the search of such journals is performed at TPRC by highly trained scientific and technical personnel, the cost of such a search is very great. In view of these factors. a two-year research program was undertaken early in 1958 to study optimization in searching through abstracting journals. As a result of this effort, TPRC has developed proven techniques whereby reading only 20 per cent of the total pages of an abstracting journal approxmately 95 per cent of the information is retrieved (see [1] and [2] for details of this procedure). Of the nearly 700 abstracting journals currently published, fourteen major journals were selected and are systematically read at TPRC and some additional ten are irregularly monitored. These fourteen major journals, in turn, give a coverage of over 12 000 technical and scientific journals providing TPRC with a most comprehensive coverage of the world literature on thermophysical properties.

TPRC's coverage of academic dissertations is accomplished through two publications entitled: *Dissertation Abstracts* and *Masters Theses in the Pure and Applied Sciences.* The former publication gives a fairly representative (but somewhat incomplete) reporting of Doctoral dissertations accepted by United States Colleges and Universities; while the latter represents the most complete listing of Masters Theses of over 180 United States Colleges and Universities [3]. This publication was initiated by TPRC for the specific purpose of maintaining a complete cognizance of academic research activities and constitutes the only publication of its kind.

For a detailed account of the substance classification procedure developed by TPRC and the mechanized storage and retrieval procedures, the reader is referred to [4] and [5], respectively.

CRITICAL TABLES OF PROPERTIES

As a rule, engineers do not have the time, resources, or the specialized training to wade through the mass of scientific information and unscramble its often conflicting knowledge. The generation of internally consistent tables of critically evaluated data on an up-to-date basis is indeed the end product which scientists and in particular, engineers need. It is highly important, however, to establish a clear distinction between compendia of data and critical tables (tables of "most probable" values). It is the intent here to bring about critical evaluation. analysis, correlation, as well as new calculations of data on a continuing basis. The effort indicated here is a highly technical one and requires the best of technical and scientific talents. In this activity, the concentration of effort must logically fall on those materials which may be identifiable, within acceptable limits of tolerances. Comprehensiveness of all known knowledge as well as the currency of the information processed, is the key to the effectiveness and usefulness in this effort. TPRC's activities in this area (1) insure the preservation of the results of basic and applied research, (2) shorten the time for research results in finding their place in design, (3) establish a "feed-back" into basic science, and (4) provide the key ingredient in avoiding costly mistakes and duplications in useless hardware development.

To perform their functions effectively, the scientific and technical personnel have at their disposal the unique facilities of TPRC's Scientific Documentation Division, which makes available to them all the original research literature pertinent to each project. The ultimate aims and functions of TPRC's Data Correlation Division may be summarized as follows:

(a) Taking one property and one material, or a group of materials, at a time, to refer to the original research literature, to extract the data, to evaluate critically, reconcile, and correlate all the available data on this property and material and, whenever possible, come forth with an internally consistent set of tables which are termed the "most probable values" of the particular property and materials as of a given date.

(b) To fill in gaps and to extend the available experimental data over higher or lower ranges of temperatures and pressures by means of semi-empirical or theoretical considerations and calculations whenever such procedures of interpolation and extrapolation seem to hold any justification.

(c) Through the methods of statistical thermodynamics to generate tables of transport properties where experimental data on such properties are nearly non-existent at the present time. (d) The recommended "most probable values" for each property are normally accompanied by a graphical representation comparing these recommended tabular values with all the available experimental data. Such a comparative plot is called a per cent "Departure" representation, "Departure" being defined as:

Per cent Departure

$$=\frac{(\text{Value})_{\text{Exp.}}-(\text{Value})_{\text{Tab.}}}{(\text{Value})_{\text{Tab.}}}\times 100.$$

Such a "Departure" plot constitutes an additional source of invaluable information since it reveals at a glance the concordance or discordance and the paucity or abundance of the experimental data in a given case. It further gives an indication of the evaluation placed on each of the works reported on a particular property.

(e) Once a specific research project, such as described above, is completed on a given date, the results are never considered final and each table is subject to periodic revision and extension in the light of new information that may become available in the literature or research being conducted by TPRC. In other words, after the initial effort, the tables of properties are constantly kept up to date.

In certain cases, tables of data (together with their graphical representation) are released prior to their final analysis. Such intermediate releases are justified on the basis that they bring valuable information to the attention of engineers and scientists at the earliest possible date. Such tables are reissued in revised form as soon as their critical analysis is completed and "most probable values" are established.

The overall organization of TPRC's data tables consists of three volumes, namely:

- Data Book, Volume 1: Metallic Elements and their Alloys (gaseous, liquid, and solid states)
- Data Book, Volume 2: Nonmetallic Elements and their Compounds (gaseous and liquid states at NTP)
- Data Book, Volume 3: Nonmetallic Elements and their Compounds (solid state at NTP).

Within each volume, tables on various properties constitute different chapters, thus bringing together all the thermophysical properties for a given material or substance. For the case of nonmetallic substances, the consideration of physical state (gas, liquid, and solid) is based on the state substances are found at "normal temperature and pressure" (NTP). From the above discussion, it is clear that the number of chapters in each of the three volumes of the Data Books will gradually increase as new projects become activated covering different thermophysical properties.

Because of the enormity of the task, in its preparation of data tables, TPRC selects specific properties and groups of substances on a priority basis. As of the Fall of 1962, the following data table projects have been initiated:

Thermal Conductivity: all metallic and nonmetallic elements, their alloys and compounds in the solid, liquid, and gaseous states.

Emissivity, absorbtivity, reflectivity: all metallic and nonmetallic elements, their alloys and compounds in the solid state.

Viscosity: selected gases, vapors, and liquids of technical importance (fifty-two substances within the initial group).

Data sheets are released in June and December of each year. They consist of both revisions and new additions. As of December 1962, over 900 sheets, 11×17 inches in size, have been released and disseminated to industrial, governmental, and academic laboratories.

EXPERIMENTAL RESEARCH

As a result of TPRC's activities in the areas of Scientific Documentation and Critical Tables Projects, it became perfectly apparent where the paucity and discord of information lie. TPRC's experimental program is therefore, strongly oriented by the two activities already discussed and has as its guiding philosophy the following aims:

(a) To conduct extensive new measurements on selectively chosen materials and systems of engineering importance.

(b) To conduct research in the engineering sciences, which will lead to a better understanding and interpretation of existing information and the reliable extrapolation of this information to materials, either as yet unstudied, or yet to be developed. (c) To develop new techniques and work towards the standardization of existing reliable techniques for the measurement of thermophysical properties over wider ranges of parameters (temperature, pressure, wavelength, etc.)

TPRC's experimental research was held in abeyance* until its activities in the other two areas were able to produce a topographic picture of the state of knowledge in specific cases requiring further systematic study. The first two research programs on subjects of major scientific and engineering importance are the following:

(a) The precise determination of the thermal conductivity of gases, vapors, and liquids up to 500 atm pressure and 500°C. As a result of this program, which will explore systematically selected fluids with varying degrees of molecular complexity, it is anticipated that it will be possible to obtain a better insight into intermolecular forces and arrive at an improved set of collision integral and intermolecular potential models for the reliable estimation of transport properties.

(b) The characterization of surfaces of solids from the standpoint of their optical properties (emissivity, reflectivity, etc.). Until such time when the surface condition of solids can be better defined, the radiative properties data for these surfaces will have little or no meaning. In general, surfaces need to be characterized geometrically, chemically and structurally for their complete description. The initial study undertaken at TPRC concerns itself with the geometric or topographic characterization.

Further development of TPRC's experimental research will involve the study of the thermal conductivity of metallic and nonmetallic solids with emphasis on high temperatures as well as equilibrium calorimetric investigations.

TPRC AS A SEPARATE RESEARCH CENTER

On 15 November, 1962, Purdue University announced TPRC's separation from the School of Mechanical Engineering and its establishment as a new unit of the Schools of Engineering. In announcing TPRC's reorganization, the University recognized that TPRC has outgrown the directive with which it started in 1957 and has become an interdisciplinary institution with a staff of chemists, physicists, chemical engineers and mechanical engineers. In fact, as the center has expanded, it has pursued studies in many areas, some of them by full-time professional investigators who are not on the teaching faculty. It is anticipated that the present staff of thirty-two members will soon be expanded by other appointments to include specialists in statistics, mathematics, and metallurgy.

In the summer of 1963, TPRC will be relocated in its new building which is being erected at McClure Park, the University's industrial research park, one and a half miles north of the campus. This new structure, which will cost approximately \$500 000 when equipped, is being constructed with the financial assistance of the Purdue Research Foundation. It will not only bring about the appropriate environment which will benefit the overall research program of TPRC; it will also provide three times the space TPRC now occupies, allowing room for needed expansion. When it is completed, the total research area being used by TPRC will be approximately 18000 ft².

IN CONCLUSION

It is quite clear that the tasks TPRC has set for itself are national, indeed international, in their implications. In the decade ahead, technology will exploit increasingly the progress of basic science. The time lag between scientific discovery and practical application must and will diminish, and the boundary between pure and applied science will often be diffused. These developments will be achieved primarily through the contributions made by what is known as supporting research, the type of research which welds pure and applied science together and, in so doing, strengthens both.

While already substantial tangible results are at hand, TPRC's first five years should be looked upon primarily as the formative years of an organization which has proved in performance the practicability of a somewhat new concept in meeting the information needs in the important area of thermophysical properties. The author is confident that, in its second five years, TPRC will grow even more rapidly to serve education,

^{*} TPRC's experimental research was activated in September 1961.



The Thermophysical Properties Research Center of Purdue University will occupy this new structure at 2595 Yeager Road, West Lafayette, by mid-1963. When completely equipped, the new facility will total nearly \$500 000. The new structure will house TPRC's laboratory, offices, shop and documentation rooms on 16 000 square feet of floor space. The center also will retain 2000 square feet of laboratory space on the campus. science, engineering, and technology with increasing effectiveness.

It is the aim of this brief presentation to acquaint scientists and engineers engaged in thermophysical properties research, as well as users of thermophysical properties information with an activity in which they have a direct interest and concern. The author hopes that he was able to achieve this goal at least in part and that such awareness will bring about better communication and exchange of information between workers in this specialized area throughout the world. TPRC attempts to achieve such communications, and the use of its resources by others and welcomes further inquiries on any aspect of its operations.

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Résumé—On étudie ici le but, le rôle et le fonctionnement d'un centre de recherche spécialisé qui s'est avéré effectif devant la nécessité de réunir des informations concernant les propriétés thermophysiques. Ce centre comprend trois branches d'activité concernant respectivement (1) la documentation scientifique (2) les tables de données des propriétés (3) les recherches expérimentales destinées à compléter les données manquantes et à discriminer les discordances des informations. On étudie le champ d'activité de ces trois sections en mettant l'accent sur les méthodes spéciales utilisées et l'esprit qui préside à leur fonctionnement. Des exemples particuliers sont cités pour illustrer les principales réalisations et contributions apportées par le centre au cours de ses 5 premières années. L'auteur présente enfin les étapes de l'extension du centre jusqu'à ce qu'il soit devenu un centre indépendant à l'Université de Purdue.

Zusammenfassung—Es werden Ziele, Aufgaben und Arbeitsweise eines spezialisierten Forschungszentrums dargelegt. Dieses Zentrum dient der thermophysikalischen Stoffwertinformation, wobei es sich den Anforderungen voll gewachsen zeigt. Das Gesamtarbeitsfeld umfasst zwar miteinander verwandte, im einzelnen jedoch scharf umrissene Teilgebiete, nämlich: (1) Wissenschaftliche Dokumentation, (2) Kritisch ausgewählte Stoffwerttabellen, (3) Experimentelle Forschung zur Ermittlung fehlender Werte und Klärung strittiger Bereiche. Der Umfang jedes einzelnen der drei Gebiete wird umrissen, mit besonderer Betonung der verwendeten Spezialverfahren und der den Arbeiten zugrundeliegenden Ideen. Beispiele zeigen die Hauptleistungen und Beiträge während der 5-jährigen Tätigkeit des Zentrums. Zuletzt verweist der Autor auf das vergrösserte Tätigkeitsfeld des Zentrums als gesonderte Abteilung der Purdue Universität.

Аннотация—Рассматриваются цели, функции и работа специализированного научноисследовательского центра, который доказал свою полезность при необходимости получения сведений о теплофизических характеристиках. Основное направление этого центра охватывает три взаимосвязанные, хотя отличающиеся друг от друга, области деятельности, а именно: 1. научная документация, 2. критические таблицы свойств материалов, 3. экспериментальное исследование для получения новых данных и для разрешения научных разногласий.

Рассматривается сфера деятельности в каждой из этих трех областей, когда особое внимание уделяется специальным технологическим процессам и методологии, которая составляет основу этих процессов. Приводятся иллюстрации основных достижений и успехов, полученных в течение первых пяти лет работы этого научно-исследовательского центра. В конце статьи автор останавливается на мерах, которые были предприияты для расширения деятельности этого центра как отдельной лаборатории при Университете Парду.