



Project Summary

The Rubber-Processing Chemicals Data Base

A. Twhigg, E. Helmes, D. Kashiwase, S. Rovito, and K. E. McCaleb

This report describes the work performed on a project to establish a Rubber-Processing Chemicals Data Base (RPCDB) as an extension of the Organic Chemical Producers Data Base (OCPDB) which has been maintained by the EPA since 1976.

The RPCDB was conceived of as the second in a series of supplements to the OCPDB to be focused on various sectors of the chemical industry. The first such supplement, the Organic Dyes and Pigments Data Base (ODPDB), is also being developed by SRI International. Specifications for the data elements and formatting closely follow the currently employed General Purpose OCPDB Update Forms, with minor modifications reflecting the nature of the entries.

Over 300 chemical products are included in the RPCDB, representing virtually all the organic chemicals used to process rubber in the U.S. at economically significant levels. The development of the data base was started by using some of the information obtained in an earlier study done by SRI for the International Agency for Research on Cancer. This study had concerned the exposure to chemical products in the rubber industry. Additional sources for the data collected include various on-line data banks, government statistical and research publications, standard industry handbooks, and the expertise of the staff in several ongoing SRI programs.

The entry format was designed to be compatible with the System 2000® data base management system implemented in 1979 and currently in use for the revised OCPDB. When placed on System 2000, retrieval of data will be

possible in the same manner as with the revised OCPDB, using a variety of "key" data elements to correlate the data needed.

This Project Summary was developed by EPA's Industrial Environmental Research 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

The Rubber-Processing Chemicals Data Base (RPCDB) was designed to be a specialized extension of the Organic Chemical Producers Data Base (OCPDB), focusing exhaustively on a specific use area within the chemical industry. The OCPDB was originally intended as a catalog of large-volume industrial chemicals; it was initiated in 1976 using a list of 380 chemicals and was revised in 1980 and expanded to include petrochemical feedstocks, priority pollutant chemicals, and other large-volume products. The RPCDB represents an emphasis distinct from the existing OCPDB, since it is an attempt at a comprehensive catalog of one specific industry rather than a cross-industry comparison of a small number of important individual products. It contains a large number of complex, closely-related products unused outside of the industry under examination, since a much lower minimum volume was employed as a basic criterion than in the OCPDB. Coupled with this is a decrease in the average amount of data per product entry, since many of the products are obscure and the particular industry is highly proprietary. Data elements which were sought but for which information was seldom or never found included use

volume and percent domestic use, Wiswesser Line Notations, specific figures for annual production volume and sales, IPPEU reference numbers, and chemical producer process capacities.

Discussion and Procedure

The intent in preparing the RPCDB was to adhere as closely as possible to the model of the revised OCPDB, given the somewhat different nature of the data available on rubber-processing chemicals. Table 1 lists the data elements included in the RPCDB.

Because the requirements of the software currently employed in the OCPDB

Table 1. Data Elements in the RPCDB

<i>Chemical Information</i>
<i>Chemical I.D. number</i>
<i>Chemical name</i>
<i>CAS number</i>
<i>New chemical marker</i>
<i>Priority pollutant marker</i>
<i>Wiswesser line notation</i>
<i>NIOSH registry number</i>
<i>Synonyms</i>
<i>Economic Information</i>
<i>Year</i>
<i>Production volume</i>
<i>Unit cost</i>
<i>Sales value</i>
<i>Use Information</i>
<i>Chemical or allied product</i>
<i>Use description</i>
<i>Amount</i>
<i>Percent domestic use</i>
<i>IPPEU reference number</i>
<i>SIC code</i>
<i>Product application</i>
<i>Product Process Information</i>
<i>Process I.D. number</i>
<i>Process description (brief)</i>
<i>IPPEU reference number</i>
<i>Reaction component</i>
<i>OCPDB number</i>
<i>ICPDB number</i>
<i>Industrial origin</i>
<i>SIC code</i>
<i>Other process material</i>
<i>Process description (extended)</i>
<i>Chemical Producer Information</i>
<i>Chemical producer name</i>
<i>Chemical producer I.D. number</i>
<i>City location</i>
<i>State location</i>
<i>Zip code</i>
<i>County location</i>
<i>River basin name</i>
<i>River basin code</i>
<i>AQCR code</i>
<i>Process capacity</i>
<i>Parent company</i>

are more sensitive to field length specifications, modifications in the data elements were generally not permitted. (For the ODPDB, different software was available and a number of field lengths had been increased and additional data elements were added.)

The criteria for inclusion of chemicals in the RPCDB were established in accordance with the United States International Trade Commission (USITC) definition of minimum commercially significant production as given in the publication *Synthetic Organic Chemicals, U.S. Production and Sales: 1,000 pounds annual production for chemicals found in the rubber-processing chemicals section of that publication, and 5,000 pounds for plasticizers, chemical intermediates, and miscellaneous products*. Many of the candidates for the RPCDB were derived from an SRI task on evaluating industrial exposure to rubber-processing chemicals performed for the International Agency for Research on Cancer (IARC) in 1981. The list of chemicals developed for IARC was evaluated with regard to their U.S. production or importation levels under the criteria given above for the period 1977-1980. A number of the IARC chemicals believed to be used only in Europe were dropped, although certain natural products for which no production figures were available were retained. Rubber by-products, monomers, and plasticizers had been excluded from the IARC study, but a decision was made to include those plasticizers used primarily for processing rubber in the RPCDB. A selection of 22 such plasticizers was compiled, bringing the total candidate list to 327 products.

It was found that 53 of the candidate chemicals were large-volume products that had previously been entered in the OCPDB. To avoid duplicating existing data, the only information gathered for the RPCDB on these chemicals consisted of economic updates and synonyms and end use data specific to rubber-processing applications. The candidates were arranged in structurally-related groupings for the purpose of data collection, as they had been in the IARC study (see Table 2).

The sequence for data entry was, however, alphabetical -- in conformity with the OCPDB. Five-digit entry ID numbers were assigned to new products beginning with number 20000 in order to distinguish the RPCDB from the ODPDB, which used numbers between 10000 and 18000.

Table 2. IARC Rubber-Processing Chemicals Arranged by Structural Class

A. Nitrogen compounds
1. <i>Phenylenediamines</i>
2. <i>Diphenylamines</i>
3. <i>Other aromatic amines</i>
4. <i>Aromatic amine-aldehyde (ketone) condensates</i>
5. <i>Quinolines</i>
6. <i>Arylguanidines</i>
7. <i>Alkyl amines</i>
8. <i>Carbamates</i>
9. <i>Miscellaneous</i>
B. Sulphur compounds
1. <i>Mercaptans</i>
2. <i>Thiocarbamates</i>
3. <i>Benzothiazoles</i>
a. <i>Sulphenamides</i>
b. <i>Miscellaneous</i>
4. <i>Xanthates</i>
5. <i>Sulphides and disulphides</i>
a. <i>Thioethers</i>
b. <i>Thiurams</i>
c. <i>Miscellaneous</i>
6. <i>Thioureas</i>
7. <i>Miscellaneous</i>
C. Oxygen compounds
1. <i>Phenols</i>
a. <i>Carbon-bridged phenols</i>
b. <i>Alkylated phenols</i>
c. <i>Aminophenols</i>
d. <i>Hydroquinones</i>
e. <i>Miscellaneous</i>
2. <i>Quinones</i>
3. <i>Carboxylic acids and salts</i>
4. <i>Anhydrides and esters</i>
5. <i>Peroxides</i>
6. <i>Aldehydes and ketones</i>
7. <i>Alcohols</i>
8. <i>Miscellaneous</i>
D. Phosphorus compounds
1. <i>Phosphites</i>
2. <i>Phosphates and phosphonates</i>
E. Halogen compounds
F. Hydrocarbons
G. Miscellaneous organic compounds

As the RPCDB was designed to be completely compatible with the revised OCPDB, information on data structure and accessing have not been provided here; the report entitled "The Revised Organic Chemical Producers Data Base System," U.S. Environmental Protection Agency, September 1980, EPA-600/2-80-164, should be consulted.

A. Twigg, E. Helmes, D. Kashiwase, S. Rovito, and K. E. McCaleb are with SRI International, Menlo Park, CA 94025.

Mark J. Stutsman is the EPA Project Officer (see below).

The complete report, entitled, "The Rubber-Processing Chemicals Data Base," (Order No. PB 84-149 137; Cost: \$8.50, subject to change) will be available only from:

*National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650*

*The EPA Project Officer can be contacted at:
Industrial Environmental Research Laboratory
U.S. Environmental Protection Agency
Cincinnati, OH 45268*

☆ U.S. GOVERNMENT PRINTING OFFICE: 1984-759-015/7313

United States
Environmental Protection
Agency

Center for Environmental Research
Information
Cincinnati OH 45268

BULK RATE
POSTAGE & FEES PAID
EPA
PERMIT No. G-35

Official Business
Penalty for Private Use \$300

• •

• •