Computerized Numeric Data for Polymers

JOHN NARDONE
Plastics Technical Evaluation Center, U.S. Army Armament Research and Development Command, Dover, New Jersey 07801

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The Plastics Technical Evaluation Center (PLASTEC) has developed a computerized engineering oriented data system for polymers. The system has the capability for accessing a broad spectrum of data and information, and includes capability for graphics of engineering data. The mechanics of the system have been demonstrated and the current PLASTEC need is for data. A scheme for the cooperative gathering of data is suggested which requires the cooperation of industry, universities, government, and professional societies.

The subject of "retrieval of polymer information" is extremely broad but normally refers to action to locate a published report or other reference document for the purpose of obtaining technical information. Currently, however, there is interest in another phase of information retrieval, that is, the remote access of numeric data.[1-3] This technique would make specific, scientific, and engineering data available directly to technical personnel, thus eliminating the costly and time-consuming retrieval and manual review of documents.

PLASTEC has recognized the need and the value of numeric data and believes that the establishment of centralized computer files is the most efficient method for storage and retrieval of material property data. This is particularly true for polymers since the number of materials and variations is continually increasing.

We have initiated a highly engineering oriented system to aid the military and industrial community. The major need of this system will be the technical data, which is discussed subsequently.

The first remote access system of this type developed by PLASTEC was called COMPAT. It was a unique file of data on the response of polymers in the presence of explosives or propellants. Following inception, a user guide was prepared describing the dial up procedures and the simplified, tutorial approach to data retrieval. This program development was beneficial in three respects. First, it provided a computerized file of information heretofore scattered throughout many documents; secondly, it proved the concept of remote data access; and thirdly, it emphasized the need for more formal procedures in reporting data.

COMPAT is still quite active and has been expanded in scope to include data on the compatibility of polymers in end use environments. However, this file is limited since the information is taken only from available failure reports.

The PLASTEC Data System, currently under development, consists of fundamental material property data for polymers. It utilizes the CDC 6000 series computers and a commercially available data management system called DRS, procured specifically for this project. The software is versatile and enables the user to retrieve data directly or to perform data manipulations, calculations, and assessments for material selection purposes.

When the software is coupled with a display-type terminal, another dimension is added to data retrieval—computer graphics, which is highly desirable in the interpretation and analysis of engineering data.[4]

The PLASTEC system was initially structured for molding type compounds with plans to expand the coverage to composites and elastomers. The data is engineering oriented and based on user needs.

The PLASTEC system was structured initially for the following basic property categories: mechanical, electrical, thermal, optical, physical, and permanence. Within each category it was then necessary to determine the specific properties of interest. This was a very selective process in that the property must be engineering oriented toward material selection. The detailed results of this effort has been published previously by PLASTEC.[5]

For the mechanical properties, the following ten basic areas are relative: creep, stress relaxation, stress vs. strain, Poisson's ratio, shear fatigue, hardness, friction, and abrasion. And within each of these, another selection process was conducted to determine the specific data formats desired, the applicable test method, and the desired test parameters. For instance, tensile and compressive creep data are desired at various stress levels and temperatures in accordance with ASTM D 2990. Impact data by use of a falling weight in accordance with ASTM D 3029 and over a range of temperatures are desired.

This process of defining the engineering relevance of data formats was also conducted for the electrical properties resulting in the following: dielectric strength and constant, dissipation factor, and volume and surface resistivity. This process, of course, was continued for each of the property categories.

It should be noted that although each material property defined in this program is oriented toward the design phase, the data are also useful for production engineering, and for specification control purposes.

The proposed content of the PLASTEC Data System can be assessed best by reviewing typical computer outputs. A hypothetical material has been used for demonstration purposes.

For instance, retrieval of tensile creep data for a specific material would be accomplished by requesting the creep information and subselecting the material trade designation. The output has been structured to list (Figure 1) the major test parameters, i.e., trade number, stress level, average strain, standard deviation, time, and test temperature. This information is not complete for engineering use and must be supplemented with supporting data, e.g., test method, relative humidity, date of test, and the pertinent specimen information. Data provided for all these fields represent that which is suggested in the ASTM test method and thus can be considered suitable for material assessments.

The graphics mode of tensile creep is generated by use of the tensile creep data points which would normally appear in the list format (Figure 2). This graphics format contains a more complete picture of tensile creep providing the basic and supporting data. It also includes a material description and a schematic of the test.

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PLASTEC DATA SYSTEM
MECHANICAL PROPERTIES
TENSILE CREEP

SUBSELECTION: S2='PT101';

TRADE NUMBER	STRESS LEVEL (MPA)	AVERAGE STRAIN (%)	STANDARD DEVIATION	TIME (HRS)	TEMPERATURE (C)
PT101	6.9MPA	.5		.1	23C
		1		1	
		1		10	
		1		100	
		1		1000	
		1		10000	
PT101	13.8MPA	1.3		.1	23C
		1.9		1	
		2.0		10	
		2.1		100	
		2.2		1000	
PT101	27.6MPA	2.5		.1	23C
		3.6		1	
		4.1		10	
		4.7		100	
PT101	48.3MPA	3.9		.1	23C
		4.7		1	
		6.0		10	

Figure 1. PLASTEC Data System mechanical properties: tensile creep.

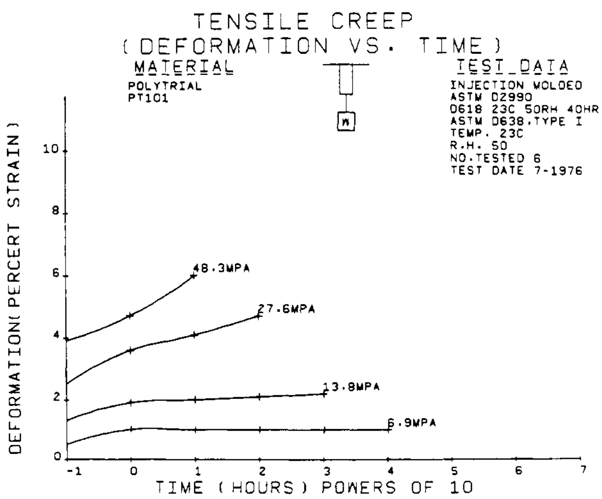

Figure 2. Tensile creep: deformation vs. time.

Considering the dielectric constant, a comparable output can be obtained. The major test parameters listed will contain the point values for dielectric constant, standard deviation, frequency, and temperature. Again there is an assortment of supporting test data, such as specimen data to accompany all the basic data. The graphics output (Figure 3) for dielectric constant will contain the point data, supporting data, material description, and a test method schematic.

The technology employed here is not unique in that data output is a normal computer function and that graphics has been around for some time. What is novel is the form of the data proposed in this system. PLASTEC will begin to acquire the needed data for the many materials of interest. This data acquisition phase remains the one difficult challenge in our program. PLASTEC is optimistic in that once our goals are defined, cooperation will follow.

Within the PLASTEC Data System, under the category of permanence, is the property dealing with chemical resistance. As these data are extensive, PLASTEC had decided to create a separate file. A review of this program will illustrate the approach to computerization of numeric data.

At the outset of creating such a file, the first question asked was, what does a user want to know? The normal reply is the response of a material in a specific chemical environment. As the specific environment parameters differ from application to application, it is necessary that the data be all encompassing. That is, resistance to hydrochloric acid must be available for each material at selected concentrations and temperatures for test periods up to a year. This is essential since, if the data are not through, we would be faced constantly with the problem of insufficient data and relying on conjecture as to

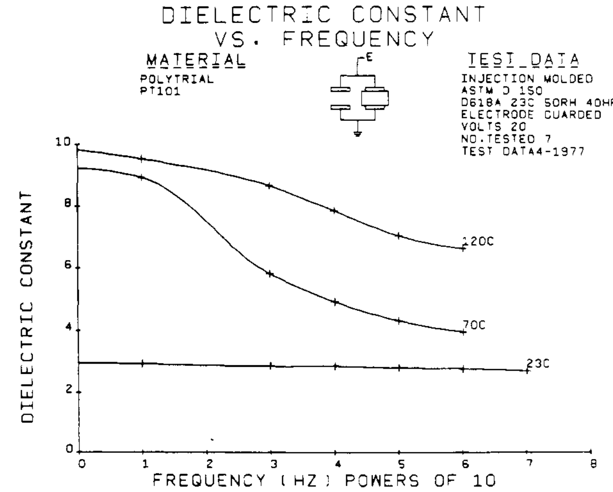

Figure 3. Dielectric constant vs. frequency.

performance capability. Thus, it was decided that the most effective data should indicate the response or interaction as a result of exposure to the major environmental factors over an extended period of time. The methods to generate and record the data are fairly well established as ASTM D 543, Resistance of Plastics to Chemical Reagents, and ASTM C 581, Chemical Resistance of Thermosetting Resins used in Glass Fiber Reinforced Structures. These methods are commonly used for testing and form the basis for the data requirements.

The data structure was initially established by considering the following types of records that are desired:

Generic Record—contains a general classification of polymeric materials. The fields included are generic name, family, and chemical formula.

Material Record—contains information for specific polymeric materials tested with the reagents contained in the test results. Fields include polymer type, trade name, code number, reinforcements, fillers, and the supplier.

Chemical Record—contains the reagent information for the test conducted. The fields include the reagent name, category, chemical formula, and, where pertinent, its trade designation and supplier.

Reference Record—contains the specific document information from which the data were obtained, linked to each test data point. The fields include title, author, contract number, data, description, report number, and source.

Test Results Record—contains the specific test data results and supporting data. Fields include changes in dimension, weight, volume, hardness, mechanical properties, and appearance as influenced by reagent concentration, temperature, stress, and time. Our program requires data on exposure for at least one year. Other fields included are the supporting data, specimen fabrication method, type, dimensions, number tested, conditions, and the test method.

It is quite obvious that if data were provided over a range of temperatures and chemical concentrations, a few conditions of stress, and for at least a year, we would then have an effective amount of data from which one can draw on to assess the particular problem. In addition, each of these records will contain a place for comments in order to provide supplemental information concerning past performance, use information, general statements, precautions, and advisements. This will contain actual experience information, which in the past has been found to be invaluable.

To facilite the computer end of the scheme, the data management system can provide a hierachical data structure. This feature provides a more efficient management of data, since each record is structured and linked internally for more 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[†]

P. F. ROUSH,* J. T. SEITZ, and L. F. YOUNG

The Dow Chemical Company, Midland, Michigan 48640

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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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