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Project Summary

Development of a Data Base on Chemical Migration from Polymeric Materials

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A data base was designed and constructed to organize and access data on the migration of chemical substances from polymeric materials. The data base was developed under an Interagency Agreement between the U.S. Environmental Protection Agency (EPA) and the U.S. Food and Drug Administration (FDA). The data base will facilitate the thorough and efficient review of chemical migration data and enable the EPA and FDA to maintain an up-to-date compilation of such data.

The migration data base was developed with the use of a commercial software package, Advanced Revelation®*, and runs on IBM personal computers and compatibles. Data elements include the identity of the polymer and migrant(s), the experimental conditions of the migration test, the diffusion coefficient, the amounts migrated as a function of time, and the data source. Data extraction guidelines and data base features for data entry, editing, searching, and reporting were developed based on EPA/FDA operational requirements. All data entered into the data base were extracted from the published literature and FDA indirect food additive petition files. Migration data were entered from 90 citations and include data for approximately 26 polymers and 81 migrants and adjuvants. A User Manual providing detailed user instructions was also prepared.

This Project Summary was developed by EPA's Risk Reduction Engineering Laboratory, Cincinnati, OH, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Migration is the movement by diffusion of low molecular weight molecules from a polymeric material to an external phase. Migrants may be additives to the polymeric material that improve its stability (e.g., an antioxidant) or that impart desirable properties (e.g., a plasticizer). Migrants may also be monomers, oligomers, or other residues of polymerization (e.g., catalysts). Furthermore, migrants may be chemicals that are absorbed by the polymer after fabrication.

Migration of chemical additives is of interest to the U.S. Food and Drug Administration (FDA), which is responsible for ensuring that materials used for packaging foods do not contribute levels of chemicals to foods that may present a health risk. Migration of chemical contaminants is of interest to the U.S. Environmental Protection Agency (EPA) because of health and safety concerns of workers wearing protective clothing (e.g., the slow release of chemicals from chemical protective garments that have not been fully decontaminated). In addition, EPA is also concerned with chemical migration from polymeric materials as a potential source of indoor air pollution and as a factor in the containment of wastes at sites where

polymers are used as waste containment liners.

The objective of the report summarized herein was to design, construct, and document a computerized data base on the migration of chemical substances from polymeric materials. The effort was performed under an interagency agreement between the EPA and the FDA to address both agencies' requirements for access to chemical migration data and to fundamental parameters associated with migration data (e.g., diffusion coefficients).

Data Base Design

The initial requirements for the data base focussed on the types of data to be stored in the data base and the capabilities for operation of the final data base system. We first developed a prototype system based on the definition of the system requirements. The applications development software package was selected, and a prototype capability for data entry and searching was constructed. After the prototype was reviewed by EPA and FDA, the fully operational data base was developed and delivered to them with a documented data set, guidelines for further data extraction, and a User Manual.

Data Elements

Each data record in the data base contains a series of data elements or fields that are required to fully define the migration test and test results. The data elements describe the data source, the identity of the polymer formulation, the chemical migrant(s), the experimental conditions under which the migration test was performed, the migration data, and the diffusion coefficient when available.

Full reference citations identify the source of the data. Each chemical and polymer is identified by using data elements for the CAS registry number as well as by using several chemical names. Data elements were also included to report properties of the polymer formulation (e.g., molecular weight, density). Data elements describing of the experimental conditions include the test temperature, the extraction medium and volume, the polymer surface area and thickness, and the analytical detection method and its sensitivity. The migration test results are reported using data elements for time, amount migrated, and diffusion coefficient.

Each data element was categorized as either essential or supplemental. Only those migration data for which values were reported for all of the essential data elements are included in the data base. This screening for essential data elements was the only screening criteria applied to the data. No analysis of data quality in terms of accuracy or precision was performed. Values of all replicate measurements were, however, entered into the data base so that data quality assessments could be made in the future if desired. The data base could be expanded to include data elements that address data quality.

Data Base Structure

Based on the definition of the data base requirements and the data elements, the data base structure was defined (Figure 1). The hierarchy begins with the data elements describing the citation or data source; these are then related to multiple polymer formulations for which migration data were measured. The polymer formulation is related to the polymer, the migrant and other adjuvants, and the physical properties reported for the formulation. The migrant is related to multiple sets of experimental conditions at which the formulation was tested. Each set of experimental conditions is then related to one set of migration test data that includes multi-valued time and amount migrated data elements, and the diffusion coefficient.

Software Selection

Several commercial software packages for IBM personal computers and compatibles were reviewed for their suitability to develop the data base system. Advanced Revelation (Cosmos, Inc., Bellevue, WA), a relational data base application development package, was selected based on the operational requirements and the required data base structure.

Data Base Features and Operation

The data base features and operation are described in detail in the User Manual. A summary of the features for data entry, searching, and reporting and for system maintenance is provided here. All data base operations are menu-driven and several function keys were defined to simplify operation of the data base.

Data Entry

Data entry is performed with the use of full-screen displays and overlay windows. Separate data entry screens are provided for entry of citations, polymer and chemical identity information, polymer formulations and properties, experimental test conditions, and migration test data. Movement through the series of entry screens is controlled through the use of function keys. Function keys also provide data editing and deletion capabilities.

Option lists provide easy reference during data entry for several data elements that have common or restricted values. Option lists are provided for the polymer class, temperature, analytical detection method, extraction medium category, polymer property test method, and data source indicator data elements. Options lists are accessed by using a function key and may be updated by using the system maintenance capability.

Search and Report

Capabilities to search the data base and generate reports are also available through a menu-driven format and full-screen displays. A search routine allows the user to define the search criteria using combinations of the polymer, chemical, temperature, and extraction medium data elements. Options are provided to review the search results on-screen, print the search report, redefine the search criteria, or perform another search. The results of the search, reviewed either on-screen or printed as a report, are presented in a predefined format.

Capabilities to perform other, user-defined data base searches are made possible through the use of Easy Writer, the menu-driven report generation capability that is part of the Advanced Revelation software. Easy Writer is a full-feature report generator that allows the user to search the data base files using any combination of data base elements and to define customized report formats.

List Reports

Three list reports are provided. The first report generates a list of all citations in the data base and allows the user to specify either author or citation number order. The second generates a list of all chemicals in the database, and the third, a list of all polymers. The chemical and polymer list reports can be specified for output in either CAS Registry number order, CAS Registry name order, or display name order. All list reports can be directed to the screen, a printer, or a disk file for output.

System Maintenance

System maintenance capabilities are included to set-up and modify printer definitions and to update the options lists.
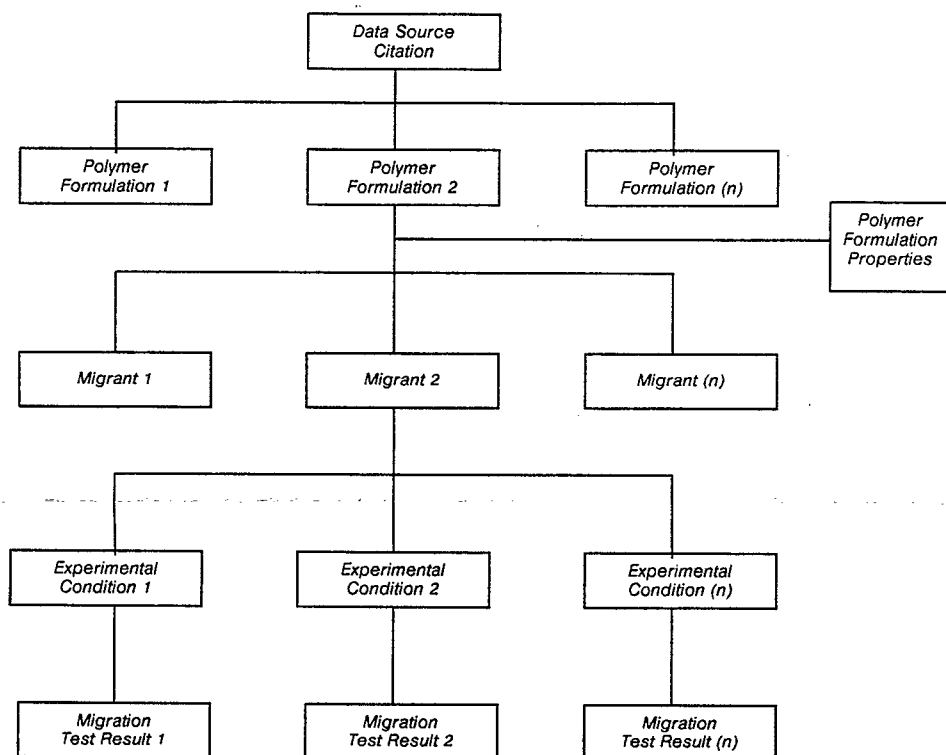
Figure 1. Data base hierarchy.

User Manual

The User Manual describes the data base capabilities and provides detailed, step-by-step instructions for data base operation. The manual documents the data base elements and data extraction guidelines and details instructions for use of the present system.

Data Extraction and Entry

The data set in the final data base system was extracted from published literature sources and from FDA indirect food additive petition files. At the outset of the assignment, an EPA Category IV Quality Assurance Project Plan (QAPjP) was prepared describing the project, the intended use of the data base, the data base quality objectives, and our mechanism for ensuring the accuracy of mathematical operations, data transcription, and entry procedures. This quality assurance plan was followed throughout the program.

Data extraction and entry efforts were conducted according to a defined set of data extraction guidelines or procedures. The guidelines address data conversion and calculation procedures required for numeric data base fields. Character or alphanumeric fields (e.g., the identity of the citation, polymer, migrant, adjuvants, extraction medium, and analytical detection method) are not considered here because they are directly transcribed from the citation. Procedures for data conversions and data calculations are described below.

Data Conversion Procedures

All numeric data base elements require specific units for data entry. Consequently, data extracted from citations must be converted if reported in other units. Generally, these conversions were straightforward and involved direct multiplication or division by a constant. Conversion procedures were documented for several common units to the required units for each numeric database element.

Data Calculation Procedures

In addition to data conversions, extraction of some numeric data elements required a calculation procedure involving one or more other parameters reported in the citation or available from the general reference literature. Calculation procedures are described for the four data elements that routinely require calculations to be performed. These elements include the amount of extraction medium, the migrant detection level, the amount migrated, and the diffusion coefficient.

Data Sources

The migration data extracted and entered in the data base are from three principal sources:

(1) Scientific journal articles,
(2) Project reports of studies conducted by Arthur D. Little, Inc., and the National Bureau of Standards (NBS) under contract to the FDA, and
(3) FDA indirect food additive petition (FAP) files.

No migration data were generated under this assignment.

A total of 95 citations were reviewed during this assignment. Data were extracted and entered from 90 of these 95 citations. Five citations were rejected for entry because values for data elements designated as essential were not reported and/or could not be calculated. For the 90 citations entered, 43 citations were scientific journal articles, 10 were project reports of studies conducted under contract to the FDA, and 37 citations were FDA indirect food additive petitions. The screening and extraction of data from the FDA petition files was conducted at the FDA facilities in Washington, DC.

Table 1 summarizes the polymers, using common names and CAS Registry numbers, included in the data base.

Conclusions and Recommendations

The migration data base provides a useful resource for both the EPA and FDA in the area of migration and diffusion in polymers. Migration data from a broad range of literature and other sources have been compiled in a detailed and consistent format that facilitates comparison and correlation. The data base will enable the EPA and FDA to thoroughly and efficiently review chemical migration data and to maintain an up-to-date compilation of such data. The data base could ultimately be used to develop models or correlations to gain a better understanding of the migration, permeation, and decontamination of polymeric materials.

3

We recommend that the extraction and entry of available migration data continue on a regular basis. Because the development of the data base system was the focus of this assignment only a fraction of the published migration data was reviewed and extracted. We also recommend that a system for characterizing the quality of the data be implemented so that the user will have an indication of the reliability of the reported migration data.

The full report was submitted in fulfillment of Contract No. 68-03-3293 by Arthur D. Little, Inc., under the sponsorship of the U.S. Environmental Protection Agency.

Table 1   Summary of Polymers Included in Migration Data Base

CAS Registry Number	Common Name	CAS Registry Number	Common Name
9003569	Acrylonitrile-butadiene-styrene copolymer	977085565*	Polycarbonate resin
977096459*	Acrylonitrile-methylacrylate copolymer, nitrile rubber modified	25748372	Polyethylene terephthalate polymer
25038362	Ethylene propylene ethylidenenorbornene terpolymer	9011147	Polymethylmethacrylate
25640146	Ethylene-1,4-cyclohexylene diethylene terephthlate	9003070	Polypropylene
9010791	Ethylene propylene copolymer	9003536	Polystyrene
24937788	Ethylene-vinyl acetate copolymer	977085838*	Polystyrene, rubber-modified
977027330*	High-density polyethylene	9002862	Polyvinyl chloride
977027341*	Low-density polyethylene	20000*	PVC-PA-PVC-PU
24937164	Nylon 12	9003547	Styrene-acrylonitrile copolymer
25038544	Nylon 6	9003558	Styrene-butadiene-styrene block copolymer
32131172	Nylon 66	9011067	Vinylidene chloride-vinyl chloride copolymer
9002817	Poly(oxymethylene) copolymer	25038726	Vinylidene chloride-methyl acrylate copolymer
9003172	Polybutadiene rubber	10009*	Wax-coated paper

*No specific CAS Registry number available; sequence number assigned by FDA.

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The complete report, entitled "Development of a Data Base on Chemical Migration from Polymeric Materials," (Order No. PB 90-235 102/AS; Cost: $17.00, subject to change) will be available only from:
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