efficient storage of data. The user can retrieve any of the dispersed chemical resistance information and data in any manner desired.

To reiterate, the mechanism for the type of data retrieval described is available. What is now necessary is the acquisition of data so desperately needed to fulfill the PLASTEC goal. If past literature is any guide, data acquistion will be a problem: more specifically, the availability of data, the inconsistency in reporting data, and the reliability of the information. PLASTEC's system dictates that these data be derived directly from the material supplier for each major grade of material marketed.

It is anticipated that the materials data requested will not be complete. This is unfortunate, since the ASTM test methods provide adequate guidance for the testing and reporting of data. What is needed is a more definitive effort at providing engineering data. Once a material is tested and the data are documented, it is valid for practically the life of the material. The plight of the material supplier, in that testing is costly, is truly appreciated. But, it is to the suppliers advantage to characterize fully and publish each material property to assure effective use. There are some who do a good job, but they are a small segment of the industry.

The solution to the problem of numberic data acquisition for the computerization involves many parties. It is not something that can be done alone, but needs broad cooperation of industry, universities, government, and the professional societies. The course to be taken is threefold:

First, the necessity to establish a systematic approach to data gathering. A commitment on the part of professional societies and universities is needed to provide guidance of data formats. Specialists need to specify what technical presentations of data are most meaningful for use and how they should be documented. We at PLASTEC have established basic formats and prepared "data capture forms", modeled after other typical computer forms, to collect and assess data. These forms, we hope, will be the stimulus for more active participation in our system and others.

Second, a long-range commitment on the part of industry to generate the data in a more comprehensive manner, that is, adhering to the standardized formats and reporting procedures. This will enable better assessments of materials for use applications.

Third, a commitment on the part of national data centers to act as repositories for such information. This implies a commitment for data gathering, assessment, and storage. The centers would in essence maintain a central file of data which is thorough, current, and validated. They would also enable remote terminal access through the time-share mode or provide updated data files on a periodic basis.

The program at PLASTEC, as discussed herein, represents one contribution to the computerization of numeric data. The technology is available and the need exists. What remains is the cooperation necessary to make this program and others the ultimate in information retrieval.

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An On-Line System for Storage and Retrieval of Polymer Data[†]

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A system for the on-line storage and retrieval of data related to polymeric substances has been developed for use by technical service, research, and marketing personnel. The database includes trade names, chemical names, structure and polymer class fragment codes, Wiswesser line notation, physical properties, and other descriptive data for about 1100 polymers. The retrieval system has two features: a report-generator, for displaying information on selected polymer names and families, and a search function for retrieving substances with certain property, substructure, and polymer class requirements.

The polymer scientist and engineer have a continual need for physical property data on a wide variety of polymers and polymer systems. The engineer may need the data for design purposes to assess a material's worth in the market place. The scientist may wish to ascertain the effects of chemical structure on certain physical properties in order to design a material to meet a particular application. The problem is that the data they need are widely scattered throughout the literature and are only accessible via long, tedious literature searches. Very often, because of the very nature of these searches, a piece of key data is missed. This can be disasterous because much time and effort may be expended in reinventing a material.

A solution to this problem would be to establish a computer-centered property database which could be accessed easily at a variety of levels to meet the broad interests of technical service, research, and marketing personnel. A system of this type could provide interactive on-line data storage and retrieval capabilities, which would greatly enhance the timeliness and availability of the data. In an industrial environment, this would allow for the comparison of competitive

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DOW ABS 500 resin	(Name)
Dow, acrylonitrile, butadiene, styrene	(Description)
/*1Y*CN/ &721 &121 /*YR&1*/ &722 &122 /*U4*/ &122	(Dow-Modified WLN)
Alkyl, CN, Phenyl, C =, CH, 1	(Substructure Fragment Codes)
AN, BD, PS	(Class Codes)

Figure 1. Descriptive data for typical polymer.

Composition codes:

AN = Acrylonitrile
BD = Butadiene
PS = Polystyrene

Substructure codes:

ALKYL = Any Alkyl group
CN = Nitrile group
1 = $-CH_2-$ or $-CH_3$

Figure 2. Some chemical substructure fragment codes and composition codes.

DOW ABS 500 resin

IZ	2.7	#BRDL76541
US	4700	BRDL76541
HDT	198	DWABS500
MFR	3.2	BRDL76541

Figure 3. Some property values for DOW ABS 500 resin.

and proprietary material properties, as well as the rapid retrieval of information on a particular product for customer service and marketing. This paper describes the development of such a system at The Dow Chemical Company.

THE DATABASE

The database for this system is composed of descriptive and physical property data for about 1100 Dow and non-Dow polymer products. A growth to a maximum of 3000 substances is predicted. Information in the database has been obtained from published information, such as product data sheets, trade journals, advertisements, books, and unpublished sources, such as Dow research reports. Since the system contains proprietary information, it is not generally available to the public.

Descriptive data consist of a trade name or chemical name, source or other descriptive comment, modified Wiswesser line notation, chemical structure fragment codes, and composition (or polymer class) codes. These data for a typical compound are illustrated in Figure 1. Chemical substructure fragment codes are selected from a dictionary of predefined descriptors for which the codes are an abbreviation (Figure 2). Similarly, composition codes represent broad classes of polymers or starting monomers (such as acrylonitrile polymers (AN), styrene polymer (PS)) (Figure 2). More than one of these codes will apply to copolymers to indicate their monomer composition. The codes represent a modification of similar codes established by the American Society for Testing and Materials (ASTM).[1]

Each element of property data consists of three parts: a property identification code, a numeric value, and a reference identification code. Some typical data are illustrated in Figure 3. Multiple values for a given property are each recorded separately. Property codes to date have been defined in terms of a single set of experimental conditions (Figure 4), and only those properties measured under such conditions have been

IZ	=	Izod impact strength, ft-lb/ in notch, ASTM D256
US	=	Ultimate tensile strength, psi, ASTM D638
HDT	=	264 psi annealed heat deflection temperature, °F, ASTM D648
MFR	=	Melt flow rate, g/10 minutes, ASTM D1238

Figure 4. Some property codes and their definitions.

BRDL76541	=	Bird, A. L., Dow Report PSN-1-76-016
DWABS500	=	Dow ABS 500 Resin, Styrene Plastics Dept Product Information, form no. 301-347-76, The Dow Chemical Company.

Figure 5. Some bibliographic citations for reference codes.

recorded. If a standard of the American Society for Testing and Materials exists for determination of a property, conditions of this procedure are used.[2] If a reference source contains only "nonstandard" property values, the existence of such values is indicated by a "zero" value in a property data item. A pound sign (#) prefaces the reference code for such items. If both standard and nonstandard data exist in a reference source, the standard value is recorded and the existence of the nonstandard material is indicated by the reference code pound sign (Figure 3). A parameter field for recording various experimental conditions is being introduced into the data items. This should obviate the need to distinguish between "standard" and "nonstandard" data, thereby enhancing the retrieval capabilities of the system.

Reference codes are 15 character mnemonic abbreviations for full bibliographic citations (Figure 5). A listing of these codes and citations is made available to all users, as are the codes and code definitions for chemical substructure fragments, compositions, and properties. Individual code definitions may be retrieved through the data retrieval program described below.

THE RETRIEVAL PROGRAM

An on-line interactive search program performs the retrieval function of the system using various commands entered by the user. Tutorial features have been incorporated into the program to assist the new or infrequent user. There are two basic types of query: (A) retrieval of all or part of the data for a given polymer or generic group of polymers (TRADENAME command); (B) retrieval of all polymers having certain chemical substructure, composition, and/or property value characteristics (SEARCH and related commands).

The first type of query (A) is actually a reporting feature for printing selected data for polymers. The user enters the TRADENAME command, in response to which the program prompts him to enter the trade name or chemical name for the desired compound. Generic searches for families of trade names may be achieved by entering the left-most portion of the name which reflects the level of specificity desired. For example:

DOW ABS

DOW ABS 500

The first item would retrieve all polymers with the root DOW ABS; the second name restricts the search to DOW ABS 500.

```
Search Query:
    Display the ultimate tensile strength and
    heat deflection temperature of Dow ABS 500
    resin

Parameters:
    DOW ABS 500
    US, HDT

Answer:
    DOW ABS 500 resin
        US 4700 BRDL76541
        HDT 198  DWABS500
```

Figure 6. TRADENAME command query for specific polymer.

```
Search Query:
    Display the ultimate tensile strength for all
    Dow ABS resins

Parameters:
    Dow ABS
    US

Answer:
    Dow ABS 213 resin
        US 3400 BRDL76541

    Dow ABS 350 resin
        US 5000 CMPSTYPLA

    Dow ABS 500 resin
        US 4700 BRDL76541
```

Figure 7. TRADENAME command query for generic polymer family.

Spaces are not significant and are ignored in matching the query name with those in the database.

All or part of the data items mentioned in the preceding section describing the database may be displayed. In addition, data may be printed at the user's terminal or on the line printer. A one-character code has been designated to indicate the print options shown in Table I.

Any combination of these codes may be entered in response to the program's request for display options. The "PP" option will prompt a further request for specific property codes to be displayed. If no options are entered, only the polymer names are displayed. Examples of specific and broad or "generic" searches of trade names are illustrated in Figures 6 and 7.

The second type of search (B) is initiated by the SEARCH command. Queries are formulated by linking parameters from the three broad categories (substructure fragment code, composition code, property code and value) using the Boolean operators AND, OR, and NOT. Property value relations are expressed with the mathematical operators GREATER THAN (>), LESS THAN (<), and EQUAL TO (=). The

Table I

code	option
D	descriptive information
W	WLN
S	chemical substructure fragment codes
C	composition codes
P	all property data
PP	partial property data
L	print report on line printer

```
Search Query:
    Find all styrenic polymers with an ultimate
    tensile strength >10000 and a vicat softening
    point >200

Parameters:
    PS AND US >10000 AND VSP >200

Answers:
    LUSTRAN* SAN 31 molding material
        US  10500 MNSLUSSAN31
        VSP   229 DLDA764989

    TYRIL**880  styrene-acrylonitrile resins
        US   10000 #DWTYR 880
        VSP    231  DWTYR 880

    *Trademark of Monsanto Chemical Company
   **Trademark of The Dow Chemical Company
```

Figure 8. SEARCH command example.

```
Search Query:
    Find polymers with high transparency (optical
    transmission > 85%) and low flammability (UL94
    flammability = 0)

Parameters:
    TR > 85% AND VE = 0

Answers:
    MERLON* SE2100 polycarbonate resin
        VE  0    PLAWAETPSEM
        TR 87   #MBYPIMR2100,71

    LEXAN** F2000 polycarbonate resin
        VE  0    GELXFTSF2000
        TR 86   #GELXFTSF2000

    *Trademark of Mobay Chemical Company
   **Trademark of General Electric Company
```

Figure 9. SEARCH command example.

user may display data for search results using the DISPLAY command (same features as the TRADENAME command) or narrow down his search with further parameters (MOD command).

The SEARCH command provides the user with the ability to compare the properties of Dow products with competitive ones or even with other Dow products in relation to a particular need. For example, if a research chemist were developing high-strength, high-heat styrenic materials for use in machine housings, he might formulate the search illustrated in Figure 8. Note that both a Dow and non-Dow material with similar properties were retrieved. Similarly, a salesman might be interested in surveying the market for materials used as windows. The search in Figure 9 would satisfy his request. If either one of these users wanted additional data about their query results, the DISPLAY command provides this capability.

In addition to the above features, the retrieval program has other commands which provide expanded definitions for search parameter codes (DICT) or reference codes (REF). The INSTRC command initiates the tutorial feature mentioned earlier.

HARDWARE

The system described above operates on a Digital Equipment Corp. PDP 11/70 with the Resource Sharing Time Sharing operating system. Software has been coded in BASIC-PLUS. Data entry is achieved through use of an Ann Arbor cathode ray tube using full screen data entry. Searching may be carried out at any terminal compatible with the PDP 11/70. A previous generation of this system was developed on an IBM 370/158, with batch mode data entry and on-line search.

CONCLUSION

Dow has developed an on-line interactive data storage and retrieval system for polymer products. Queries to the system may retrieve information for a particular trade name or family of trade names, or any group of substances with certain substructure, composition and/or property criteria. The system will provide the polymer scientist, engineer, or salesman with rapid access to current data for the specific needs of their particular occupation. The system will also serve as a prototype for other small in-house data management systems.

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A Classification System for Polymer Literature in an Industrial Environment†

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Polymer science and technology has evolved over the past 35 years into a significant and fast-growing literature with a unique nomenclature and language, and as an extension rather than a part or subclass of physics, chemistry, and engineering. A book classification system is described that treats polymer science and technology as a major class oriented to the information needs of polymer scientists and engineers in an industrial environment.

Classification is a process of differentiation in which objects or ideas are brought together by similarities and separated by differences. Languages are replete with classificatory concepts: solids/liquids/gases; plants/animals; land/water; and night/day, to name a few. Languages rich in synonyms and antonyms have enabled scientists to observe and study nature and to think with a great spectrum of similarities and differences.

Classification schemes have been of great importance in the history of knowledge and education. An outstanding example of a classification system was the family–genus–species concept that Linnaeus introduced in 1738, and which marks the beginning of the systematization of botany. The outstanding example of a classification system in chemistry was Mendeleev's introduction of the periodic table in 1869. This paradigm in chemistry pointed out not only potential errors of existing information but predicted the discovery of new elements and their properties. The periodic table motivated and advanced research and it remains a powerful teaching aid.[11,12]

The classification of knowledge has played an important role in how documents are arranged in libraries, especially large libraries. Well into the 19th century, the majority of libraries arranged books alphabetically by author or by title, size, color, or accession. A few libraries employed a classification system based on academic fields of study, and some even used a decimal system—for the shelves, not the books. We are indebted to Melvil Dewey for the Decimal Classification System which he introduced in 1876 for the arrangement of documents in libraries and which quickly was adopted as such or modified by many libraries.

The major library book classification systems used today are: Dewey; the Universal Decimal Classification or UDC,

Table I. Some Principal Classes in the Dewey System

	500	Pure Science
	540	Chemistry, Crystallography, Mineralogy
	541	Physical Chemistry
	542	Apparatus and Equipment
	543	Analytical Chemistry
	546	Inorganic Chemistry
	547	Organic Chemistry
2	547.013	Polymerization: Organic Chemistry
3	547.92	Special fields of organic chemistry
		starch
		cellulose
		high polymers
		rubber
		synthetic resins
	600	Applied Science
4	660.28	Chemical Engineering
	661	Industrial Chemicals
	668	Other Organic Chemical Materials and Products
	668.4	Plastics Industries, Resins, Gums
	668.422	Condensation Plastics, e.g., Phenolics
	668.423	Linear Polymer Plastics (except fibers), e.g., polyethylene
1	668.44	Plastics from cellulose
	677	Textile and Other Fiber Manufacturers
	677.46	Rayon
	678	Rubber
	678.3	Natural and Synthetic Rubber
	678.7	Elastomers
	678.72	Synthetic Rubber
	678.722	Polymerization: Synthetic Rubber

See Table V for identification of 1, 2, 3, and 4

which is a modified Dewey; and the Library of Congress or LC.[4,5,9]

Libraries using the Dewey system adhere to the classes shown in Table I.

Libraries using the UDC system arrange books according to the classes shown in Table II.

Polymerization in UDC is assigned the number 542.952.6

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