outlier types, while GM does both at the same time. The Abraham and Box procedure is less likely to be useful than GM because it was designed to consider only one type of outlier.[1] The relationship between GM and the Chernick et al.[8] procedure is discussed elsewhere.[4,5]

CONCLUSIONS

On the basis of these results it can be concluded that the GM procedure is an effective method for the quick discovery of the effects of catalytic poisons, as long as care is taken to ensure that all model assumptions are met prior to drawing any conclusions about the process based on this method. The computational procedure may be implemented quickly on a laboratory microcomputer so that results become immediately available to a quality-control laboratory. Related procedures, involving quality-control charts, which may be useful in some circumstances for catalytic processes, are discussed in Booth and Isenhour.[6]

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Method for Estimating the Human and Environmental Exposure Potential of Chemicals Having Designated Uses†

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This paper describes a methodology that was designed to assist the Environmental Protection Agency in setting priorities for regulating chemicals in accordance with requirements of the Toxic Substances Control Act by indicating the extent of exposure potentially associated with a particular use of a chemical. Development and application of the methodology to actual chemical uses proceeded in four stages: (1) development of an exposure classification scheme, (2) development of a chemical use list, (3) assignment of exposure category scores to chemical uses, and (4) merging of exposure scores into ranked groups, creating the Index of Exposure. The purpose of the Index was to identify those chemical uses having the greatest potential for human and environmental exposure. Theoretically, the objectivity of the scoring methodology is such that, given the same data for a chemical use, different scorers will be able to arrive at the same exposure score for that use.

INTRODUCTION

The Toxic Substances Control Act (TSCA), which became effective on January 1, 1977, makes the Environmental Protection Agency (EPA) responsible for regulating chemical substances "whose manufacture, processing, distribution in commerce, use or disposal may present an unreasonable risk of injury to health or the environment."[1] Under TSCA, manufacturers, processors, and importers may be required to submit certain data to EPA prior to the commercial production, processing or distribution of a new chemical or of a previously produced chemical intended for a new use. EPA is also authorized to collect the same data for existing chemicals in existing uses. Such data may include the chemical's molecular structure, its intended use, estimated production volume for each intended use, the byproducts resulting from

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FACTOR 1 MODE OF HUMAN EXPOSURE	FACTOR 2 MODE OF ENVIRONMENTAL EXPOSURE	FACTOR 3 AMOUNT OF HUMAN EXPOSURE	FACTOR 4 AMOUNT OF ENVIRONMENTAL EXPOSURE
A. ROUTE OF EXPOSURE		A. NUMBER OF PEOPLE EXPOSED	
0 NO EXPOSURE	0 NO EXPOSURE	0 < 200,000	0 NO EXPOSURE OR EXPOSURE AS CONSTITUENT OF A BULK SOLID
1 ORAL, TOPICAL, INHALATION	1 EXPOSURE VIA AIR, WATER OR SOIL	1 200,000 - 2,000,000	1 UP TO 1% OF SUBSTANCE
2 ANY TWO OF THE ABOVE	2 EXPOSURE VIA ANY TWO OF THE ABOVE	2 2,000,000 - 20,000,000	2 1 - 10% OF SUBSTANCE
3 ALL OF THE ABOVE	3 EXPOSURE VIA ALL OF THE ABOVE	3 > 20,000,000	3 10 - 100% OF SUBSTANCE
B. FORM OF EXPOSURE		B. FREQUENCY OF EXPOSURE	
0 NOT APPLICABLE		0 YEARLY OR LESS OFTEN	
1 LIQUID,* SOLID OR GASEOUS**		1 MONTHLY	
2 ANY TWO OF THE ABOVE		2 WEEKLY	
3 ALL OF THE ABOVE		3 DAILY OR CONTINUOUSLY	
		C. EXTENT OF CONTACT	
		0 TRACE CONTACT	
		1 LIGHT CONTACT	
		2 MODERATE CONTACT	
		3 HEAVY CONTACT	
		D. DURATION OF EXPOSURE	
		0 FLEETING EXPOSURE	
		1 SHORT EXPOSURE	
		2 MEDIUM EXPOSURE	
		3 LONG EXPOSURE	

* INCLUDES SUSPENSIONS AND SOLUTIONS
** INCLUDES GASES, VAPORS, MISTS, AEROSOLS AND RESPIRABLE-SIZE PARTICULATES

Figure 1. Exposure classification scheme.

manufacture, processing, use or disposal of the chemical, estimates of the related occupational exposure levels, and any known environmental and health effects of the chemical.

This paper describes a methodology that was designed to assist EPA in setting priorities for regulating chemicals in accordance with TSCA requirements by indicating the extent of exposure potentially associated with a particular use of a chemical. Since the same chemical can present different exposure potentials depending on the use, it is essential to estimate the exposure potential of chemicals destined for a particular use in order to assess their potential impact on humans and the environment.

Chemical manufacturing companies, faced with the prospect of having to test those of their products that present the greatest risk of deleterious effects, might want to use this methodology to estimate the exposure potential associated with selected uses of their products. Knowledge of the exposure potential of a chemical in one or more given uses could serve as an adjunct to other information affecting the decision of whether to test, such as actual or anticipated production volume, byproducts, environmental fate, and any already known health or environmental effects.

Development and application of the methodology to actual chemical uses proceeded in four stages: (1) development of an exposure classification scheme, (2) development of a chemical use list, (3) assignment of exposure category scores to chemical uses, and (4) merging of exposure scores into ranked groups, creating the Index of Exposure. The purpose of the Index was to identify those chemical uses having the greatest potential for human and environmental exposure.

The exposure scoring procedure was based on two elements: (1) the exposure classification scheme, which gives numerical values to categories of exposure, and (2) the data related to a chemical use that enables the scorer to assign an appropriate exposure score to the chemical use. The scoring methodology was designed to be an objective measurement tool, so that, given the same data for a chemical use, different scorers will be able to arrive at the same exposure score for that use. However, results may not be replicable if scoring is based on incomplete or varying data. Because development of the scoring methodology was essentially a feasibility study, the contract under which this work was performed imposed a time limit of 1 h per chemical use to be spent in scoring. Thus, the contractor was not usually able to obtain complete data and had to rely on what data was readily available, and the participating chemical engineers and industry specialists had to frequently estimate scores, on the basis of their experience. Others using the same methodology may be permitted more time to amass input data, thereby refining the results of such an assessment.

PHASE 1: DEVELOPMENT OF THE EXPOSURE CLASSIFICATION SCHEME

The exposure classification scheme contains the parameters related to human and environmental exposure, divided into four major categories and subsets thereof: (factor 1) mode of human exposure; (factor 2) mode of environmental exposure; (factor 3) amount of human exposure; (factor 4) amount of environmental exposure. These factors and the subfactors they subsume are illustrated in Figure 1. Definitions of the exposure classification parameters are given in Figure 2. As is apparent from Figure 1, multiple modes of exposure are scored progressively higher than a single mode. For example, if the route of human exposure is either oral, topical, or by inhalation, a score of 1 is assigned. A combination of any two of the three routes would receive a score of 2, and a combination of all three routes would be scored 3.

PHASE 2: DEVELOPMENT OF THE CHEMICAL USE LIST

In order to provide a source of chemical uses for scoring, a list of approximately 800 chemical uses, representing the

FACTOR	DEFINITION
MODE OF HUMAN EXPOSURE	MEANS BY WHICH HUMANS MAY BE EXPOSED DURING NORMAL USE OF A SUBSTANCE,* EXPRESSED AS A CUMULATION OF TWO SUB-FACTORS
ROUTE OF EXPOSURE	POINT OF HUMAN CONTACT WITH A SUBSTANCE DURING NORMAL USE
FORM OF EXPOSURE	PHYSICAL STATE OF THE PRODUCT BEING USED
MODE OF ENVIRONMENTAL EXPOSURE	ROUTE BY WHICH A SUBSTANCE IS RELEASED TO THE ENVIRONMENT DURING NORMAL USE
AMOUNT OF HUMAN EXPOSURE	AMOUNT OF HUMAN EXPOSURE EXPRESSED AS A CUMULATION OF FOUR SUBFACTORS
NUMBER OF PEOPLE EXPOSED	NUMBER OF PEOPLE WHO WOULD COME INTO CONTACT WITH A SUBSTANCE DURING NORMAL USE. CATEGORIES WERE CHOSEN TO REFLECT PERCENTAGE OF U.S. POPULATION, SUCH THAT: 200,000 = 0.1% 2,000,000 = 1% 20,000,000 = 10%
FREQUENCY OF EXPOSURE	FREQUENCY WITH WHICH THOSE PEOPLE EXPOSED TO A SUBSTANCE WOULD COME INTO CONTACT WITH IT DURING NORMAL USE
EXTENT OF CONTACT	AMOUNT OF SUBSTANCE TO WHICH A PERSON WOULD BE EXPOSED DURING NORMAL USE. THIS SUBFACTOR MAY BE EXPRESSED AS THE PERCENTAGE COMPOSITION OF THE FUNCTIONAL CHEMICAL IN THE PRODUCT OR AS THE PERCENTAGE CONCENTRATION OF THE FUNCTIONAL CHEMICAL IN THE IMMEDIATE AREA OF USE. • TRACE CONTACT - SUBSTANCE OCCURS ONLY INCIDENTALLY IN THE FINISHED PRODUCT (E.G., A POLYMERIZATION INTERMEDIATE WHICH MAY EXIST ONLY AS AN IMPURITY IN A TEXTILE FIBER), OR IS PRESENT IN THE WORKPLACE IN TRACE AMOUNTS AS A RESULT OF INCIDENTAL LOSSES DURING PROCESSING IN TOTALLY ENCLOSED OPERATIONS. • LIGHT CONTACT - FINISHED PRODUCT CONTAINS UP TO 1% BY WEIGHT OF THE SUBSTANCE, OR THE SUBSTANCE IS PRESENT IN THE WORKPLACE AS A RESULT OF INCIDENTAL LOSSES FROM BATCH OPERATIONS. • MODERATE CONTACT - FINISHED PRODUCT CONTAINS 1-10% BY WEIGHT OF THE SUBSTANCE. OCCUPATIONAL EXPOSURES ARE MOST LIKELY TO BE LIGHT OR HEAVY, RATHER THAN MODERATE, SINCE INDUSTRIAL OPERATIONS ARE LARGELY EITHER AUTOMATIC, IN WHICH CASE THE EXPOSURE IS LIGHT, OR MANUAL, IN WHICH CASE THE EXPOSURE IS HEAVY. • HEAVY CONTACT - FINISHED PRODUCT CONTAINS 10-100% BY WEIGHT OF THE SUBSTANCE, OR THE SUBSTANCE IS PRESENT IN THE WORKPLACE AS A RESULT OF SUCH OPERATIONS AS SPRAY DRYING AND PAINT SPRAYING, OR THE SUBSTANCE IS CONTACTED BY DIRECT HANDLING, AS IN UNLOADING BAGS AND DRUMS OR WEIGHING IN OPEN CONTAINERS.
DURATION OF EXPOSURE	LENGTH OF TIME FOR WHICH A PERSON WOULD BE IN CONTACT WITH A SUBSTANCE DURING NORMAL USE: • FLEETING EXPOSURE - EXPOSURE OF UP TO 1 SECOND DURATION • SHORT EXPOSURE - EXPOSURE OF 1 SECOND TO 1 MINUTE • MEDIUM EXPOSURE - EXPOSURE OF 1 MINUTE TO 1 HOUR • LONG EXPOSURE - EXPOSURE OF LONGER THAN 1 HOUR DURATION
AMOUNT OF ENVIRONMENTAL EXPOSURE	EXTENT OF ENVIRONMENTAL EXPOSURE IN TERMS OF THE APPROXIMATE AMOUNT OF SUBSTANCE WHICH ENTERS THE ENVIRONMENT DURING NORMAL USE. FOR EXAMPLE, UP TO 100% OF AN AEROSOL SPRAY MIGHT ENTER THE ENVIRONMENT, WHILE LESS THAN 1% OF AN AUTOMOTIVE FUEL MIGHT ENTER THE ENVIRONMENT IN ITS ORIGINAL FORM WITHOUT UNDERGOING COMBUSTION.

*AS USED HERE, THE TERM "SUBSTANCE" DOES NOT REFER TO A PARTICULAR CHEMICAL COMPOUND, BUT TO ANY CLASS OF COMPOUNDS PROVIDING A GIVEN FUNCTION (E.G., PROPELLANT, TACKIFIER, EXTENDER).

Figure 2. Definitions of exposure factors.

	FUNCTION		APPLICATIONS
001	ABLATIVES	1705	ROCKET WARHEADS AND EXPLOSIVE COMPONENTS
		281	GUIDED MISSILES AND SPACE VEHICLES AND PARTS
002	ABRASIVES	03200	CARPENTRY
		0323	MASONRY, STONEWORK, TILE SETTING AND PLASTERING
		06	FABRICATED METAL PRODUCTS
		⋮	
		25114	METAL POLISH
0020	BLASTING ABRASIVES	04003	OFFICE AND PUBLIC BUILDING CLEANING AND MAINTENANCE
		06	FABRICATED METAL PRODUCTS
		0645	SURFACE CLEANING AND CONDITIONING
⋮			
130	COAGULANTS	0407	SEWERAGE TREATMENT AND REFUSE DISPOSAL
		04080	WATER PURIFICATION
		192	PAPER MILL PRODUCTS
		⋮	
		211	NATURAL RUBBER
		214	SYNTHETIC RUBBER
		⋮	
151	DEFOLIANTS	012	CROP PRODUCTION
		014	FORESTRY
		1700	BIOLOGICAL AND CHEMICAL WARFARE AGENTS
171	DESIZING AGENTS	0412	LAUNDRY AND DRYCLEANING
		273	MISCELLANEOUS TEXTILE PRODUCTS
263	KIER ASSISTANTS (TEXTILE TECHNOLOGY)	270	FINISHED TEXTILE PRODUCTS
264	LACHRYMATORS	0405	LAW ENFORCEMENT
		1700	BIOLOGICAL AND CHEMICAL WARFARE AGENTS
290	OPTICAL BRIGHTENERS	04122	LAUNDERING
		18	PAINT AND ALLIED PRODUCTS
		19	PAPER AND ALLIED PRODUCTS
		2700	BLEACHED AND WHITE FINISHED FIBERS, YARN AND FABRICS
315	PULPING RETENTION AIDS	195	PULP MILL PRODUCTS
⋮			
358	STRIPPERS	2312	PHOTOENGRAVING
3580	DYE STRIPPERS	04120	DRYCLEANING AND DYEING
		2702	PLAIN DYED AND FINISHED FIBERS, YARN AND FABRICS
3581	PAINT STRIPPERS	0325	PAINTING, PAPER HANGING AND DECORATING
		0421	FURNITURE REPAIR AND REFINISHING WORK
		0645	SURFACE CLEANING AND CONDITIONING
3582	WAX STRIPPERS	0400	CLEANING AND MAINTENANCE
		0642	ENGRAVING AND ETCHING EXCEPT FOR PRINTING
		0645	SURFACE CLEANING AND CONDITIONING
		1436	SEMICONDUCTORS AND RELATED SOLID STATE DEVICES

Figure 3. Excerpt of the Chemical Use List.

contractor's estimate of the most significant uses in industry, was derived from the Chemical Use Classification System previously designed by the contractor for EPA.

The Chemical Use Classification System, completed in October 1977, classifies all significant industrial chemical uses in the U.S. to allow manufacturers, processors, and importers of chemicals to report current or intended chemical uses in a form that will facilitate analysis by EPA. For the purposes of the Classification System, chemical use is defined as a combination of function and application. A function is an action for which a chemical is specially fitted or used. An application is a process or product in which a chemical is used. For example, a chemical may *function* as a soil release agent for *application* to yarns and fabrics.[2] An excerpt of function–application combinations from the chemical use list is presented in Figure 3. The complete chemical use list appeared in the Federal Register on July 25, 1978.

PHASE 3: ASSIGNMENT OF EXPOSURE CATEGORY SCORES TO CHEMICAL USES

In phase 3, exposure classification scheme categories were applied to uses from the chemical use list developed in phase

SUMMARY INFORMATION:		CHEMICAL USE: (FUNCTION/APPLICATION)		
FACTOR	OCCUPATIONAL EXPOSURE	S/M* VALUE	CONSUMER EXPOSURE	S/M VALUE
1A ROUTE OF EXPOSURE		/6		/6
1B FORM OF EXPOSURE		/6		/6
2 MODE OF ENVIRONMENTAL EXPOSURE		/3		/3
3A NUMBER OF PEOPLE EXPOSED		/12		/12
3B FREQUENCY OF EXPOSURE		/12		/12
3C EXTENT OF CONTACT		/12		/12
3D DURATION OF EXPOSURE		/12		/12
4 AMOUNT OF ENVIRONMENTAL EXPOSURE		/3		/3

* S IS THE ACTUAL NUMERICAL VALUE OF THE ASSIGNED EXPOSURE VARIABLE; M IS THE MAXIMUM NUMERICAL VALUE OBTAINABLE FOR THAT EXPOSURE VARIABLE.

Figure 4. Scoring work sheet.

2. This scoring task consisted of determining a numerical score for each chemical use. The score was a total of the numerical values of the parameters within each factor of the exposure classification scheme that best characterized the potential for exposure associated with a given use. The score was computed according to the following formula:

$$r_j = \sum_{i=1}^{4} w_i \frac{s_{ij}}{m_i}$$

where w_i is the weight assigned to the ith factor group, s_{ij} is the actual numerical value of the exposure variable assigned to the jth chemical use, m_i is the maximum numerical value obtainable for that exposure variable, and r_j is the score of the jth chemical use, from which its rank will be derived. (The weighting factor permits subjective modification of scores to reflect any special significance that the scoring organization wishes to attach to a variable.)

It was felt that the major prerequisite for satisfactory scoring was that the scorer have a broad background in chemical technology and marketing, which would enable him to make the required judgmental decisions in the face of sparse or nonexistent data and the contractually prescribed time limitation of 1 h per chemical use.

Each chemical was scored separately for occupational and/or consumer (i.e., general population) exposure, as appropriate. For example, both workers and consumers could be exposed to wet strength agents used in sanitary paper products, but only workers would be exposed to soaping-off assistants for printed and finished fabrics, as these assistants are discarded in the plant waste water. Scores were assigned only for intended use; accidental exposure was not considered. Figure 4 shows the scoring work sheet.

PHASE 4: MERGING OF EXPOSURE SCORES INTO RANKED GROUPS

In phase 4, the exposure classification scores assigned to chemical uses were merged into ranked groups representing the lowest to the highest exposure potentials associated with the chemical uses. All chemical uses whose exposure classification scores fell within a particular ranked group were considered to have equivalent exposure potentials.

Prior to performing the scoring and ranking operations, a manual was written to describe the step by step procedure to be followed by scorers in assigning exposure scores to chemical uses. The purpose of the manual was to ensure that any two scorers, given the same data for a chemical use, would assign the same exposure classification categories, and thus the same score, to that use. The following sections, excerpted from the manual, outline the materials and techniques required for scoring chemical uses.

METHOD FOR ASSIGNING EXPOSURE SCORES TO CHEMICAL USES

To begin scoring, the following materials are required: (1) the exposure classification scheme (Figure 1), (2) definitions of the exposure factors (Figure 2), (3) the chemical use list (Figure 3), and (4) scoring work sheets (Figure 4). The same four steps, described below, are to be completed for each chemical use.

Select Chemical Use. The chemical use list contains approximately 800 uses that require scoring. Each scorer has been assigned a section of the list to score. Select chemical uses in the following order: (1) well-established uses; (2) uses with which the scorer is most familiar; (3) uses with which the scorer is least familiar. Selection of uses in this order maximizes scoring efficiency and ensures that the most significant uses receive scores.

Note Use on Work Sheet. A separate work sheet must be filled out for each chemical use. As the initial step in completing a work sheet, write both name and number of the selected chemical use on the work sheet where indicated. Place a check or similar notation next to this use on the chemical use list, so that the use will not be scored a second time.

Obtain Data Required for Scoring. In order to correctly score a chemical use, data pertaining to amount and mode of human and environmental exposure associated with the use must be acquired. Because the time allotted to scoring has been limited to an average of 1 h per chemical use, it may be necessary to estimate exposures on the basis of ones experience in the chemical industry, if the requisite information is not readily available. Information should be obtained from the following categories of sources, in the order specified: (1) general reference sources (see Figure 5, part 1, for examples); (2) specialized reference sources (see Figure 5, part 2, for examples); (3) companies, associations or experts likely to have knowledge of the chemical use in question (see Figure 6 for examples); (4) personal knowledge of chemical use characteristics based on experience in the field.

In most cases, it will be necessary to determine the kinds of chemicals likely to be employed for a particular use, and their physical form, in order to determine the associated exposure modes and amounts. (However, when starting with a known chemical, it will only be necessary to know its uses.)

Assign Exposure Scores. Using the exposure classification scheme and the exposure factor definitions, select from the classification the category of exposure that most closely describes the exposure associated with the use in question. Write the number corresponding to the selected exposure category in the proper box on the work sheet. In addition, write the verbal description of the category selected to identify the nature of the exposure. For example, a score of 1 for factor 1A (route of exposure) could indicate either oral, topical, or inhalation exposure. Specify which of these is the correct route. Finally, write a capsule summary, in the space allotted on the work sheet, of the information on which score assignment was based.

SPECIFIC METHODS FOR FACTOR BY FACTOR SCORING

Specific methods for scoring each of the four factors are described in this section and then illustrated for a sample chemical use.

Factor 1 Scoring (Mode of Human Exposure). The two components of factor 1, route and form of human exposure,

PART 1. GENERAL REFERENCE SOURCES

DICTIONARY OF SCIENTIFIC & TECHNICAL TERMS
pH & p ION: CONTROL IN PROCESS & WATER STREAMS
CHEMICALS & FORMULAS. EASTMAN KODAK COMPANY
THE CONDENSED CHEMICAL DICTIONARY
MATERIALS HANDBOOK
OPD BUYERS' DIRECTORY
CHEMICAL WEEK BUYERS' GUIDE
THE MERCK INDEX
KIRK-OTHMER ENCYCLOPEDIA OF CHEMICAL TECHNOLOGY
THE CHEMICAL FORMULARY

PART 2. SPECIALIZED REFERENCE SOURCES

TEXTILE FLAME RETARDANTS
FIRE JOURNAL
WELLINGTON SEARS HANDBOOK OF INDUSTRIAL TEXTILES
WHITTINGTON'S DICTIONARY OF PLASTICS
FAIRCHILD'S DICTIONARY OF TEXTILES
WATER SOLUBLE POLYMERS
WATER CONDITIONING FOR INDUSTRY
TEXTBOOK OF POLYMER SCIENCE
NOISE REDUCTION
INTRODUCTION TO THE TECHNOLOGY OF POTTERY
INTRODUCTION TO FORESTRY
WELDING ENCYCLOPEDIA
THE CHEMISTRY AND USE OF FIRE RETARDANTS
CONSERVATION OF LIBRARY MATERIALS: A MANUAL AND BIBLIOGRAPHY ON THE CARE, REPAIR AND RESTORATION OF LIBRARY MATERIALS
ADHESIVES AGE
AMERICAN ASSOCIATION OF TEXTILE CHEMISTS AND COLORISTS BUYERS' GUIDE
AMERICAN SOCIETY OF HEATING, REFRIGERATING AND AIR CONDITIONING ENGINEERS' GUIDE
APPLIED BASIC TEXTILES
METALS HANDBOOK
NATIONAL PAINT DICTIONARY
DICTIONARY OF CEMENT MANUFACTURING AND TECHNOLOGY
LOCKWOOD'S DIRECTORY OF THE PAPER AND PULP INDUSTRY
HANDBOOK OF ADHESIVES
PAPER TRADE JOURNAL
RUBBER AGE BUYERS' GUIDE
SEWAGE TREATMENT
HANDBOOK OF NOISE CONTROL
INDUSTRIAL POLLUTION CONTROL HANDBOOK
RADIATION BIOPHYSICS
POLYMER HANDBOOK
RUBBER RED BOOK
ENCYCLOPEDIA OF BASIC MATERIALS FOR PLASTICS
SOAP & SANITARY CHEMICALS
PAPER YEAR BOOK
MODERN PLASTICS
AMERICAN DYESTUFF REPORTER
CHEMISTRY AND TECHNOLOGY OF RUBBER

Figure 5. Reference sources consulted during exposure scoring.

are scored on the basis of physical properties of the chemical(s) likely to be involved in the use. For example, a volatile liquid could have a topical and inhalation route of exposure and a liquid and gaseous form of exposure.

Factor 2 Scoring (Mode of Environmental Exposure). The mode of environmental exposure is determined on the basis of the processing and handling procedures involved during use and ultimate disposal. For example, soaping-off assistants are used to wash out excess dye and dyeing assistants from the fabric after printing. The wash bath is disposed of in the plant waste water, and the ingredients of the bath could therefore enter environmental waters. (The possible presence of pollution controls is not to be taken into account, since it cannot be determined, in the allotted time, whether they are applied uniformly throughout an industry.)

Factor 3 Scoring (Amount of Human Exposure). For occupational exposure, subfactor A (number of people exposed) scoring is based on data supplied by publications such as the

ALDAN RUBBER COMPANY, PHILADELPHIA, PA
ALGONQUIN CHEMICAL COMPANY, HAMBURG, PA
ALLEGHENY BALLISTICS, CUMBERLAND, MD
AMERICAN CAN COMPANY, UNION, NJ
AMERICAN CYANAMID, PHILADELPHIA, PA
ARCO, PHILADELPHIA, PA
BRUDER, M.A., COMPANY, PHILADELPHIA, PA
CABOT CORPORATION, BOSTON, MA
CALGON CORPORATION, PITTSBURGH, PA
CENTURY ENGRAVING COMPANY, FULLERTON, CA
CHASE BAG, PHILADELPHIA, PA
CIBA-GEIGY, ARDSLEY, NY
CONOCO COAL DEVELOPMENT LABORATORY, PITTSBURGH, PA
CONSOLIDATED COAL, PHILADELPHIA, PA
COSAN CHEMICAL CORPORATION, CLIFTON, NJ
CROMPTON & KNOWLES, SOMERSET, NJ
CRYSTAL X CORPORATION, PHILADELPHIA, PA
DEGUSSA, INC., NJ
DIAMOND SHAMROCK, MORRISTOWN, NJ
DOW CHEMICAL COMPANY, MIDLAND, MI
DuPONT, WILMINGTON, DE
EAST CAROLINA STATE UNIVERSITY, GREENSVILLE, NC
EASTMAN-KODAK, NEW YORK, NY
FIRESTONE PLASTICS, POTTSTOWN, PA
FOLEY MACHINERY, PISCATAWAY, NJ
FOOD & DRUG ADMINISTRATION, WASHINGTON, DC
FRANKLIN MAINTENANCE, PHILADELPHIA, PA
GATES ENGINEERING, WILMINGTON, DE
GIVAUDAN CHEMICAL, CLIFTON, NJ
GLOBE DYE WORKS, PHILADELPHIA, PA
GULF & WESTERN, READING, PA
HENKEL INC., HOBOKEN, NJ
HERCULES, INC., WILMINGTON, DE
HOUGHTON, E.F., COMPANY, PHILADELPHIA, PA
HUBER, J.M., COMPANY, HAVRE DE GRACE, MD
ICI AMERICA, WILMINGTON, DE
INSTITUTE OF MAKERS OF EXPLOSIVES, NEW YORK, NY
JERSEY STATE CHEMICAL, HALEDON, NJ
JOHNSON-MARCH CORPORATION, PHILADELPHIA, PA
KERR-McGEE CHEMICAL CORPORATION, PHILADELPHIA, PA
KEYSOR CHEMICAL, NEW CASTLE, DE
LAUREL PRODUCTS, PHILADELPHIA, PA
LONE STAR INDUSTRIES, BETHLEHEM, PA
LUKENS STEEL COMPANY, PITTSBURGH, PA
NATIONAL PAINT AND COATINGS ASSOCIATION, WASHINGTON, DC
NATIONAL PRINTING INK INSTITUTE, BETHLEHEM, PA
NAVAL ORDNANCE LABORATORIES, WHITE OAK, MD
NEW YORK SANITATION DEPARTMENT, NEW YORK, NY
PENNWALT COMPANY, KING OF PRUSSIA, PA
PHILADELPHIA COLLEGE OF TEXTILES & SCIENCE, PHILADELPHIA, PA
PHILADELPHIA INQUIRER, PHILADELPHIA, PA
PHILADELPHIA QUARTZ COMPANY, VALLEY FORGE, PA
PHILIPS AND JACOBS, PHILADELPHIA, PA
POLAROID COMPANY, BOSTON, MA
REICHHOLD CHEMICAL COMPANY, WHITE PLAINS, NY
ROCKLAND COLLOIDS CORPORATION, PIERPORT, NY
ROHM & HAAS COMPANY, PHILADELPHIA, PA
SCOTT PAPER COMPANY, PHILADELPHIA, PA
STAUFFER CHEMICAL, NEW CASTLE, DE
SUPERIOR INK, NEW YORK, NY
THIOKOL CHEMICAL, TRENTON, NJ
TOMS RIVER CHEMICAL, TOMS RIVER, NJ
TROY CHEMICAL CORPORATION, NEWARK, NJ
UNIVERSAL ATLAS CEMENT, SADDLEBROOK, NJ
VULCANIZED RUBBER & PLASTICS, MORRISVILLE, NJ
WARNER COMPANY, PHILADELPHIA, PA
WATER POLLUTION CONTROL FEDERATION, WASHINGTON, DC
WESTLAKE PLASTICS, PHILADELPHIA, PA
WESTMORELAND COAL, PHILADELPHIA, PA
WITCO CHEMICAL COMPANY, NEW YORK, NY

Figure 6. Companies and associations contacted during exposure scoring

SUMMARY INFORMATION: COAGULANTS ARE USED IN SYNTHETIC RUBBER MANUFACTURE TO PRECIPITATE OUT THE RUBBER CRUMB AFTER POLYMERIZATION. CHEMICALS USED AS COAGULANTS ARE GENERALLY ALUM OR HYDRATED ALUMINUM CHLORIDE IN AN AQUEOUS SOLUTION, WHICH IS EITHER MADE UP AT THE PLANT OR PURCHASED FROM A SUPPLIER. BECAUSE THE RUBBER CRUMB IS WASHED REPEATEDLY TO REMOVE THE COAGULANT AND OTHER REACTIVE MATERIALS, THERE IS NO CONSUMER EXPOSURE TO THE COAGULANT.

CHEMICAL USE: COAGULANTS FOR SYNTHETIC RUBBER (No. 130-214)

FACTOR	OCCUPATIONAL EXPOSURE	S/M VALUE	CONSUMER EXPOSURE N.A.	S/M VALUE
1A ROUTE OF EXPOSURE	TOPICAL	1/6		
1B FORM OF EXPOSURE	LIQUID AND/OR SOLID	2/6		
2 MODE OF ENVIRONMENTAL EXPOSURE	WATER OR SOIL	1/3		
3A NUMBER OF PEOPLE EXPOSED	< 200,000	0/12		
3B FREQUENCY OF EXPOSURE	DAILY	3/12		
3C EXTENT OF CONTACT	HEAVY	3/12		
3D DURATION OF EXPOSURE	LONG	3/12		
4 AMOUNT OF ENVIRONMENTAL EXPOSURE	1-10%	2/3		

Figure 7. Completed scoring form for coagulants used in synthetic rubber manufacture.

Statistical Abstracts of the U.S., the *Census of Manufactures of the Department of Commerce*, Department of Labor figures for various industries, and specialized trade magazines. Consumer exposures are based on estimates. For example, interior paint applications may be assumed to involve over 10% of the general population, since so many people do their own housepainting.

Subfactors B–D (frequency of exposure, extent of contact, and duration of exposure) are all scored on the basis of processing and handling procedures (for occupational exposure) and common knowledge of chemical applications (for consumer exposure), as well as physical form of the chemical(s). For example, in a plant batch operation in which a powdered substance must be loaded into machinery several times a day, exposure could be daily, heavy, and long, for A–C, respectively, according to the definitions given in Figure 2. As an example of a consumer exposure, a brightener in a laundry detergent could be scored weekly, moderate, and medium for A–C, respectively.

Factor 4 Scoring (Amount of Environmental Exposure). Amount of environmental exposure is also scored on the basis of processing and handling procedures during use and ultimate disposal. For example, environmental exposure to a dishwashing compound would fall into category 3, with 10–100% environmental exposure, because the compound is disposed of in the wash water. On the other hand, environmental exposure to a cross-linking agent in a permanent press fabric would be scored as zero, because it is a constituent of a bulk solid and, as such, does not enter the environment either during use or disposal.

EXAMPLE OF SCORE GENERATION FOR A SPECIFIC USE

The following example describes category by category score generation for coagulants used in the manufacture of synthetic rubber (no. 130-214 on the chemical use list). The scoring form for this use is presented in Figure 7. Information used in scoring was based on the scorer's own experience, verified, to the extent possible, in the *Kirk-Othmer Encyclopedia of Chemical Technology*.

Factors 1A and 1B: Route and Form of Human Exposure. Chemicals used as coagulants for synthetic rubber are generally alum or hydrated aluminum chloride, although any electrolyte can be used. Coagulants are used in water solution, which is either made up at the plant from the solid material or purchased in liquid form from a supplier. Although little human exposure occurs when the coagulant solution is introduced into the reaction vessel by gravitational flow or mechanical pumping, splashing and leakage do occur but may be largely ignored, as the coagulant materials are generally considered innocuous. In addition, workers may observe the mixing operation through a hole in the reactor (the "manhole"), getting splashed in the process. Thus, the route of exposure of plant workers to coagulants would be topical, with a score of 1, and the form of exposure would be either liquid, with a score of 1, or solid and liquid (for solutions made up at the plant), with a score of 2.

Factor 2: Mode of Environmental Exposure. Coagulants are used to precipitate out the crumb (i.e., the rubber polymer) from the reaction mixture, which contains any unreacted monomer, as well as a catalyst, activator, modifier, and antioxidant; coagulants do not enter into the reaction. The crumb rubber is washed repeatedly to remove the coagulant and other chemicals. Coagulant may also be lost during solution make-up (as solid and/or solution) and charging to the reactor (as solution). Dissolved coagulant could enter the environment through the sewage system (i.e., via water), and solid coagulant could enter the environment through the disposal of sweepings (i.e., via soil). Thus, the mode of environmental exposure is via water or soil, with a score of 1.

Factor 3: Amount of Human Exposure. As reported in the *Census of Manufactures*, the number of people employed in the synthetic rubber industry is less than 200 000. Therefore, the number of people exposed (factor 3A) to coagulants for synthetic rubber would be under 200 000, with a score of 0. Because coagulants are used daily in synthetic rubber manufacture, frequency of exposure (factor 3B) is daily, with a score of 3. Because coagulants are used in batch, rather than in continuous, operations, with significant worker exposure, extent of contact (factor 3C) is considered to be heavy, with a score of 3. Because reaction times run between 2 and 5 h (depending on whether a solution or emulsion medium is used) and the batch must be charged to the reactor between reactions, duration of exposure (factor 3D) for the worst case is considered to be long, with a score of 3. This score also takes into account leakage and splashing during reaction.

Factor 4: Amount of Environmental Exposure. Coagulant is lost during solution make-up, charging of solution to the reactor, and washing of the crumb rubber to remove residual coagulant. The process water itself, containing the bulk of the coagulant, is recycled indefinitely, with replacement amounts of coagulant and other materials. Thus, combined loss of coagulant to the environment probably does not exceed 10% of the amount used, for a score of 2.

Because coagulant is rinsed off the crumb rubber in the plant, there is no consumer exposure to coagulants used in synthetic rubber manufacture.

RESULTS OF SCORING AND RANKING

According to the formula shown earlier, where the rank of a chemical use equals the sum of the actual numerical values of the assigned exposure variables (s) divided by the sum of the maximum numerical values obtainable for all exposure variables (m), the lowest possible value of s was 0, and the highest possible score was 24; m equalled 24. Figure 8 illustrates the score range for each factor. The possible exposure scores fell into 25 groups, calculated, as shown in Figure 9, by dividing the values of s by the value of m, resulting in a series of fractions beginning with 0 and ending with 1 (i.e., 24/24).

Scores for the 800 chemical uses were ordered, as expected, in a bell-shaped distribution, with few uses having exceptionally

	S/M
1A	0/6 - 3/6
1B	0/6 - 3/6
2	0/3 - 3/3
3A	0/12- 3/12
3B	0/12- 3/12
3C	0/12- 3/12
3D	0/12- 3/12
4	0/3 - 3/3

S/M = 0/24 TO 24/24

Figure 8. Range of scores by factor.

$$R_j = \sum_{i=1}^{4} W_i \bullet \frac{S_{ij}}{M_i}$$

SCORE:	0/24	1/24	2/24	3/24	...	8/24	...	12/24	...	15/24	...	21/24	...	24/24
RANK:	0.0	0.41	0.83	.124		.333		.50		.625		.875		1.0

Figure 9. Computation of ranks.

low or high scores and the majority of uses having various intermediate scores within a relatively narrow range. This result was acceptable and consistent with the goal of the scoring activity, which was to identify those chemical uses having the greatest potential for exposure. Whoever is responsible for selecting uses having the greatest exposure potential can establish any desired cutoff point along the curve. Should the entity conducting such a scoring and ranking operation desire to highlight one or more exposure parameters, weighting values can be assigned to selected parameters in accordance with the ranking formula. The result will be higher scores assigned to those uses characterized by the selected parameters of exposure. Furthermore, scoring for human and environmental exposure can be completely disassociated, if exposure to only one or the other is of interest.

Scores for the individual chemical uses can be made more accurate by devoting personnel time to accumulate more data in preparation for scoring. However, the basic concept of scoring and ranking chemical uses according to the methodology described above appears to be valid for its stated purpose.

REFERENCES AND NOTES

(1) U.S. Congress, Senate "Toxic Substances Control Act"; 94th Congress, 2nd Session: Washington, DC, 1976; S. 3149, Oct 11, 1976, Publication L. 94-469.
(2) Byer, W. L.; Landau, H. B.; Stalder, E. W. "Development of a Chemical Use Classification System to Facilitate Reporting under the Toxic Substances Control Act." *J. Chem. Inf. Comput. Sci.* **1977**, *17*, 197-200.

Use of MACCS within ICI†

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ICI is developing a new system called SAPPHIRE—a user-friendly, interactive system for the storage and rapid retrieval of chemical structures and related property data, with interfaces to other systems such as molecular modeling, reaction design, and biological data handling. The chemical structure part of SAPPHIRE will be handled by MACCS software, written by Molecular Design Limited and enhanced by them in 1983 to meet ICI requirements for handling databases of over 400 000 compounds. Interfaces will use the Molecular Design program MACCSLIB.

INTRODUCTION

The Company Compound Center database shared by five ICI divisions contains about 360 000 compounds. Of these, nearly 190 000 are Pharmaceuticals Division compounds that have huge numbers of related biological test results. In addition, there is a file of commercially available compounds, and there are several smaller specialized files. Since the 1960s, all this data has been handled by the ICI CROSSBOW system,[1-6] with Wiswesser line notation (WLN) as the tool for structure representation. Chemists are unfamiliar with WLN and have therefore needed the intervention of information experts to search scientific data on their behalf. Moreover, structure display in CROSSBOW is a batch process, and the end-user has had to wait 24 h or more for his answers. His creative scientific ideas have therefore not been put to best use because his valuable train of thought is interrupted. In a truly interactive system this should not happen, and as each idea leads to another, the scientist should be able to pursue each train of thought to its logical conclusions when and how he himself wants.

ICI is therefore developing the SAPPHIRE system (*S*tructures *a*nd *P*roperties *P*roduced by *H*elpful *I*nteractive *R*apid *E*nquiry), a user-friendly, interactive system for the storage and rapid retrieval of chemical structures and related property data. The system will have interfaces to other ICI systems such as molecular modeling, reaction design, and biological data handling and even, it is hoped eventually, to systems external to ICI for handling information from the scientific literature.

The SAPPHIRE project is being developed by a team of about six analysts and programmers at ICI Pharmaceuticals Division but is funded by three of the five divisions who share the Company Compound Center database, namely, ICI Organics, Pharmaceuticals, and Plant Protection Divisions. The views of end users at all relevant ICI sites are being carefully considered in the system design.

The chemical structure part of SAPPHIRE will be handled by software written by Molecular Design Limited (MDL) and, in particular, by a version of MACCS enhanced to furnish rapid search on very large databases. This product is at present referred to as MACCS-BV (for "the big version" of MACCS) and is being beta-tested at ICI Pharmaceuticals Division. Later in 1984, MACCS-BV will be the standard version of

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