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Direct access to material properties for modeling and simulation

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Abstract. For developing or verifying material science models and simulation techniques, it is frequently important to have access to reliable material properties in electronic format. New sources of such data are becoming more readily available now, and one notable example of this is the services of STN International. STN is the worldwide scientific and technical information network, operated jointly by the American Chemical Society in the USA, Fachinformationzentrum-Karlsruhe in Europe, and the Japanese Information Center for Science and Technology in Asia. The numeric properties data services available on STN, notably the Material Property Data Network (MPD Network) and the Chemical Property Data Network (CPD Network) are described in some detail below, and their applicability to expert modeling and simulation programs discussed.

1. Introduction

Considerable progress is being made in the development of constitutive equations relating material performance to processing parameters and microstructure, leading in turn to the potential of new optimization procedures for alloy development. For developing or verifying such material models and related simulation technology, it is frequently important to have access to reliable material property in electronic format.

Among the major new means of access to diverse worldwide sources of reliable materials data are the Material Property Data Network (MPD Network) and the Chemical Property Data Network (CPD Network), available via STN International. STN is the worldwide scientific and technical information network, operated jointly by the American Chemical Society in the USA, Fachinformationzentrum-Karlsruhe in Europe, and the Japanese Information Center for Science and Technology in Asia.

The nature and status of development of these resources are described in some detail below, and their applicability to expert modeling and simulation programs discussed.

The scope of the paper thus includes:

- an overview of user needs,
- a description of the unique aspect of property data,
- capabilities of the CPD and MPD services:

(a) single-point access to vast data array,
(b) direct access from PC or terminal,
(c) menu interface,
(d) cluster searching,

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(e) numeric search software, and
(f) logic-based presentation.

2. Addressing user needs

In laying out the plans for the CPD and MPD services for providing easy online access to worldwide sources of reliable chemical and material property data, we utilized background information gathered from many sources on the needs of property data users [1]. The principal sources were a series of eight workshops that were held jointly with our associates in the Standard Reference Data Program at the National Institute for Standards and Technology (NIST) (e.g. [2–4]), our operation of a pilot MPD Network operation for four years from Stanford University [5], and from user groups whose reaction and assessments were obtained. From the experience gained, we not only learned much about the specific needs of scientists and engineers but also gained some insights into the broader interpretation of searchers' needs in addressing computerized systems of all types.

The primary need identifed was single-point access to a wide variety of reliable numeric (quantitative) material performance and application data. Material selection and design decisions are constantly being made, and indeed will be made with the best data that can be readily obtained in the time available. Most technical decisions cannot be delayed too long to await new information, and so the quality of decision is based upon the applicability of the specific data available at the time. Thus the preferred source of data will be that with the greatest combination of breadth and depth of property data, without this 'critical mass' of data, potential users will quickly lose interest.

Once a substantial data resource or aggregate of resources is available, the next important need (and often a principal motivator) is ease of access. The selection of one of several candidate sources may well be based upon relative convenience and support available. Regrettably, even quality of data sometimes seems secondary at this level, though for direct application to modelling and simulation, a clear measure of the reliability is required. Difficulties in accessing a source (e.g. the complexity of telecommunication connection to search online sources or getting 'hung up' or stranded in search and retrieval software) may be sufficient to cause the search to be abandoned and reliance placed upon readily available (though lesser quality) data.

If problems of access to either local or online sources are solved, this level of need is succeeeded by one relating to the interface software for the search and retrieval system. Relative motivation to use system A or B is likely to depend upon the relative simplicity, clarity, and flexibility of the search software for the candidate systems. An easily understood and logical menu-driven search software may well be sufficient to get the user to choose one system over another similar source for which searching involves use of a command language requiring training and frequent use for retention.

If concerns of access and interfacing are met satisfactorily, users' motivations shift to factors of system support. A broad and valuable glossary interfacing with the search and retrieval system, for example, may provide the added motivation for a user to select one system over another. Finally, if all other needs are met, the searcher's concern shifts to what may or must be done with the data, and the selection of one data source over another may well be based upon the presence of software packages for analytical treatment, graphics, or computer-aided design and manufacturing.

The important point to take from this illustration is simply that to be of value to the materials modeling and simulation expert, a potential data source must provide:

- a critical mass of numeric data; a high probability of useful answers;
- ease of access; a 'quick connection';
- flexible search and retrieval software; multiple search paths;
- strong system support; integrated thesaurus, help functions; and
- capabilities for handling and downloading the data.

These are precisely the objectives behind the development of the CPD and MPD Networks on STN International.

3. Nature of numeric property data

Adding to the complexity of developing the CPD and MPD Networks is the fact that numeric property data have several important characteristics not shared by more conventional bibliographic data [6–8]. First the obvious: They are quantitative and thus have implied precision, come in ranges as well as discrete values, and may vary over many orders of magnitude within a single data record containing four or five properties. Second, they have units associated with them from which they can never be separated and still retain meaning: the numbers in any one record may have multiple units, some of them involving two or three unit types (e.g. length, time, pressure, and temperature). Finally, they are usually dependent upon a number of independent variables or combinations of variables called parameters, which influence their value or behavior in certain situations.

These factors all make the handling of numeric data more complex than the handling of textual data, which typically is searched for 'strings' of characters without other modifiers except perhaps other strings that may be added together in various boolean modes. Numeric data must be stored and searched keeping in mind at least three major elements—the name of the property, its value, and the units of that value —and often more. For example, the property may be dependent upon time of exposure at a particular combination of temperature and pressure, and so three more factors—time, temperature, and pressure—must be included as delimiters in every query about that property.

4. CPD and MPD network service on STN international—fulfilling user needs

The National Materials Property Data Network (NMPDN) Inc. was formed in 1985 with the mission of providing easier access for engineers and material scientists to reliable materials properties. In 1987, the NMPDN began working jointly with Chemical Abstracts Service (CAS) to implement and distribute the MPD Network service on STN International. The prototype production version of the MPD Network Service became available early in 1991.

In December 1991, a second service, the Chemical Property Data (CPD) Network Service, was implemented on STN International as a complement to the MPD service. The CPD service provides physical and chemical property data for a wide range of chemicals.

STN International is the premier online scientific and technical information

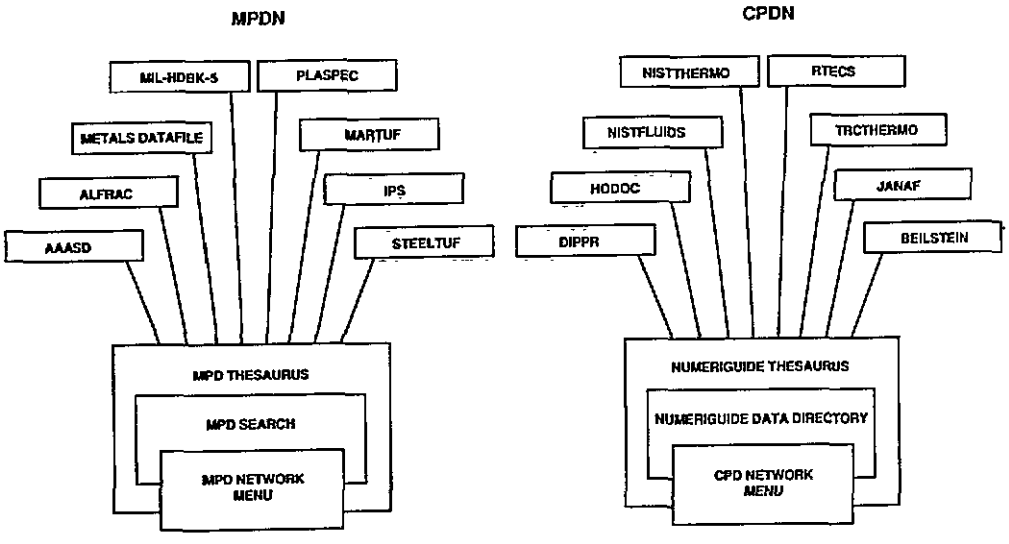

Fig. 1. MPD and CPD Network schematic.

network operated jointly by CAS, a division of the American Chemical Society, in Columbus, OH, USA, FIZ Karlsruhe, a scientific and educational organization in Karlsruhe, Federal Republic of Germany, and Japan Information Center of Science and Technology (JICST) in Tokyo, Japan [9].

These two services, the CPD Network and the MPD Network, are referred to as 'networks' because, within each, the databases are networked physically by the search software and intellectually by the search strategies and the associated thesauri, which cross-link the terminology in the various databases, as illustrated by the schematic in figure 1. Thus, these are truly network services within the context of the broader scientific and technical network known as STN International, and permit concurrent searching of all of the databases networked in each cluster, regardless of which of the three service centers the individual databases reside on (illustrated schematically in figure 2).

5. STN International provides single-point access to a vast array of property data

Through the CPD and MPD services, STN International provides single-point access to a significant volume of property data. The combined services provide access to over 500 properties, 25 000 chemicals, 20 000 materials, and 20 databases. The coverage is being extended continuously, both for chemical substances and for materials.

The CPD service includes such classes of properties as thermodynamic, electrochemical, spectral, safety, and transport.

Among the specific databases currently available through the prototype version of the CPD service are

DIPPR—textual and numeric information on the pure component physical property data for commercially important chemical substances;

HODOC—an electronic version of much of the CRC Handbook of Data on Organic Compounds, including the chemical and physical properties of over 25 000 organic

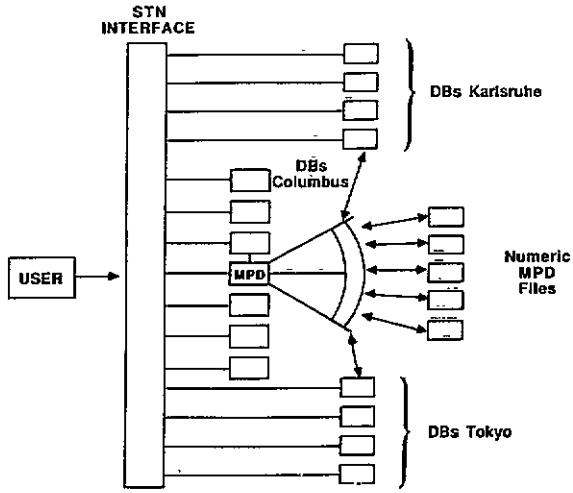

Fig. 2. Functional schematic of the MPD Network on STN International.

substances;

JANAF—critically evaluated thermodynamic properties from the Joint Army–Navy–Air Force Thermodynamic Tables;

NISTTHERMO (formerly NBSTHERMO)—the NIST Tables of Chemical Thermodynamic Properties, containing critically evaluated chemical thermodynamic properties of over 8000 inorganic and organic substances;

NISTFLUIDS (formerly NBSFLUIDS)—the NIST calculation package covering the thermophysical and transport properties of fluids as a function of temperature and pressure;

TRCTHERMO—from the Thermodynamic Research Center–the evaluated thermodynamic properties of 7000 compounds.

In addition, and partially transparent to the user, the CPD service makes significant use of the NUMERIGUIDE and CAS REGISTRY databases to identify properties and chemicals, respectively, and to locate the databases that will likely contain the data the user desires. NUMERIGUIDE is a property thesaurus and data directory that provides

- property names and hierarchies,
- definitions/descriptions,
- aliases,
- abbreviations,
- identification of databases that address each property,
- default units, and
- variables associated with property (e.g. temperature).

The REGISTRY database provides a reliable means for searching chemicals by chemical name, molecular formula, or CAS Registry number. REGISTRY also provides identification of databases that address each chemical.

Numeric information available on the MPD service includes not only mechanical, physical, and other performance data for all structural materials, including metals, polymers, ceramics, and composites, but also the properties of connections and joints in these materials.

Among the specific databases available through the MPD service are

AAASD—from the Aluminum Association—typical and minimum tensile properties, typical mechanical and physical properties, and fabricating and application information on more than 150 commercial aluminum alloys;

ALFRAC—from NIST/SRD, the Materials Properties Council, and the Aluminum Association—plane strane fracture toughness data for about 25 high-strength aluminum alloys, with validity documentation;

COPPERDATA—from the Copper Data Association—mechanical, electrical, thermal and other physical properties of 166 wrought and 95 cast US coppers and copper alloys;

IPS (International Plastics Selector)—from DATA Business Communications, a division of IHS;

MIL-HDBK-5—from the MIL-HDBK-5 Coordination Committee publication—design tables covering the design mechanical and physical properties of ferrous and non-ferrous alloys;

MARTUF—from the Materials Property Council —about 10 000 individual toughness test results for steels for marine applications;

METALS DATAFILE—from Materials Information (ASM International and the Institute of Metals)—data from more than 40 000 literature citations from technical journals;

MPDSEARCH—an international directory of sources for material property information that contains both databases and data centers—organizations who will research information for you;

NISTCERAM—from NIST—properties of structural ceramics—silicon carbides and silicon nitrides;

PDLCOM—from the Plastics Design Library—chemical and environmental compatibility of plastics;

PLASNEWS—a daily news file for the plastics industry;

PLASPEC—from the publishers of Plastics Technology—typical properties from producers of about 10 000 plastics; and

STEELTUF—from the Electric Power Research Institute and the Materials Properties Council—results of more than 20 000 individual tests of steels for the power and petroleum industries.

There are also a number of materials-related bibliographic databases on STN International, and these are readily accessible in cross-over searching from the numeric files, except that such cross-overs are limited to command-mode searching (as contrasted to menu searching; see section 7). So background files like COMPENDEX,

METADEX, EMA, and INSPEC may provide useful complementary information to that in the numeric files.

6. Direct access from user's PC or terminal

Modelers and simulation experts may access both the CPD and MPD services from anywhere in the world directly through their own computer or a terminal together with a modem. Users may use their own telecommunication software or, if they wish, use a specially designed diskette that, with a single command, dials, connects, logs in, and accesses the CPD and MPD Network services directly.

7. Numeric data software capabilities

In order to provide search and retrieval software that deals with the complexities of numeric properties data, NMPDN and CAS have over the years enhanced the STN search and retrieval software to provide certain capabilities that are especially useful in meeting users' needs in handling numeric data. All the features listed below are available on the CPD and MPD services:

- range searching—the ability to search for chemicals or materials with combinations of properties in specific ranges or above or below certain limiting values;
- unit conversion—the ability to convert to any of the worldwide standard systems of units—International Standard (SI), meter-kilogram-second (MKS), centimeter-gram-second (CGS), engineering (ENG), and the STN user-friendly SI system;
- tolerance setting—the ability to define ranges of search values by the tolerance on the search value (e.g. 50 000 ±1000 psi);
- table display—the ability to obtain tabular display of data that match your specific query and to predefine certain types of tabular displays; and
- calculation packages—the capability for interpolation and estimation of additional information or the application of parametric analysis of multi-variant properties, valuable in providing specific answers to some complex materials questions.

8. Menu interface

Most materials experts are not experienced in searching by the conventional online command modes, and since such searches are done only occasionally have little incentive to learn the relatively complex terms needed. Therefore, NMPDN and CAS have developed and implemented menu-driven search-and-retrieval interfaces for both the CPD and MPD Network services that are easy to use, even for someone with no previous online experience. Among the major features of these interfaces are

- very logical, easy-to-use, menu-driven search paths;

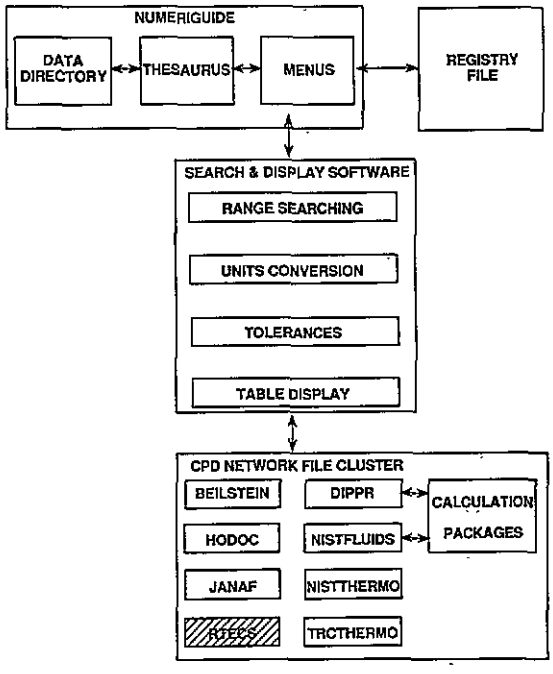

Figure 3. Key elements of the CPD Network.

- a variety of search paths, recognizing that different types of users and different applications will require different queries;
- a 'metadata' system in the form of an interactive thesaurus that both deals with user queries, translating them to all other acceptable nomenclature and terminology, and responds quickly to clarify the meaning of names, terms, and abbreviations;
- the ability to define and include in the search variables associated with both the substances and properties of interest; and
- a directory of data sources, including those outside the services.

By nature of the detailed searching done in numeric files in contrast to the broader subject searching done in textual files, these menus are much more detailed and sophisticated than those used to guide searchers to appropriate bibliographic files. They truly are 'expert systems' of a sort, capable of taking the basic input from the user, determining the proper databases to search, and building the appropriate command-language searches required to conduct the search.

The functionality, built into the menu interface is suggested by the schematic architecture in figure 3, using the Chemical Property Data (CPD) Network as the illustration; the architecture of the MPD Network is quite similar. The menu interface links the data directory and theseaurus encompassed within Numeriguide and the Chemical Abstracts REGISTRY file, as a material/substance locator, to the numeric search and retrieval discussed above, and ultimately to the appropriate cluster of liles, providing the cluster search capability described below.

9. Cluster searching

The conventional approach to database access and searching has been based upon the assumption that each database stands alone and is accessed and searched largely independently of the others. With numeric properties databases, which each tend to be relatively small and well focused, this approach is often not very useful for several reasons. First, a number of databases may need to be accessed to provide all the property data required for many applications. Second, the user may not know which of several databases will be most responsive to the particular needs at any given moment. Thus, to best serve the needs of searchers for properties data, it has proven desirable to link many databases together into a logical 'cluster' and permit easy cross-file searching of those files.

Depending upon the nature of a query, CPD and MPD service users may approach the database cluster with different pieces of information at the heart of their query:

- a specific database with a certain type of data, e.g. design values;
- a specific chemical or material for which a variety of types of data are sought;
- a specific property or properties for which a comparison of chemicals or materials is required, perhaps involving a specific range of values, notably those equaling or exceeding certain limiting values.

The CPD and MPD services enable the user to search all of the databases in the cluster simultaneously, with no requirement that the user know which databases are most likely to contain the data. Further, from such a cluster, all reasonable data sets responsive to the query will be provided, always with clear evidence of why they were provided and from where they have come along with all of the associated parametric support data. In the case where answers to the same query are located in two or more different databases, the user is always given the option of selecting individual answers or comparing all of them; no analysis is made, but rather the user may decide which to use based upon the relative mertis of the replicate values.

The flow of operation of the system is suggested by the representative sequence of screens presented in figure 4: (*a*) illustrates the starting point at the basic query building screen, where the user may specify what chemicals and/or properties are needed, may specify a database or let the system locate the appropriate databases, and set the desired units system for search and display; (*b*) illustrates the chemical identification options, and (*c*) and (*d*) the screens for choosing the properties needed; (*e*) illustrates the completed query for a user searching for the Gibbs energy function at temperatures above 1000 K, and (*f*) the concise direct answer to the query.

10. Presentation formats

Property data are typically sought to support some analytic use in a specific application, perhaps ranging from developing a new, improved chemical or material to designing some specific structure. To facilitate the analysis efforts of data users, the CPD and MPD services provide a wide range of data display options that take the following factors into account.

- types of users—engineers and scientists tend to expect data to be presented in a

(a)

CPD Network BEGIN SPECIFYING YOUR SEARCH Screen: qb1.i

Select the category with which you would like to begin.

1 Specify Databases
2 Specify Chemicals
3 Specify Properties

U Specify Units System STN

If you do not specify databases, the CPD Network will specify appropriate databases based upon your other selections. If you do not specify a units system, the STN unit system will be used.

Enter your selection:

Enter ? for help Enter MC to view list of Menu Control Options

(b)

CPD Network CHEMICAL SPECIFICATION Screen: chselect.i

Indicate how you wish to specify chemicals for search:

1 Chemical Name
2 Molecular Formula
3 CAS Registry Number

Enter your selection:

Enter ? for help Enter MC to view list of Menu Control Options

(c)

CPD Network PROPERTY SPECIFICATION Screen: propmenu1.i

Select from the following classes of properties --

1 Atomic and Molecular
2 Crystal
3 Density and Volume
4 Electric/Magnetic
5 Electrochemical
6 Mechanical
7 Multicomponent System
8 Optical
9 Safety
10 Spectral
11 State of Aggregation
12 Structure/Energy
13 Thermodynamic
14 Transport

Enter your selection:

Enter ? for help Enter MC to view list of Menu Control Options

Figure 4. Representative menu interface screen for CPD Network (*a*)–(*f*).

(d)

```
CPD Network        THERMODYNAMIC PROPERTIES        Screen: prop.thermo.i

Select from the following Thermodynamic properties --

 1  Critical Constant              9  Linear Expansion Coefficient
 2  Energy Properties             10  Mass Properties
 3  Enthalpy Properties           11  Pressure Properties
 4  Entropy Properties            12  Second Virial Coefficient
 5  Equilibrium Properties        13  Temperature Properties
 6  Gibbs Energy Function         14  Thermal Conductivity
 7  Gibbs Energy of Formation     15  Volume Properties
 8  Heat Capacity Properties

Enter your selection:

Enter ? for help                  Enter MC to view list of Menu Control Options
```

(e)

```
CPD Network          CURRENT SEARCH STATUS          Screen: qb3.i

Your current search terms are:

 1  Databases          SYSTEM WILL SELECT DATABASES
 2  Chemicals          TOLUENE
 3  Properties         GIBBS ENERGY FUNCTION
 4  Property Variables 1000 <= TEMPERATURE <= 99999 K

Select line number to insert, replace, or delete search term, or select

 S  to conduct search
 U  to change Units System   STN

Enter your selection:

Enter ? for help                  Enter MC to view list of Menu Control Options
```

(f)

```
CPD Network        *** Result 1 TRCTHERMO ***        Screen: disp.primary

RN   ***108-88-3*** TRCTHERMO
MF   C7 H8
CN   Methylbenzene

GIBBS ENERGY FUNCTION
TBLNO:23-2-(33.11000)-s  PGNO: s-3200
Revision date (RDAT): 31 Oct 1986

SSTA  Temperature   Value
      GEF.T         GEF
        K           J/mol*K
=====+==========+========
  IG      1000      384.62
  IG      1100      400.09
  IG      1200      415.05
  IG      1300      429.51
  IG      1400      443.49
  IG      1500      457.01

Enter GO to continue:
```

Figure 4. *Continued.*

logical, use-oriented tabular or graphic display rather than bunched together or in a long, disorganized litany. Wherever appropriate, property data are presented in tabular matrix displays.

- types of query—special display formats, known as 'query-related' displays, are utilized to focus specific properties and the variables or parameters that define the applicability of the data. Searchers do not have to wade through extraneous data, yet they have all of the pertinent related information.
- Number of answer sets—brief summary displays have been designed to allow searchers to scan large numbers of records to locate those of particular interest, which can then be displayed more fully.
- Documentation required to define the source and applicability of data—as noted earlier, a number of variables such as time and temperature, or in the case of the materials, form and dimensions, are often required to define the range of utility of specific data. Displays are designed to accomodate reporting of these variables along with the specific data requested.

The provision of supporting documentation in the displays is a particularly important point that is often taken for granted or omitted completely in reporting data. This may go well beyond what a specific user requests. Basic facts such as the type of data (design value or individual test result) and the applicable orientation (longitudinal or short transverse) are included.

11. Downloading, analytical and graphical analysis

As noted earlier, once useful materials data are located, engineers and material scientists typically have great interest in carrying out some types of analytical or graphical parametric evaluation of the data. Such functions might be carried out with the search and retrieval software itself, but more likely will be done after downloading into their own specific software programs. As a result for the MPD and CPD Network services, a higher priority has been placed upon the development of a downloading capability incorporating a variety of standard formats than on the analytical and graphical functions themselves.

Work underway in ASTM Committee E49 on Computerization of Material and Chemical Property Data will soon lead to some new interchange protocols for the properties and chemical structures of certain materials and these will be accomodataed in the STN downloading capabilities. Such downloading, especially in the new standard STEP protocols now being evaluated in ASTM Committee E49, will be especially important for application to CAD/CAM operations where complete electronic data exchange is desired.

12. Summary

In developing the CPD and MPD Network services on STN International, an innovative approach was taken to addressing the needs of engineers and scientists for easy access to and flexible interaction with worldwide sources of numeric chemical and material property data. The distinct added complexities of storage, search, and retrieval

of numeric property data have been addressed with special search software and a user interface to aid the scientists and engineers who are the end users of such highly technical information. Provision has been made to ensure that a variety of types of user and their queries may be handled with ease on the system and that the confusion of names, terms, and abbreviations can be removed.

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