

Toxic Substances



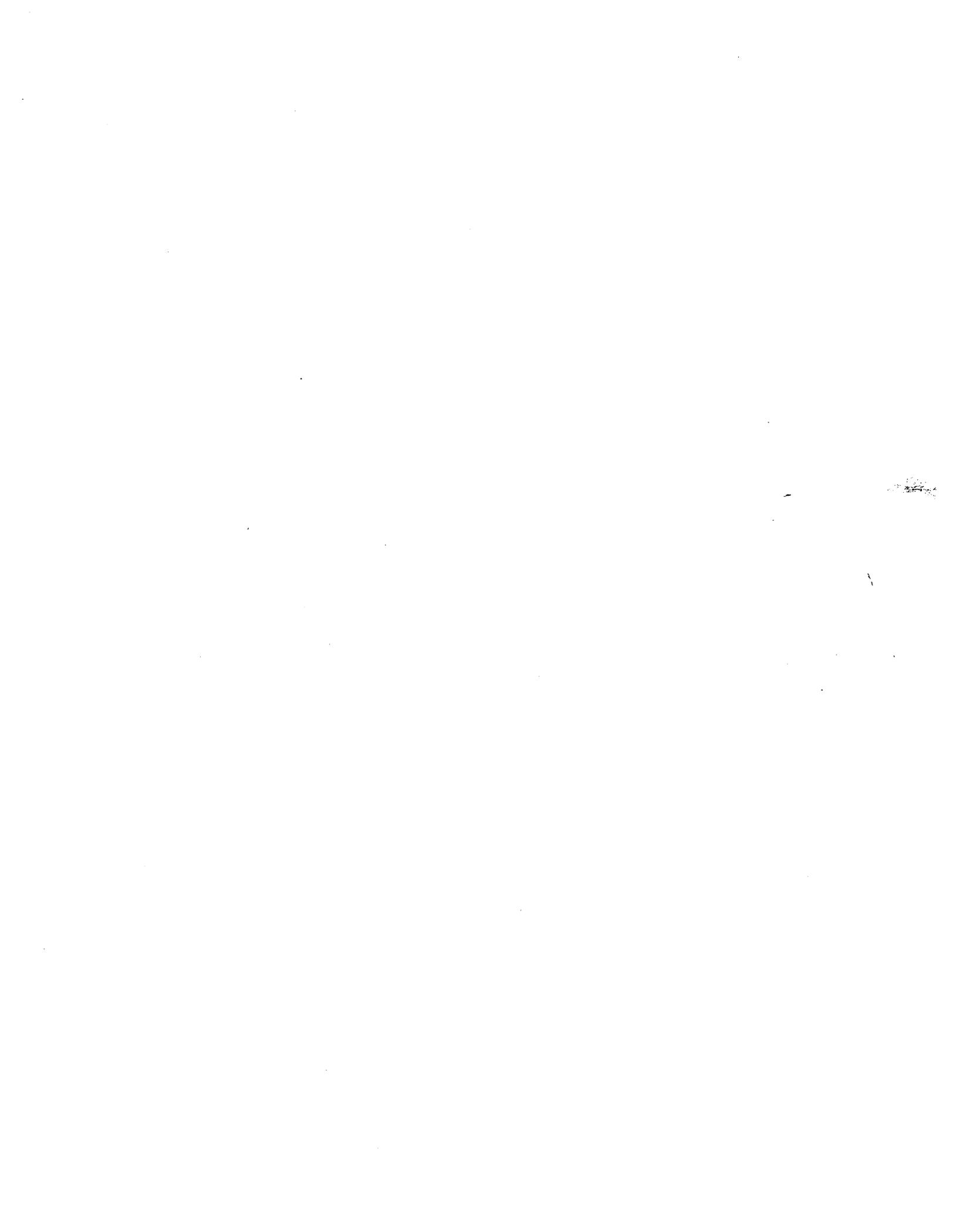
Methods for Assessing Exposure to Chemical Substances

Volume 7

Methods for Assessing Consumer Exposure to Chemical Substances

Checklist
1. Identifying
2. OIS





EPA 560/5-85-007
APRIL 1987

METHODS FOR ASSESSING EXPOSURE
TO CHEMICAL SUBSTANCES

Volume 7

Methods for Assessing Consumer Exposure
to Chemical Substances

by

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EPA Contract No. 68-02-3968

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FOREWORD

This document is one of a series of volumes, developed for the U.S. Environmental Protection Agency (EPA), Office of Toxic Substances (OTS), that provides methods and information useful for assessing exposure to chemical substances. The methods described in these volumes have been identified by EPA-OTS as having utility in exposure assessments on existing and new chemicals in the OTS program. These methods are not necessarily the only methods used by OTS, because the state-of-the art in exposure assessment is changing rapidly, as is the availability of methods and tools. There is no single correct approach to performing an exposure assessment, and the methods in these volumes are accordingly discussed only as options to be considered, rather than as rigid procedures.

Perhaps more important than the optional methods presented in these volumes is the general information catalogued. These documents contain a great deal of non-chemical-specific data which can be used for many types of exposure assessments. This information is presented along with the methods in individual volumes and appendices. As a set, these volumes should be thought of as a catalog of information useful in exposure assessment, and not as a "how-to" cookbook on the subject.

The definition, background, and discussion of planning exposure assessments are discussed in the introductory volume of the series (Volume 1). Each subsequent volume addresses only one general exposure setting. Consult Volume 1 for guidance on the proper use and interrelations of the various volumes and on the planning and integration of an entire assessment.

The titles of the nine basic volumes are as follows:

- Volume 1 Methods for Assessing Exposure to Chemical Substances
(EPA 560/5-85-001)
- Volume 2 Methods for Assessing Exposure to Chemical Substances in the
Ambient Environment (EPA 560/5-85-002)
- Volume 3 Methods for Assessing Exposure from Disposal of Chemical
Substances (EPA 560/5-85-003)
- Volume 4 Methods for Enumerating and Characterizing Populations Exposed
to Chemical Substances (EPA 560/5-85-004)

- Volume 5 Methods for Assessing Exposure to Chemical Substances in Drinking Water (EPA 560/5-85-005)
- Volume 6 Methods for Assessing Occupational Exposure to Chemical Substances (EPA 560/5-85-006)
- Volume 7 Methods for Assessing Consumer Exposure to Chemical Substances (EPA 560/5-85-007)
- Volume 8 Methods for Assessing Environmental Pathways of Food Contamination (EPA 560/5-85-008)
- Volume 9 Methods for Assessing Exposure to Chemical Substances Resulting from Transportation-Related Spills (EPA 560/5-85-009)

Because exposure assessment is a rapidly developing field, its methods and analytical tools are quite dynamic. EPA-OTS intends to issue periodic supplements for Volumes 2 through 9 to describe significant improvements and updates for the existing information, as well as adding short monographs to the series on specific areas of interest. The first four of these monographs are as follows:

- Volume 10 Methods for Estimating Uncertainties in Exposure Assessments (EPA 560/5-85-014)
- Volume 11 Methods for Estimating the Migration of Chemical Substances from Solid Matrices (EPA 560/5-85-015)
- Volume 12 Methods for Estimating the Concentration of Chemical Substances in Indoor Air (EPA 560/5-85-016)
- Volume 13 Methods for Estimating Retention of Liquids on Hands (EPA 560/5-85-017)

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ACKNOWLEDGEMENTS

This report was prepared by Versar Inc. of Springfield, Virginia, for the EPA Office of Toxic Substances, Exposure Evaluation Division, Exposure Assessment Branch (EAB) under EPA Contract Nos. 68-01-6271 and 68-02-3968. The EPA-EAB Task Managers for this task were Karen A. Hammerstrom and Stephen H. Nacht; the EPA Program Managers were Michael A. Callahan and Elizabeth F. Bryan. The support and guidance given by these, and other EPA personnel, is gratefully acknowledged.

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1. INTRODUCTION

This volume is the seventh in a series of thirteen volumes presenting methods for assessing exposures to chemical substances; the reports are being developed for the U.S. Environmental Protection Agency, Office of Toxic Substances. This volume presents methods and supporting information for estimating exposures to chemical substances in consumer products. The methods that are presented in this volume to estimate inhalation and dermal exposure are the basis of user-friendly, personal computer programs that comprise the Computerized Consumer Exposure Models (CCEM). CCEM was developed for the Exposure Evaluation Division of the Office of Toxic Substances. Much of the supporting information included in this volume is also included in CCEM. Such data include room air exchange rates, human inhalation rates, skin surfaces areas, film thickness values for liquids on skin, mixing factors, and body weights of humans. The background and purpose of this report, the consumer products considered by this methods report, and its methodological framework, are discussed in the following subsections.

1.1 Background and Purpose

The Toxic Substances Control Act (TSCA) of 1976 (PL94-469) authorizes the U.S. Environmental Protection Agency (EPA) to assess human and environmental exposure to chemical substances. An exposure assessment for a chemical substance attempts to determine the amounts of that chemical substance to which populations are exposed, as well as to identify and estimate the size of exposed populations. The EPA Office of Toxic Substances (OTS), Exposure Evaluation Division (EED), is responsible for conducting exposure assessments for new and existing chemical substances in support of Sections 4, 5, and 6 of TSCA.

Exposure assessments for each of the exposure categories (i.e., ambient, occupational, food, drinking water, and consumer) have historically been limited by a lack of complete and reliable data. Accurate calculation of exposure to a chemical substance relies on actual monitoring data from the media (e.g., air, water, food, surfaces) containing the chemical and the entire time period during which exposure occurs. For most chemical substances, however, these data are insufficient, difficult to obtain, or non-existent, necessitating estimation of exposure. The goal of this report is to catalog pertinent information, data bases, and tools, and to provide a systematic approach or methodology whereby the exposure to a given chemical substance in consumer products can be estimated at any desired level of detail.

1.2 Consumer Products Considered by This Methods Report

Consumer products are defined in this report as products containing chemical constituents to which human or environmental exposure may occur

as a result of the use of the consumer product. This is a broad definition, which incorporates a multitude of products and product groups and crosses several regulatory boundaries.

The product groups that have been specifically excluded from the scope of this exposure assessment methods report are listed below. These product groups pose analytical complications not addressed at this time, are covered by other methods reports, or are excluded from TSCA authority.

- Tobacco and tobacco products.
- Non-consumer pesticides and fertilizers.
- Business products (i.e., copying machines).
- Firearms, ammunitions, and explosives.
- Food, food products, and food additives/preservatives.
- Products containing radioactive materials.
- Products used exclusively for hobbies and crafts.
- Drugs and medical devices.

The criteria used by the FDA to distinguish between cosmetics and drugs state that any preparation used only for cleansing or beautification of the skin, hair, or fingernails is considered a cosmetic. Any claim of a medicinal nature, even if it is only implied, immediately places the product in the drug class. (Products such as bandages, lip balms, and suntan lotions are included in this methods report because of their intended protective, not medicinal, purposes.)

Finally, exposures resulting from the use of any form of transportation are limited to cleaning, waxing, and polishing automobiles and exposures to synthetic interior materials.

As part of the general data collection portion of this methods report, a comprehensive list of consumer products found in typical American households was compiled and is presented in Table 1. This is a working list that is believed to reflect those products and product groups of commonly used items which, through various modes of consumption (exposure scenarios), lead to exposure to chemical constituents. This list is somewhat arbitrary and subjective. Creating a finite set of products, however, was necessary to begin the task of collecting the vast amount of product-specific information. Definitions of product types, such as aerosol and liquid, are cited in Table 2.

1.3 Overview of Methodological Approach

This report presents methods and data recommended for estimating exposure to chemical substances in consumer products. Methods for estimating both "active" and "passive" exposure to chemical substances in consumer products are presented. Active exposures are defined as

CONSULTANT
OF CIPRA
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Table 1. Consumer Products Found in the
Typical U.S. Household¹

Consumer product category	Consumer product
<u>Cosmetics hygiene products</u>	Adhesive bandages Bath additives (liquid) Bath additives (powder) Cologne/perfume/aftershave Contact lens solutions Deodorant/antiperspirant (aerosol) Deodorant/antiperspirant (wax and liquid) Depilatories Facial makeup Fingernail cosmetics Hair coloring/tinting products Hair conditioning products Hairsprays (aerosol) Lip products Mouthwash/breath freshener Sanitary napkins and pads Shampoo Shaving creams (aerosols) Skin creams (non-drug) Skin oils (non-drug) Soap (toilet bar) Sunscreen/suntan products Talc/body powder (non-drug) Toothpaste Waterless skin cleaners
<u>Household furnishings</u>	Carpeting Draperies/curtains Rugs (area) Shower curtains Vinyl upholstery, furniture

Table 1. (continued)

Consumer product category	Consumer product
<u>Garment conditioning products</u>	Anti-static spray (aerosol) Leather treatment (liquid and wax) Shoe polish Spray starch (aerosol) Suede cleaner/polish (liquid and aerosol) Textile water-proofing (aerosol)
<u>Household maintenance products</u>	Adhesive (general) (liquid) Bleach (household) (liquid) Bleach (see laundry) Candles Cat box litter Charcoal briquets Charcoal lighter fluid Drain cleaner (liquid and powder) Dishwasher detergent (powder) Dishwashing liquid Fabric dye (DIY) Fabric rinse/softener (liquid) Fabric rinse/softener (powder) Fertilizer (garden) (liquid) Fertilizer (garden) (powder) Fire extinguishers (aerosol) Floor polish/wax (liquid) Food packaging and packaged food Furniture polish (liquid) Furniture polish (aerosol) General cleaner/disinfectant (liquid) General cleaner (powder) General cleaner/disinfectant (aerosol and pump) General spot/stain remover (liquid) General spot/stain remover (aerosol and pump) Herbicide (garden-patio) (liquid and aerosol)

Table 1. (continued)

Consumer product category	Consumer product
<u>Household maintenance products</u> (continued)	Insecticide (home and garden) (powder) Insecticide (home and garden) (aerosol and pump) Insect repellent (liquid and aerosol) Laundry detergent/bleach (liquid) Laundry detergent (powder) Laundry pre-wash/soak (powder) Laundry pre-wash/soak (liquid) Laundry pre-wash/soak (aerosol and pump) Lubricant oil (liquid) Lubricant (aerosol) Matches Metal polish Oven cleaner (aerosol) Pesticide (home) (solid) Pesticide (pet dip) (liquid) Pesticide (pet) (powder) Pesticide (pet) (aerosol) Pesticide (pet) (collar) Petroleum fuels (home) (liquid and aerosol) Rug cleaner/shampoo (liquid and aerosol) Rug deodorizer/freshener (powder) Room deodorizer (solid) Room deodorizer (aerosol) Scouring pad Toilet bowl cleaner Toilet bowl deodorant (solid) Water-treating chemicals (swimming pools)

Table 1. (continued)

Consumer product category	Consumer product
<u>Home building/improvement products (DIY)</u>	Adhesives, specialty (liquid) Ceiling tile Caulks/sealers/fillers Dry wall/wall board Flooring (vinyl) House Paint (interior) (liquid) House Paint and Stain (exterior) (liquid) Insulation (solid) Insulation (foam) Paint/varnish removers Paint thinner/brush cleaners Patching/ceiling plaster Roofing Refinishing products (polyurethane, varnishes, etc.) Spray paints (home) (aerosol) Wall paneling Wall paper Wall paper glue
<u>Automobile-related products</u>	Antifreeze Car polish/wax Fuel/lubricant additives Gasoline/diesel fuel Interior upholstery/components, synthetic Motor oil Radiator flush/cleaner Automotive touch-up paint (aerosol) Windshield washer solvents

Table 1. (continued)

Consumer product category	Consumer product
<u>Personal materials</u>	Clothes/shoes Diapers/vinyl pants Jewelry Printed material (colorprint, newsprint, photographs) Sheets/towels Toys (intended to be placed in mouths)

DIY = Do It Yourself.

¹ A subjective listing based on consumer use profiles conducted by Versar.

Table 2. Product Form Terminology Adopted
for Use in This Report

Term	Descriptive definition
Aerosol	Any product dispensed from a pressurized can. The state of the product following delivery from the aerosol can includes mists/aerosols, foams, liquids, and powders.
Pump	Any liquid product dispensed from an unpressurized container via a pumping trigger.
Liquid	Any liquid product dispensed by pouring from its container. This includes a "roll-on" or similar liquid dispensing container.
Powder	Any powdered product that can be poured or "dusted" from its container. Powdered products include crystals and granules.
Solid	A solid product; e.g., moth balls, though they are crystalline in nature and are poured from their containers, are considered a "solid" product.
Gel/wax	Any viscous liquid, gel, wax, or paste squeezed or scooped from its container.

exposures resulting to the user of a consumer product during active use of the product (e.g., exposures to chemical substances in paints during the act of painting). Passive exposures pertain to exposures that occur (1) to the user after active use has ceased, (2) to non-users who are passively exposed as a result of user activities, and (3) to persons in the environs of products, such as solid air fresheners, that result exclusively in passive exposures.

The methods for performing consumer exposure assessments are discussed in the following five sections:

- Section 2 - Physical-Chemical Properties
- Section 3 - Product-Specific Data Required to Assess Exposure
- Section 4 - Methods for Estimating Release of Chemicals from Consumer Products and Concentrations of Chemicals in External Media
- Section 5 - Exposed Populations
- Section 6 - Exposure Analysis

Appendix A of this report contains methods for estimating inhalation exposure to particulates discharged from consumer products. Appendix B includes guides to the individual Simmons Market Research Bureau (SMRB) reports and to the products included in each volume, respectively. Appendix C includes an alphabetical listing of all variables used in Volume 7 of Methods for Assessing Exposure to Chemical Substances. A definition of each variable and the units in which it is expressed are also included in Appendix C.

In developing the methods, a series of chemical-, product- and environment-specific questions were addressed:

- Chemical-specific:
 - How much of a chemical is in the product?
 - How much is permanently bound in the product and unavailable for exposure?
- Product-specific:
 - How is the product used, and for how long?
 - How are chemical constituents released through use?
 - How much of the product is used and by whom?
- Environment-specific:
 - Where is the product used?
 - How do ventilation, dilution, etc., affect available concentrations?

By answering these questions for a range of consumer products, this methods report attempts to supply the analytical tools necessary for estimating exposures resulting from various typical consumer activities and the means by which other analytical tools can be developed to

calculate values for more unusual consumer exposure situations. An effort is made throughout the report to explain the rationale behind the approaches followed, the derivation of all equations and models, the assumptions and estimates used, and any inherent limitations.

The basic steps for performing a consumer exposure assessment for a given chemical are to identify the products in which it appears, identify appropriate exposure scenarios (detailed circumstances in which consumer exposure occurs) for each of the products, gather the data required by each scenario, calculate an exposure or dose based on the equation and parameter values delineated in each scenario, and enumerate the populations exposed (both actively and passively). A more detailed scheme of methodological operations is presented in Table 3. These method components are intentionally called operations instead of steps to discourage the notion that they must be fulfilled in sequential order.

Methods for assessing exposure to chemical substances in consumer products are delineated in this volume for several pathways of exposure. Sections of this volume to use in estimating inhalation exposure during use of consumer products are presented in Table 4. Sections of this volume to use in estimating dermal and ingestion exposure during use of consumer products are presented in Table 5.

Table 3. Operations for Performing a Consumer Exposure Assessment for a Given Chemical

Relate based on exposure assessment data to identify + measure relevant (S)

Method operations	Related data needs
Identify consumer products that contain chemical	<ul style="list-style-type: none"> • Synonyms and CAS # • Information on whether chemical will be a product constituent or residual of product processing
Identify pertinent exposure routes	<ul style="list-style-type: none"> • Physical-chemical properties • Basic information on product use patterns • States of products before, during, and after use
Develop/select appropriate exposure scenarios	<ul style="list-style-type: none"> • Identification of key parameters (e.g., frequency of product use, duration of each use, amount of product delivered in each use, inhalation rates, etc.)
Based on scenario, select appropriate values for key parameters (ranges and typical values)	<ul style="list-style-type: none"> • Physical-chemical properties • Specific information on product use patterns • Environmental parameters (e.g., room size, ventilation)
Determine amount of chemical in each product	<ul style="list-style-type: none"> • Chemical engineering processes related to product formulation • Weight percentages of constituents in each product • Weight percentages of chemical in each constituent

Handwritten notes: Relate based on exposure assessment data to identify + measure relevant (S)



Table 3. (continued)

Method operations	Related data needs
Determine release of chemical from product	<ul style="list-style-type: none"> • Physical-chemical properties • Release mechanism analysis
Determine concentration of chemical available for exposure	<ul style="list-style-type: none"> • Input from previous three operations
Calculate exposure	<ul style="list-style-type: none"> • Input from all previous operations
Calculate dose (optional)	<ul style="list-style-type: none"> • Exposure value • Physical-chemical properties • Pharmacokinetics data
Enumerate exposed populations (active and passive)	<ul style="list-style-type: none"> • Input from product identification and key scenario parameters • Market data • General population/housing statistics

to be according to

Table 4. Sections of Volume 7 to Use in Estimating Inhalation Exposure

Exposure pathway	Release rate of chemical substance to air	Concentration of chemical substance in air	Levels to which consumers are exposed
Inhalation of a chemical substance that is a component of aerosols formed while spilling or pouring a liquid or powder	4.3.1	4.4.2	6.2.2
Inhalation of a chemical substance during continuous release of the contents of a pressurized aerosol product	4.3.1	4.4.2	6.2.2
Inhalation of a chemical substance during intermittent release of the contents of a pressurized aerosol product, in which the time between releases is on the order of a few seconds	4.3.1	4.4.2	6.2.2
Inhalation of a chemical substance during its evaporation from a container of liquid or from a wet film or coating spilled or applied instantaneously to a surface	4.3.2	4.4.2	6.2.2
Inhalation of a chemical substance during its evaporation from a wet film or coating applied to a surface, in which the period of application is more than a few minutes	4.3.2	4.4.3	6.2.2
Inhalation of a chemical substance released from a solid that sublimes (e.g., from solid room deodorizer, moth balls, etc.)	4.3.1	4.4.2	6.2.2
Inhalation of a chemical substance released from a dry coating or polymer	4.3.3	4.4.2	6.2.2

*Public
Sector MCCC
INDOOR
RTD
SUBSTANTIAL
MIST
MIGRATION*

Table 5. Sections of Volume 7 to Use in Estimating Exposure via Dermal Contact with and Ingestion of Consumer Products

Exposure pathway	Estimate levels to which consumers are exposed
Exposure to a film of liquid deposited on the skin	6.2.3(1)
Exposure to dusts and powders deposited on the skin	6.2.3(2)
Dermal exposure to chemical substances contained in or adhering to solid matrices	6.2.3(3)
Ingestion exposure to chemical substances leached out of objects designed to be used in the mouth	6.2.4(1)
Ingestion exposure from unintentionally swallowing liquids used in the mouth	6.2.4(2)

*One bank
- after 1000s
- 1000s
- 1000s*

*Look at models
+ structure*

2. PHYSICAL-CHEMICAL PROPERTIES

One of the initial efforts in any exposure assessment for a chemical substance is identification of its physical-chemical properties. Physical-chemical properties data are essential for a thorough understanding or prediction of environmental fate (i.e., transport and transformation) and the eventual environmental or exposure concentrations. The mechanisms of release of a chemical substance from a consumer product, the exposure media, and the exposure route are determined by the chemical substance's properties. The purpose of this section is to (1) briefly discuss properties that are relevant to developing exposure assessments for chemicals in consumer products and (2) catalog information sources for obtaining experimental property data and methods for estimating properties where such data are lacking.

2.1 General Property Information

Table 6 summarizes the physical-chemical properties that are relevant to performing exposure assessments for chemicals in consumer products. Not all the properties listed are required for each chemical. Required properties are dictated by the physical state of the chemical and the physical-chemical nature of the consumer product that contains it. Many of the properties listed may be required only when it is necessary to estimate exposure concentrations based on chemical release algorithms. The chemical release algorithms are discussed in Section 4 of this document.

2.2 Data Gathering

The physical-chemical properties of a chemical substance can be gathered from the scientific literature or, where experimental data are lacking, they can be estimated. The following subsections discuss sources of information for experimental data and methods for estimating physical-chemical properties.

2.2.1 Sources of Experimental Data

Information sources from which experimental data can be gathered are divided into those that are computer based and accessed on-line and those that are published documents or "hard copy." The major on-line systems including address, telephone, number, and contact for "help" information are listed in Table 7. Published documents that summarize and present experimental data are listed in Table 8.

Prior to initiating any data collection, the investigator should obtain for the chemical substance of interest the Chemical Abstracts

Table 6. Summary of Physical-Chemical Properties
Relevant to Consumer Exposure

Property/parameter	Units	Comments
Molecular weight	Dimensionless	Required input for estimation of many other properties. Required for stoichiometrically derived chemical release estimates.
Physical state	-	Solid, liquid, or gas. Assists in identification of exposure routes.
Particle size	Length (usually micron)	Used for entrainment (dispersion) analysis of dusts and powders and identifying area of respiratory tract deposition.
Density	Mass/volume (e.g., g/cm ³)	Useful for calculating film thickness of liquids on skin. Indicative of whether gases (or liquids) are heavier or lighter than air (or water).
Melting point/ boiling point	Degrees Celsius	Input for calculating vapor pressure and volatilization rates. Identifies physical state of substance at ambient conditions.
Vapor pressure	mm Hg; torr; atmospheres	Essential for predicting the behavior and fate of chemicals in the environment: rates of evaporation, equilibrium air concentrations (worst case).
Heat of vaporization	Calories/mole	Quantity of heat required to convert a unit mass of liquid into a vapor without a rise in temperature. Required input for estimating other properties such as vapor pressure.
Henry's law constant	Dimensionless or atm-m ³ /mol	Indicative of a chemical's propensity to volatilize from water. Required input for calculating volatilization rates.
Solubility	Mass/volume	Maximum amount of the chemical that will dissolve in pure liquid at a specified temperature. Facilitates calculation of worst case concentrations. Required input for calculating volatilization rates of chemicals from solutions.

Table 6. (continued)

Property/parameter	Units	Comments
Diffusion coefficients (i.e., air, water, solids)	Length ² /time (e.g., cm ² /s)	Indicative of a chemical's ability to move in a liquid, gas, or solid based on intermolecular collisions (not turbulence or bulk transport). Diffusion coefficients through gas range from 10 ⁻¹ to 10 ⁻² cm ² /s; through liquids from 10 ⁻⁵ to 10 ⁻⁶ cm ² /s; and through solids from 10 ⁻⁷ to 10 ⁻²⁰ cm ² /s. Required input for calculating volatilization rates and migration through solid matrices.
Octanol/water partitioning coefficient (K _{OW})	Dimensionless	Ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous (water) phase. Important indicator of a chemical's fate.
Volatilization rates	Length/time (e.g., cm/hr)	Required for estimating air concentrations of chemicals evaporating from liquids and solids.
Activity coefficient	Dimensionless	A factor for compensating for non-ideal behavior of compounds in solution. Required input for estimating properties of mixtures.

Table 7. Major Computerized Data Bases for Obtaining Physical-Chemical Properties

Data base name	Sponsor/contract support	Help information	Comments
Chemical Information System (CIS)	NIH/EPA Computer Science Corp. P. O. Box 2227 Falls Church, VA 22042	Mike Keller 703-237-1333 800-368-3432	Access to a wealth of computerized information including structure and nomenclature, chemical evaluation, clinical toxicology, registry of toxic effects, and oil and hazardous materials technical assistance data.
HAZARDLINE	Physicians World Communication Group Occupational Health Services, Inc. 400 Plaza Drive Secaucus, NJ 07094	Kay Sloves 800-223-8978	Access to environmental and occupational information on hazardous substances including physical and chemical properties, personal protective equipment, and chemical surveillance to test requirements, waste disposal and leaks, spills, and fire fighting information.
Medical Literature Analysis and Retrieval System (MEDLARS)	National Institutes of Health National Library of Medicine MEDLARS Management Section 8600 Rockville Pike Bethesda, MD 20014	301-496-6193 800-638-8480	On-line chemical dictionary access (CHEMLINE) and a wealth of information on toxicology and bibliographic data on chemical substances.
Chemicals in Commerce Information System (CICIS)	USEPA OTS/MSD-SDB Office of Toxic Substances Management Support Division Washington, DC 20460	Geri Nowak 202-382-3568	1977 TSCA Inventory of Chemical Substances. Chemical properties, structures, production, and use. Note: Data base has not been updated since 1977 and is therefore somewhat out-of-date.

Table 8. Major Published References for Obtaining
Physical-Chemical Properties

Document	Comment
CRC Handbook of Chemistry and Physics	Good source for general properties of a large variety of chemicals.
Chemical Engineers Handbook	Good source for general properties of a large variety of chemicals.
Lange's Handbook of Chemistry	Good source for general properties of a large variety of chemicals.
The Merck Index	Good source for pharmaceutical or medicinal chemical properties.
Kirk-Othmer Encyclopedia of Chemical Technology	Good source for general properties of a large variety of chemicals.
Farm Chemicals Handbook	Good source for properties of farm chemicals, particularly pesticides.
Handbook of Environmental Data on Organic Chemicals	Good source for properties of organic chemicals.
Physical Properties of Chemical Compounds (Volumes I, II, III)	Cyclic, acyclic, and aliphatic compounds.
Physical Properties of Hydrocarbons (Volumes I and II)	Paraffinic, halogenated, and oxygenated hydrocarbons (alcohols, oxides, glycols) (Volume I); organic acids, ketones, aldehydes, ethers, esters, nitrogen compounds, aromatics, cyclic hydrocarbons, and sulfur compounds (Volume II).
The Aldrich Catalog - Handbook of Organic and Biological Chemicals	General properties of many organic chemicals of environmental interest.
Vapor Pressure of Organic Compounds	Good source for experimental vapor pressure data.

Table 8. (continued)

Document	Comment
Technical Data Book - Petroleum Refining (Volumes I and II)	Basic properties of organic compounds that are petroleum derived.
Handbook of Vapor Pressures and Heats of Vaporization of Hydrocarbons and Related Compounds	Vapor pressure of hydrocarbons.
The Properties of Gases and Liquids	Covers most general properties.
Faith, Keyes, and Clark, Industrial Chemicals	General properties for a small number of chemicals.
Publications of the National Bureau of Standards (NBS); National Standard Data Reference System (NSRDS) <ul style="list-style-type: none"> - Journal of Physical and Chemical Reference Data - NSRDS - NBS publication series - Miscellaneous technical society publications 	See Appendix A of <u>Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Chemicals</u> for additional information. NSRDS is a good source for industrial process data including information on thermodynamic, transport, and physical properties of industrial chemicals.
Publications of the Engineering Sciences Data Units, Ltd. For example: <ul style="list-style-type: none"> - Viscosity of liquid aliphatic hydrocarbons: alkanes - Thermal conductivity of liquid carboxylic acids - Heat capacity and enthalpy of liquids: aliphatic alcohols - Vapor pressures and critical points of liquids. XIV: aliphatic oxygen-nitrogen compounds 	Information on ESDU and publications can be obtained from: <p style="margin-left: 40px;">ESDU 251-259 Regent Street London W1R 7AD England</p>

Service (CAS) number and synonyms for the name of the chemical substance. Most current on-line data bases and published documents catalog chemical data according to CAS number. This minimizes confusion inherent in storing and retrieving chemical data according to chemical name since most chemicals have more than one name. The CAS number for a chemical substance can be obtained from:

Toxic Substances Control Act Chemical Substances Inventory
Volumes I-IV (Initial Inventory, Cumulative Supplement, User
Guide and Indices to the Initial Inventory, and Trademarks and
Product Names)
U.S. Environmental Protection Agency
Office of Toxic Substances (TS-799)
Washington, DC 20460

Chemical name synonyms are particularly important because consumer product manufacturers frequently list consumer product chemical formulations according to trade or generic chemical names. For example, specific solvents in paints may simply be listed as "cellosolves" or "glycols." A list of specific chemical names and generic names is extremely useful for securing physical-chemical property data and other chemical use data related to consumer products. Many of the on-line data bases and published documents found in Tables 7 and 8 include chemical name synonyms.

2.2.2 Methods for Estimating Physical-Chemical Properties

Methods for estimating physical-chemical properties can also be found in on-line computerized data bases and in the published literature. The on-line methods are those contained in EPA-OTS's Graphical Exposure Modeling System (GEMS). Information on GEMS and inclusive data bases can be obtained from GSC (1983) or by contacting the

Modeling Section
U.S. Environmental Protection Agency
Office of Toxic Substances (TS-798)
Washington, D.C. 20460
(202) 382-2256

Table 9 lists the chemical property estimation systems and methods included in GEMS, as well as published documents that contain additional methods for estimating physical-chemical properties.

2.3 Summary

The functional steps in securing physical-chemical properties for a chemical substance are summarized as follows:

Table 9. Sources of Information for Estimating
Physical-Chemical Properties

Source/methods	Comment
<u>Computerized systems</u>	
<ul style="list-style-type: none"> • Graphical Exposure Modeling System (GEMS) USEPA Office of Toxic Substances Chemical Fate Modeling Team Washington, D.C. 20460 (202) 382-2256 	GEMS User's Guide.
<ul style="list-style-type: none"> (1) CHEMEST <ul style="list-style-type: none"> - Solubility in water - Soil absorption coefficient - Bioconcentration factors for fish - Activity coefficients - Boiling point - Vapor pressure - Rate of volatilization from water - Henry's law constant 	CHEMEST User's Guide (CHEMEST is a computerized version of the procedures listed below in <u>Handbook of Chemical Property Estimation Methods - Environmental Behavior of Organic Compounds.</u>)
<ul style="list-style-type: none"> (2) Molecular Structure File (S File) 	SFILES User's Guide.
<ul style="list-style-type: none"> (3) CLOGP (Log K_{OW} - octanol/water partition coefficient) 	CLOGP User's Guide.
<u>Published documents*</u>	
<ul style="list-style-type: none"> (1) <u>Handbook of Chemical Property Estimation Methods - Environmental Behavior of Organic Compounds</u> <ul style="list-style-type: none"> - Octanol/water partition coefficient - Solubility in water - Solubility in various solvents - Adsorption coefficient for soils and sediments - Bioconcentration factor in aquatic organisms - Acid dissociation constant 	Not recommended for fate of chemicals via hydrolysis and photolysis. See documents listed below.

Table 9. (continued)

Source/methods	Comment
<ul style="list-style-type: none"> - Rate of hydrolysis - Rate of aqueous photolysis - Rate of biodegradation - Atmospheric residence time - Activity coefficient - Boiling point - Heat of vaporization - Vapor pressure - Volatilization from water - Volatilization from soil - Diffusion coefficients in air and water - Flash points of pure substances - Densities of vapors, liquids, and solids - Surface tension - Interfacial tension with water - Liquid viscosity - Heat capacity - Thermal conductivity - Dipole moment - Index of refraction 	
<p>(2) <u>Structure Activity Correlations for Environmental Reactions</u></p>	
<ul style="list-style-type: none"> - Rate of hydrolysis - Rate of photolysis - Rate of oxidation - Rate of volatilization - Absorption to sediment and soils 	
<p>(3) <u>Validation of Estimation Techniques for Predicting Environmental Transformation of Chemicals</u></p>	<p>Supplemental data and update of <u>Structure Activity Correlations for Environmental Reactions</u>.</p>
<ul style="list-style-type: none"> - Oxidation in water - Oxidation in air - Rate of hydrolysis - Metal complexation 	

*Note: Documents listed are those principally used by EPA-OTS. The scientific literature, much of it referenced in the above documents, includes a wealth of background information and methods for estimating physical-chemical properties.

1. Obtain CAS number and compile list of chemical synonyms. Tables 7 and 8 list information sources for obtaining CAS numbers and synonyms.
2. Retrieve or gather experimental data for physical-chemical properties of interest from on-line systems or published documents. Table 7 lists computerized systems, and Table 8 cites published documents from which physical-chemical property data can be obtained.
3. Where experimental data are lacking, estimate required properties according to appropriate methods. Methods and systems for estimating physical-chemical properties are listed in Table 9.
4. Summarize all data in tabular format, and clearly indicate all units of measurement and sources of information including methods used to estimate properties where experimental data were lacking.

Note: For each physical-chemical property of interest, all immediately available data should be gathered. It is possible that different isomers of a chemical substance may have vastly differing property values. Property data may also vary because values were derived under different laboratory conditions or controls; errors in experimental data are also not uncommon. All property values gathered from the experimental literature should be carefully reviewed and any inconsistencies noted. Estimation techniques can be used to help verify or resolve inconsistencies in experimental data.

3

3. PRODUCT-SPECIFIC DATA REQUIRED TO ASSESS EXPOSURE

Prior to estimating the concentration of a chemical substance in an external medium, the assessor should estimate the quantity of the chemical released during use. In general, release of a chemical substance to air from a consumer product can occur by three mechanisms:

1. Direct application to a surface, including skin.
2. Release of a chemical substance from pressurized aerosol products and poured products that aerosolize releasing mists or particulates.
3. Migration through the solid matrix of a consumer product and subsequent volatilization or leaching.

The following sections discuss factors required to estimate the amount of a chemical substance that can be released from a consumer product during an exposure period. Methods for estimating the values of these factors for specific products are also presented in the sections that follow. Section 3.1 presents data for products that are applied as liquid films, while Section 3.2 contains data for aerosol products. Section 3.3 discusses sources that can be used to determine the presence and the amounts of specific chemicals in consumer products. A generic approach for determining weight fractions of specific chemicals in consumer products is also presented in Section 3.3.

3.1 Amount of Chemical Substance Applied Directly to Surfaces

The amount of a chemical substance that is applied to a surface can readily be estimated from the following product-specific data.

1. Surface area to which the consumer product is applied.
2. Surface area that a given amount of the consumer product can cover (material consumption rate).
3. Density of the consumer product.
4. Weight fraction of the chemical substance in the product.
5. Surface area that can be covered by the consumer product in a given amount of time (labor production rate).

Sources of information concerning material consumption rates include product labels and the Estimating Guide - 1982 published by the Painting and Decorating Contractors of America (PDCA 1982). Material consumption rates for a number of generic types of products are also reported in PDCA (1982) and are differentiated according to: (1) method of application (e.g., brush, roller); (2) type of surface to which the generic product is being applied (e.g., plywood, smooth siding, smooth finish plaster, sandfinish plaster, concrete); (3) which coat is being applied (e.g., primer, first coat, second coat, third coat); and (4) type of sheen of the product (e.g., flat finish, semi-gloss, gloss). Table 10 presents material consumption rates in units of square feet per gallon for a number of labor categories as reported in PDCA (1982). Table 11 presents values for densities of selected products in units of grams per cubic centimeter (g/cm^3) based on actual laboratory measurements of specific name-brand products (Versar 1984c). Material consumption rates and densities reported for generic types of products presumably differ very little from material consumption rates and densities for specific name-brand products within a given product group. Values for material consumption rates and densities for specific brands can be used in place of values for generic product types where generic product values are not readily available. The converse situation also applies.

The following example illustrates how surface area covered, material consumption rate, product density, and weight fraction of a chemical substance in a product can be used to determine the mass of a chemical substance applied to a surface.

A table with surface area of 27 square feet is covered with one coat of varnish. Assuming a chemical substance comprises 5 percent by weight of the varnish, what mass of chemical substance is applied to the surface?

Step 1 Divide the surface area covered by the material consumption rate reported in Table 10 to obtain the number of gallons of varnish required to cover the surface of the table.

$$27 \text{ ft}^2 / 600 \text{ ft}^2/\text{gallon} = .045 \text{ gallons}$$

Step 2 Multiply the number of gallons determined in Step 1 by the density of varnish reported in Table 11 and by the factor for the number of cm^3 per gallon to obtain the number of grams of product applied to the surface.

$$0.45 \text{ gallons} \times .879\text{g}/\text{cm}^3 \times 3785 \text{ cm}^3/\text{gallon} = 150 \text{ grams}$$

Table 10. Labor Production and Material Consumption Rates for Coatings Applied to Surfaces by Labor Category and Method of Application

Labor category	Method of application	Labor production rate (ft ² /hr)	Material consumption rate (ft ² /gallon)
Paint doors	Brush	125	400
	Roller	275	400
	Spray	400	300
Paint picture mouldings, chair rails, window frames, and other trim up to 6-inch width	Brush	200	1,000
Paint windows (no frame)	Brush	150	450
Stain	Brush	220	500
Shellac	Brush	200	600
Varnish	Brush	175	600
Lacquer interior trim	Spray	250	275
Lacquer interior doors and cabinets	Spray	275	250
Lacquer interior panelling	Spray	450	250
Remove varnish with liquid remover from a flat surface	--	45	180
Remove paint with liquid remover from a flat surface	--	30	175
Wax and polish floors	--	200	1,080

Table 10. (continued)

Labor category	Method of application	Labor production rate (ft ² /hr)	Material consumption rate (ft ² /gallon)
Apply floor seal to maple and pine	--	400	500
Apply floor seal to oak	--	450	500
Flat finish paint on plywood in a new residence	Roller	350	300
Flat finish paint on smooth siding in a new residence	Roller	325	300
Flat finish paint on smooth finish plaster in a new residence	Brush	245	500
	Roller	325	475
	Spray	500	550
Gloss/semi-gloss paint on smooth finish plaster in a new residence	Brush	260	500
	Roller	350	475
	Spray	550	550
Gloss/semi-gloss paint on sandfinish plaster in a new residence	Brush	150	295
	Roller	275	280
	Spray	400	320
Latex flat finish paint on smooth finish plaster in a new residence	Brush	225	400
	Roller	340	380
	Spray	475	440
Latex flat finish paint on rough finish plaster in a new residence	Brush	175	300
	Roller	265	285
	Spray	475	325

Source: PDCA (1982).

Table 11. Experimentally Determined Density Values for Selected Consumer Products

Product	Density* (g/cm ³)
Minwax wood stain	0.800
Semi-gloss interior latex paint	1.168
Marine spar varnish	0.879
Polyurethane clear satin finish	0.866
Varathane plastic gloss paint	1.084
Anti-rust oil-based enamel paint	0.884
Furniture polish-lemon oil	0.834
Pure shellac	0.896
Gloss black enamel paint	0.903
Latex flat wall paint	1.240
Floor shine cleaner/wax	1.017
Fiberglass resin	1.106
Car wax finish restorer	1.017
Antique oil finish	0.832
High gloss car wax	1.022
Redwood latex stain	1.332
Carpenters wood glue	1.084
Floor deck enamel paint	1.067
Interior acrylic latex wall and trim paint	1.233
White interior ceiling paint	1.182

* At room temperature (~25°C).

Source: Versar (1984c).

Step 3 Multiply the weight fraction of chemical substance in the product by the number of grams of product estimated to be applied to the surface of the table (from step 2) to derive the mass of chemical substance applied to the surface of the table.

$$150 \text{ grams} \times .05 = 7.5 \text{ grams}$$

To assess the amount of a chemical substance to which an individual may be exposed requires knowledge of the amount of a chemical substance that may potentially enter an external medium from liquids or films applied to a surface and of the duration of application of the product. The period of application can be readily estimated from information regarding the rate at which a specific product is applied to a surface. This rate, often referred to as the labor production rate, is reported for a number of labor categories in PDCA (1982). Labor production rates obtained from PDCA are presented in Table 10. Like the material consumption rates shown in this table, the labor production rates are also differentiated according to method of application, type of surface to which the generic product is being applied, which coat is being applied, and type of sheen of the product. Data regarding the time for application of a product is not only useful for estimating the period of active exposure, but is also useful in itself as an input for an algorithm that predicts room air concentrations of a chemical substance under conditions in which the release of the chemical is time-dependent (see Section 4.4.3.).

The following example illustrates how the surface area covered and the labor production rate can be used to estimate the duration of application of a consumer product in the form of a liquid or film applied to a surface.

The walls of a room 8 feet high, 8 feet wide, and 11 feet long (304 square feet) are covered with one coat of a flat finish paint using a roller. Assuming the walls are of smooth siding, how long does it take to apply the first coat?

Divide the value for the surface area of the walls of the room by the labor production rate value from Table 10 reported for the first coat of flat finish paint applied to smooth siding with a roller to obtain the value for duration of application.

$$\frac{304 \text{ ft}^2}{325 \text{ ft}^2/\text{hr}} = .94 \text{ hours}$$

This duration accounts only for roller application. It excludes brush painting of corners, moulding, and trim.

3.2 Amount of a Chemical Substance Released by Use of Aerosol and Pump Spray Products and by Pouring or Spilling Liquids and Powders

Estimation of the amount of a chemical substance released from consumer products that generate aerosols requires knowledge of the weight fraction of chemical substance in the consumer product, the mass of product released during the period of active use or active discharge, and the fraction of product that does not contact its intended target. Guidelines for determining the weight fraction of chemical substance in a consumer product are presented in Section 3.4. Data on the mass of product released during the period of actual discharge are needed for scenarios in which products are discharged for only a few seconds (instantaneously) during each exposure event. Data on the mass of product released during the period of active use, however, are needed for scenarios in which products are discharged for more than a few seconds and for scenarios consisting of more than one active discharge, provided each discharge occurs within short intervals of the other (e.g., on the order of seconds).

Table 12 presents estimated ranges of values for mass of product released per use based on responses received from roughly 40 households as part of an informal survey (Cote et al. 1974). The values shown in Table 12 were derived from information provided on rate and frequency of use by survey respondents. Rates of use were estimated from the numbers and sizes of containers which the respondents reported using over a given period of time. Cote et al. (1974) note that they have less confidence in the value reported for oven cleaner than for other products because oven cleaner is used infrequently and, therefore, the raw data used to derive these estimates were not as plentiful.

Aerosol that does not contact its intended target is referred to as overspray. The amount of overspray that occurs during application is a function of the pressure exerted on the contents of the container and the size of the orifice through which the contents are discharged, the size and shape of the target, and the size of the particles composing the spray. No specific information on values for overspray for aerosol consumer products has been found. Estimates of paint loss, or overspray, during application, however, are available for several methods of application (Gross 1970). These estimates are presented in Table 13. Conventional air spray systems atomize the paint fluid by intersecting jets of compressed air (Gross 1970). Airless or hydraulic spray systems atomize paint by the sudden release of high pressure as the fluid is ejected through a small orifice (Gross 1970). Electrostatic spray systems atomize fluids through the application of high voltage static electricity as the paint flows off a sharp edge or point (Gross 1970).

Table 12. Mass of Aerosol Product Released Per Use

Aerosol product	Mass (grams/use)
Deodorant spray	2.5 - 3.0
Hair spray	7.0 - 9.3
Shaving foam	3.0 - 4.0
Air freshener	7.0 - 14.0
Disinfectant	9.4
Furniture polish	14.0
Dust spray	7.0 - 14.0
Oven cleaner	200 - 250

Source: Cote et al. (1974).

Table 13. Estimates of Overspray During Application

Method of application	Overspray fraction
Conventional air spraying	.20 - .40
Airless spraying	.10 - .20
Electrostatic spraying	.05 - .15

Source: Gross (1970).

Aerosol products used by consumers are discharged in a manner similar to airless spray systems. For reasonable worst case estimates of exposure to aerosol consumer products that are surface sprays (e.g., spray paints), a value of 0.40 for fraction of overspray is suggested. A value of 1.0 for fraction of overspray is suggested for aerosol consumer products that are space sprays (e.g., air fresheners). Additional effort is needed to obtain values for overspray fractions of aerosol consumer products.

A recent study on aerosols formed during free-fall of liquids and powders in static air (Sutter et al. 1982) reported that an average weight fraction of 0.00003 of a "spilled" liquid and 0.00019 of a "spilled" powder can be expected to become airborne in static air when spilled from a height of one meter onto the floor of a room-sized enclosure (Versar 1985). The mass of chemical substance unintentionally released to air from accidental spills of liquids and powders can be estimated by multiplying the value for fraction of material entrained in air by the total mass of powder or liquid spilled and by the weight fraction of chemical substance in the spilled product.

3.3 Identification of Consumer Products and Formulations

A key step in assessing consumer exposure is to identify the products containing the chemical of interest. Identification of the consumer products in which a particular chemical substance will appear directs the exposure analyst to the appropriate exposure routes and relevant generic scenarios necessary to calculate consumer exposure.

A chemical may appear in a consumer product as an ingredient or as a residual (impurity) of the product manufacturing process. Most of the information sources presented in this section deal only with those chemicals intentionally incorporated as an ingredient. Chemicals that occur as impurities in consumer products are not as easily identified through conventional sources; identification of such consumer products will rely heavily on process engineering estimates and qualitative estimates from knowledgeable contacts in the subject industries.

The information sources found most useful for identifying pertinent consumer products are listed below.

- Clinical Toxicology of Commercial Products (CTCP)
- Consumer Product Safety Commission (CPSC) - economic analysis
- Organic Chemical Producers Data Base (USEPA)

- Literature:
 - The Merck Index
 - The Condensed Chemical Dictionary
 - Kirk-Othmer Encyclopedia of Chemical Technology, 3rd edition.
 - The weekly Chemical Marketing Reporter

Once the consumer products are identified, the typical amount of chemical found in each product is determined. This formulation information satisfies the weight percent (WF) parameter used in the exposure calculation (discussed in Section 6). The information sources found most useful in determining product formulations are:

- Clinical Toxicology of Commercial Products (CTCP)
- Consumer Product Safety Commission (CPSC) - CHIP Data Base
- The Chemical Formulary (Chemical Publishing Co.)
- Independent investigation:
 - Related patent literature
 - Industry and trade association contact
 - Spot surveys of products currently on shelf
 - Literature (product- or brand-specific)

Clinical Toxicology of Commercial Products, 4th edition, (Gosselin et al. (1984) Williams and Wilkins Co., Baltimore, MD), is by far the most useful resource with regard to product coverage and detail of product formulations. CTCP is kept up-to-date on a computerized format (available to Chemical Information System, CIS-USEPA, subscribers) and has the advantage of allowing search by chemical constituent, product name, product use, manufacturer, and other criteria.

The Chemical Formulary, by H. Bennett (Chemical Publishing Co., Inc., NY), is a valuable complement to CTCP in the determination of formulations for a variety of consumer products. The 23 volumes of The Chemical Formulary (from 1933 to 1981) represent a vast collection of commercial formulas, which include exact amounts and percentages of constituent chemicals and notes on preparative techniques. Complete or partial sets of volumes are available in select professional and public libraries in the Washington, D.C., area.

The Economics Division of the Consumer Product Safety Commission investigates the occurrence of selected chemicals in consumer products. In its evaluations, CPSC uses many of the same tools mentioned above;

however, it also identifies consumer products and their formulations through economic analyses and CPSC's CHIP data base. The CHIP data base is an in-house, on-line system developed from various resources collected by CPSC. Some of CHIP's components are: (1) CTCP (discussed above); (2) elements from the NIOSH trade name ingredient data base, which contains formulations of industrial, commercial, and consumer products. (This data base is being updated; estimated availability is September 1985.) Existing data are limited and largely out-of-date. Contact is Mr. David Sundin, NIOSH, Cincinnati, Ohio, 513-684-4491); (3) some occupational chemical exposure data (of unknown origin); (4) formulation data for some drugs and cosmetics collected from the FDA; and (5) consumer product formulation data compiled independently by a CPSC contractor (Auerbach) in 1975. After CPSC makes their evaluation for a particular chemical substance (based on its economic analysis, CHIP results, and independent field investigation), the results are kept on file. These files (by chemical) can provide information and data found nowhere else in the literature and are considered a primary resource to this phase of the exposure assessment. Non-proprietary portions of the file for a particular chemical can be retrieved through a freedom of information request to:

The Freedom of Information Officer
Office of the Secretary
Consumer Product Safety Commission
Washington, DC 20207

The remainder of the sources for product identification and formulation are more commonly available data or reference tools that do not provide consumer product or formulation information as their primary function. Such resources are generally used to identify consumer products that may contain the chemical in question. The presence of the chemical may be verified through other resources (usually manufacturers, trade associations, or laboratory analysis).

The availability of information regarding the weight fraction of a specific chemical in a consumer product varies with the chemical and the consumer product, and can also be a function of the time and resources available to the assessor. In some instances, time and resources will not allow an assessor to thoroughly investigate the sources useful in determining formulations for products identified as containing the chemical of interest. In such cases, a generic approach to determining weight fractions of chemical substances in consumer products is suggested. The first step of the generic approach is for the assessor to ascertain the function of the chemical substance in the consumer product for which weight fraction information is being sought. Once the function is known, the assessor can refer to readily available resources for information regarding the weight fraction of the functional component in

the consumer product. An unpublished source of information that includes this type of data is Standard Scenarios for Estimating Exposure to Chemical Substances During Use of Consumer Products (Versar 1986). Tables 14 through 19 present data on weight fractions of general components of six selected consumer products as presented in Versar (1986).

Table 14. List of Functional Components as Weight Fraction in Latex Wall Paint

Functional component	Weight fraction in product	Examples
Binder	.10-.25	Polyvinyl acetate, acrylic, and/or styrene butadiene elastomers
Vehicle		
Thinner	.25-.60 0-.10	Water Vegetable oil; resin
Pigment	.10-.20	Titanium dioxide
Extender pigment/ inert filler	.20-.55	Calcium carbonate; alumino silicate
Coalescing solvent	.002-.02 ^a	Ethers or ether esters of ethylene or propylene glycol
Plasticizer	0-.003 ^a	Adipates; phthalate esters
Freeze-thaw stabilizer	0-.02 ^b	Ethylene and/or propylene glycol
Surfactant	.0004-.002 ^a	Sulfosuccinates
Defoamer	.002-.005 ^a	Aliphatic hydrocarbons and fatty acid ester mixtures
Dispersing/Emulsifying agent	.005-.012 ^a	Carboxylic acid salts; trialkyltin fluoride
Preservative	.0002-.0025 ^a	Sulfones; mercury compounds

^aThe range of values for weight fraction for this functional component were derived from information on formulas reported for latex flat wall paint in JRB (1982).

^bAccording to Gosselin (1984), latex wall paint can contain up to 2 percent ethylene glycol; the specific function(s) of ethylene glycol in latex wall paint was not, however, reported. Schurr (1981) reports that ethylene and propylene glycols are used as freeze-thaw stabilizers and as slow-evaporating solvents. The range reported here is based on the assumption that ethylene glycol is functioning only as a freeze-thaw stabilizer.

Sources: Flick (1982)
Gosselin et al. (1984)
JRB (1982a)
JRB (1983a)
Schurr (1981).

Table 15. List of Functional Components as Weight Fraction in Aerosol Furniture Polish

Functional components	Weight fraction	Examples
Film-forming ingredients	0 - .05	Natural/synthetic waxes
Film-forming ingredients	0 - .04	Silicone oils
Film-forming ingredients	0 - .02	Mineral oils
Emulsifiers	.01 - .03	Surfactants
Solvent	0.0 - .30	Petroleum or synthetic naphthas, aliphatic hydrocarbons
Odor-Forming ingredients	.0005 - .003	Essential oils, perfumes
Preservative	.0005 - .002	Fungicides, bacteriocides
Propellants		
- Compressed gas	.01 - .02	Nitrous oxide
- Compressed liquid	.04 - .15	Hydrocarbons
Carrier	.40 - .90	Water
Refractive index modifier	0 - .05	Natural/synthetic waxes, resins

Sources: Gosselin (1984)
 JRB (1983b)
 Randall and Dwyer (1982).

Table 16. List of Functional Components as Weight Fraction in All-Purpose Liquid Cleaner*

Functional component	Weight fraction in product	Examples
Carrier	Up to .96	Water
Cleaning agent (includes surfactants, detergents, foamants)	.03 - .32	Sodium carbonates, alkyl sulfates
Builder**	Trace - .33	Complex phosphates
Abrasive	.10 - .15	Calcium carbonate
Dispersing agents	.01 - .24	Quaternary ammonium compounds
Emulsifying agents	.01 - .04	Sulfated fats and oils
Wetting agent	.01 - .04	Dialkyl sulfosuccinates
Ammonia	.01	-
Opacifier	.01	-
Fragrance	.01	-
Color agent	Trace - .01	-
Disinfectant/deodorizer	.01 - .07	Pine oil
Stabilizer	Trace	-
Water softener	?	Anti-streaking agent, film reducer

Sources: USEPA (1984); JRB (1982b)

* Best characterized by its use on indoor household surfaces (e.g., countertops, floors, appliances).

** Upgrades cleaning efficiency of surfactants (JRB 1982a).

Table 17. List of Functional Components as Weight Fraction in Motor Oil

Functional components	Weight fraction	Examples
Petroleum lubricating oil or basestock	0.75 - 1.00	Paraffinic, aromatic, and/or alicyclic (naphthenic) components
Dispersant	0.03 - 0.05 ^A	Polymeric succinimides; olefin/P ₂ S ₅ reaction products; polyesters; benzylamides
Detergent	0.025 - 0.05 ^A	Barium sulfonate; calcium sulfonate; magnesium sulfonate; barium phenate; calcium phenate; phenol sulfides; barium phosphonates
Oxidation/corrosion inhibitor	0.01 - 0.02 ^A	Zinc dithiophosphates; barium dithiophosphates; calcium dithiophosphates
Anti-rust agent	0 - 0.10	Amine succinates; alkaline earth sulfonates
Viscosity index improver	0.02 - 0.20 ^A	Methacrylate polymers; acrylate polymers; olefin polymers and copolymers; styrene-butadiene copolymers; polyisobutylenes; poly-alkylstyrenes
Anti-foam agents	0 - trace ^B	Silicone polymers
Pour-point depressants	0 - 0.05	Alkylaromatic polymers; polymethacrylates

Table 17. (Continued)

Functional components	Weight fraction	Examples
Extreme-pressure agents	0 - 0.01	Compounds containing sulfur, chlorine, or phosphorous alone or in combination
Anti-wear additives	0 - 0.01	Fatty acids; esters; ketones; organic chlorine compounds; organic sulfur compounds; organic phosphorus compounds; organic lead compounds

Sources: Booser (1981)
 Wills (1980)
 Gosselin et al. (1984).

^ADave Pavlich, Lubrizol Corporation, (216) 943-4200; personal communication with D. Arrenholz, Versar Inc., May 22, 1986.

^BTrace amounts are considered to be no more than a few ppm.

Table 18. Weight Fractions of Functional Components -
Floor Wax/Polish

Functional component	Weight fraction	Examples
Carrier	0 - 0.88	Water
Cleaning ingredients/ surfactants/emulsifiers	0 - 0.084	Ammonium hydroxide, morpholine, alkyl phenyl ethoxylates, potassium hydroxide, ammonia, diethylaminoethanol
Coalescing agents	0 - 0.04	Glycol ether and derivatives, zinc octoate
Fugitive ligand complex	0 - 0.0029	Zinc octoate
Film-forming ingredients	0.05 - 0.96	Acrylic copolymer, styrene copolymer, natural and synthetic resins, waxes, tall oil fatty acid, polyethylene emulsion
Minimum film-forming temperature (MFT) modifier	0 - 0.0703	Glycol ether and derivatives, plasticizers, ethylene glycol, tall oil fatty acid, dibutyl phthalate, tributoxyethyl phosphate
Preservatives	0 - 0.0032	Phenyl mercuric acetate, sodium metabisulfite
Refractive index modifier	0 - 0.39	Resins, waxes
Solvents	0 - 1.0	Mineral spirits, diethylene glycol monoethyl ether, diethylene glycol monomethyl ether, petroleum distillate
Viscosity modifiers	0 - 0.19	Resins
Colorant	0 - trace	

Source: Gosselin et al. (1984), Flick (1984), JRB (1983b).

Table 19. Functional Components as Weight Fraction in Vinyl Upholstery Cleaners

Functional Component	Weight fraction	Examples
Carrier	0.67 - 0.84	Water, Isopropyl alcohol
Cleaning agent	0 - 0.002	Nitrous acid, sodium salt (corrosive inhibitor); Soaps
Coalescing agents	0.05 - 0.053	Diethylene glycol monoethyl ether; Dimethyl polysiloxane fluid; 2-butoxyethanol; Polyethylene, Mono (p-(1,1,3,3-tetramethyl-butyl) phenyl) ether glycols; Propylene glycol methyl ethers; Polyglycol ether.
Film forming ingredients	0 - >0.02	Carboxyvinyl polymer, Fatty acid.
MFT Modifier	0.05 - <0.06	Diethylene glycol monoethyl ether; Fatty acid; Triethanolamine; 2-butoxyethanol; Polyethylene, mono (p-(1,1,3,3-tetramethyl-butyl) phenyl) ether glycols; Propylene glycol methyl ether; Polyglycol ether.
Odor forming ingredients	0 - 0.01	Amyl acetate, Lemon perfume oil, Perfume.
Propellant	0 - 0.08	Propane, Isobutane
Solvent	0.04 - 0.19	Odorless mineral spirits; Isopropyl alcohol; Amyl acetate.
Surfactants	0 - 0.10	Nonionic surfactant; Nonionic nonyl phenoxypoly (ethyleneoxy) ethanol surfactant; Polyoxyethylene alcohol surfactant; Triethanolamine.

Sources: Battelle (1977); JRB (1983b); Gosselin et al. (1984); CIS (1986).

4

METHODS FOR ESTIMATING RELEASE OF CHEMICAL SUBSTANCES FROM CONSUMER PRODUCTS AND CONCENTRATIONS OF CHEMICAL SUBSTANCES IN INDOOR AIR

Calculation of exposure to a chemical substance released from a consumer product is best accomplished by the use of monitoring data for the chemical in the exposure setting and media of concern. Monitoring data, however, are generally limited, if available at all. Assessment of consumer exposure, therefore, must often rely upon the use of methods to estimate releases of chemical substances from consumer products and the resulting concentrations to which consumers are exposed.

The purpose of this section is to briefly review methods that can be used to estimate the release rate of chemical substances to air and the resultant concentrations to which a consumer may be exposed. A detailed review is outside the scope of this report, as such information can be obtained from the numerous technical documents on the subject in the scientific literature. A considerable portion of the available information has already been surveyed and evaluated in two companion volumes. Both are part of this series, Methods for Assessing Exposure to Chemical Substances. The two related volumes are the following:

- Methods for Estimating Concentrations of Chemicals in Indoor Air. Volume 12. EPA 560/5-85-016 (Versar 1984b).
- Methods for Estimating the Migration of Chemical Substances from Solid Matrices. Volume 11. EPA 560/5-85-015 (Schwope et al. 1985).

Much of the information included in this section has been extracted from the above documents. The investigator, therefore, should refer directly to them for detailed information. An overview of mechanisms of chemical release and factors affecting concentrations to which consumers are exposed is presented in Section 4.1. A brief review of relevant consumer environment monitoring data is presented in Section 4.2. Section 4.3 describes methods for estimating release rates of chemical substances from consumer products. Methods for estimating concentrations to which consumers are exposed are cited in Section 4.4.

4.1 Overview of Mechanisms of Chemical Release and Factors Affecting Concentrations to Which Consumers Are Exposed

Releases of chemical substances from consumer products involve many physical and chemical mass transfer mechanisms. They can be collectively grouped as follows:

- Instantaneous releases - generally short-term or momentary release of a chemical substance to an exposure medium. An example of an

R800

*Modeling
SCIES, M.C.M.
Mass balance*

*AA Modeling
AB Model Estimate
Unit mass emission*



instantaneous release is a single discharge of the contents of a pressurized aerosol product for a period of a few seconds or less.

- Continuous releases - generally long-term releases of a chemical substance from a consumer product to an exposure medium. An example of a continuous release is the discharge of the contents of a pressurized aerosol product several times, where the intervals of time between the discharge are on the order of a few seconds.
- Time-dependent releases - generally long-term volatilization of a chemical substance from a consumer product applied to a surface. The time required to apply the product to the surface is more than a few minutes. Therefore, the rate of application of the product to the surface affects the total mass of chemical substance available for release from a given area of surface at any point in time during exposure. An example of a time-dependent release is the volatilization of a chemical substance from a film or coating applied to a surface at a constant rate, where the period of application is more than a couple of minutes.

Mechanisms included in each of these groups are discussed in Section 4.1.1. Factors affecting dispersal of a chemical in an exposure medium and the resulting exposure concentrations are reviewed in Section 4.1.2.

4.1.1 Chemical Release Mechanisms

Release or mass transfer of a chemical from a consumer product can be thought of as the migration of the chemical in a mixture, either within the same phase (e.g., dispersion of a vapor in air), or from phase to phase (e.g., liquid to gas). The chemical in the consumer product may be either a direct additive or a residual contaminant. Mass transfer occurs by diffusion, where the driving force is based on the phenomenon that systems not in equilibrium will tend to move toward equilibrium. There are actually two types of diffusion processes: molecular diffusion and eddy diffusion. In both cases, diffusion occurs as a result of a concentration gradient; however, in eddy diffusion, the mass transfer is greatly aided by the dynamic characteristics of air turbulence (Welty et al. 1976).

Models describing mass transfer and concentration changes in the consumer environment are based on a number of simple physical laws. These include Dalton's Law, Raoult's Law, Henry's Law, Graham's Law, the Ideal Gas Law, and Fick's Law. A general knowledge of these laws helps the investigator to fully understand chemical release processes and models. A review of these laws is presented in Volume 12 and Volume 11 of Methods for Assessing Exposure to Chemical Substances.

Instantaneous chemical releases to air include aerosolization and dust entrainment or suspension. Examples of each process include the spraying (e.g., either pressurized or by pump) of a cleaner in the home and the air suspension of soap powders poured from a container. A brief description of each is as follows:

- Aerosolization: Aerosols are particles or droplets, ranging in size from about 0.15 to 5 microns, which are suspended or dispersed in a gaseous medium such as air (Sciarra and Stoller 1974). The phenomenon of aerosolization is related to the expenditure of energy for the propulsion or agitation of a liquid. Movement of the aerosol is initially controlled by the expenditure of energy, and thereafter, by the processes of molecular and eddy diffusion, depending upon the aerosol size.
- Entrainment: The suspension and movement of particulates are also controlled by energy (i.e., energy of agitation and/or dynamics of air flow); the aerodynamic behavior of particles is determined by particle size, shape, and density. The size, shape, and density of the particulate affects settling by dictating the extent to which gravity pulls the particle.

Continuous and time-dependent chemical releases may involve the mass transfer of a chemical substance across phase boundaries. Processes relevant to consumer exposure include volatilization of chemical substances to air from liquids or solids and leaching from solids to liquids. Migration via molecular diffusion controls the rate of movement of a chemical to a phase boundary. (The term migration is used here only to describe the movement of a chemical within a solid (e.g., a polymer).) Following is a brief review of the processes of volatilization, leaching, and migration:

- Volatilization - The process by which a chemical transfers into the vapor phase from a solid or liquid. Examples include the release of constituents from paints, cleaning solutions, and plastic materials.
- Leaching - This term will be used to refer to the release of a chemical from a solid to a liquid, for example, the leaching of chemicals from food containers (e.g., plastic, cardboard) to the enclosed food. Leaching rates are controlled by the migration of the chemical to the surface of the solid and the solubilities of the chemical in the two media.
- Migration - This term will be used to refer to the movement of a chemical within a solid matrix to the surface of a solid. For consumer products, this process is generally only considered for the movement of relatively low molecular weight substances from

polymers (e.g., plastic and elastomeric materials). Molecular diffusion usually controls the rate of migration. The diffusion rate of a compound is affected by the size of the molecule, the structure and characteristics of the surrounding matrix, and the attractive forces of the matrix constituents. The migration phenomenon within polymer matrices is described in detail in Volume 11 of Methods for Assessing Exposure to Chemical Substances.

Models or algorithms and required input parameters for estimating the above types of mass transfer rates are reviewed in Section 4.3.

4.1.2 Factors Affecting Exposure Concentrations

Once a chemical is released into a medium (e.g., air, water) or to a surface to which exposure may occur, a number of environmental factors affect the concentration of the chemical in the media or on the surface. These factors include the medium volume, surface area, room ventilation rate, and mixing factor. Each of these is briefly described below:

- Volume - This refers to the amount of air or liquid into which the chemical is released. For chemicals emitted to air, this generally refers to the room volume.
- Surface Area - This factor is included in scenarios where coatings are applied, spilled, or sprayed onto surfaces. A quantitative value for the area of a surface covered by a consumer product is needed to estimate several parameters required to assess exposure. These include duration of application of a consumer product in the form of a film or coating applied to a surface, mass of chemical substance applied to a surface, and release rates for volatile chemical substances (e.g., solvents) in films or coatings applied to surfaces. As the area of surface covered by a film or coating increases, the mass of chemical substance on the surface increases, the amount of chemical substance released to air from the film or coating on the surface increases, and the resulting concentration of the chemical substance in air increases.
- Ventilation Rate - Air ventilation effectively reduces the concentration of a chemical substance released to indoor air by diluting the chemical. The ventilation rate, therefore, is important for calculating concentrations of chemicals in indoor air. This is usually expressed in terms of an air exchange rate, which is defined as the rate at which indoor air is replaced by outdoor air. Generic ventilation rates for various building types or rooms are discussed in Section 4.4. Ventilation rates are also discussed in Volume 12 of Methods for Assessing Exposure to Chemical Substances.

- Mixing Factor - The mixing factor, m, is an empirical number that accounts for room-specific effects on transport of chemical substances (Repace and Lowrey 1980). Removal of chemical substances is more rapid in a well-mixed atmosphere than in a poorly mixed, stable one. Factors that affect the mixing factor include type and placement of ventilation grills, ventilation flow rates, inhomogeneous distribution of a chemical substance in a room, physical barriers, circulation fans, and room traffic (Repace and Lowrey 1980). A mixing factor of 1 means that the room has ideal, perfect mixing. Actual values usually range from 1/2 to 1/10 (Repace and Lowrey 1980).

Models or algorithms including required input parameters and generic data for calculating exposure concentrations are discussed in Section 4.4.

4.2 Monitoring Data

The most accurate method of estimating exposure to a chemical substance is via the use of monitoring data for the chemical in the media of concern throughout the duration of exposure. Initial efforts in a consumer exposure assessment, therefore, should focus on gathering all available monitoring data, including the following:

- Indoor air concentrations
- Surface concentrations
- Concentrations in consumer products of contaminants of interest.

Currently, there is no automated data base or repository for any of these types of data. However, indoor air data have been found in independent scientific studies through a computer search of the scientific literature (e.g., chemical abstracts, NTIS holdings, and other bibliographic files such as those in the DIALOG Information Retrieval Service).

The Department of Energy and the CPSC sponsored a successful pilot research study of selected indoor air pollutants from which development of a more extensive data base is planned. Studies included monitoring of highly volatile organics such as benzene, halogenated hydrocarbons, other chemicals released from plastics and resins, and data on environmental factors, such as air exchange rate, temperature, and humidity of indoor environments sampled. In general, however, assessment of exposure to chemicals in consumer products must rely primarily upon the estimation procedures, models, or algorithms discussed below.

4.3 Methods to Estimate Release of Chemical Substances from Consumer Products

The release rate is a key parameter required to estimate the concentration of a chemical substance in an exposure medium as a result

of a continuous or time-dependent release. The factors that determine the release rate of a chemical substance from a product vary depending upon whether the release is continuous or time-dependent. These factors also differ for releases of chemical substances from (1) pressurized aerosol products; (2) liquid films on surfaces; and (3) bulk liquids and solids. More than one mechanism of release may be applicable for a given consumer product. For example, to account for all the release mechanisms occurring as a result of spray painting the walls of a room, one must consider (1) the rate at which the chemical substance is being discharged from the container; (2) the rate at which the chemical substance volatilizes from the liquid paint film applied to the surface of the wall; and (3) the rate at which the chemical substance migrates through the film that forms once the paint has dried.

4.3.1 Release Rate of Chemical Substances in Aerosol Consumer Products

This method is recommended for estimating the continuous release rate of the contents of a pressurized aerosol container to air. The continuous release can consist of one continuous discharge of the contents of a pressurized container or many discharges of the contents during the period of active use, provided the discharges occur within short intervals of one another (i.e., on the order of seconds). The following equation is used to estimate the release rate of a chemical substance from a pressurized aerosol product.

$$G = \frac{WF \times M \times OV}{DD} \quad (4-1)$$

where

- WF = weight fraction of chemical substance in product (unitless)
- G = release rate of chemical substance (mass/hr)
- M = mass of product discharged during active use (units of mass)
- OV = fraction of product that is overspray and does not contact intended target (unitless)
- DD = duration of active discharge of the pressurized aerosol product (hours).

General guidelines for estimating the parameters of equation (4-1) are presented in Section 3 of this volume.

If the product is designed to be released into air rather than directed at a surface, the entire mass of product released may be considered overspray, and the value for OV may be set equal to one. Products of this type include aerosol air fresheners, pesticide space fumigants, and solid room deodorizers.

If the contents of the pressurized aerosol product are applied to a surface, release of a chemical substance in the product will occur via two pathways: direct discharge to air with the contents of the aerosol container and evaporation of the material deposited on the surface. Much of the overspray from direct discharge will be deposited on unintended surfaces. The overspray, or portion of material that misses the intended target, is the maximum amount of product that can be discharged directly to air. Equation (4-1) is recommended only for estimating the continuous release rate of a chemical substance via direct discharge to air. The method for estimating the rate at which the chemical substance evaporates from the material deposited on the surface is presented in the section that follows.

4.3.2 Release Rate of Chemical Substances from Liquid Films Applied to Surfaces

(1) Assumptions. The equations required to estimate the rate of release of a chemical substance from a liquid film applied to a surface differ for continuous and time-dependent releases. Rate of release will be considered continuous if the liquid is instantaneously sprayed or spilled onto the surface; otherwise, the release will be time-dependent so that the rate at which the film is applied and the change in mass of the chemical substance released from the surface with time as the film is being applied are taken into account. For practical applications, it is best to consider the release rate to be continuous if the liquid film is instantaneously spilled or sprayed onto a surface or if the time required to cover the surface with the liquid film is less than a few minutes. If the time required to cover the surface with the liquid film is more than a few minutes, it is best to consider the rate of release to be time-dependent.

The difference between the continuous release rate and the time-dependent release rate is as follows. For a scenario in which the release rate is continuous, the amount of chemical substance remaining on the surface is the same for each unit of area at any given point in time. For a scenario in which the release rate is time-dependent, however, the amount of chemical substance remaining on the surface is different for each unit of area at any given point in time. The difference between these two scenarios is the rate at which the film is applied to the surface. For a scenario in which the release rate is continuous, the film is instantaneously applied to the surface. Therefore, the rate at which the film is applied is not a parameter of concern. For a scenario in which the release rate is time-dependent, however, the rate at which the film containing the volatile chemical substance is applied affects the total mass of chemical substance available for release from a given area at any point in time.

The following example illustrates the concept of a time-dependent release. An individual paints a board that has a surface area of five

square feet. The paint that is ultimately applied to the board contains five grams of a volatile chemical substance distributed evenly throughout the paint applied to the board. In other words, the surface of the board will be coated with one gram of the chemical substance for every square foot of board. Assume that the time required for the chemical substance to evaporate from the surface once it is applied is five minutes. Further assume that the individual paints the board at a constant rate of one square foot per minute. Therefore, the time required to apply the paint to the board is five minutes. Figure 1 depicts the mass of volatile chemical substance remaining on the surface for each square foot of board as a function of time. Values for the cumulative mass of chemical substance applied, the cumulative mass remaining on the surface of the board, and the cumulative mass released to air are also presented for each minute after painting is initiated. Values for the mass released to air during each minute are shown as well.

It must be noted that, for this illustration, instantaneous application of coating to a surface area of one square foot was assumed at each minute during application. In theory, each square foot could be divided into any number of units and could be analyzed in the same way as the five square foot board used in this example. The foundation of the time-dependent release is the assumption of instantaneous application of coating to some fixed area of the total surface and initiation of chemical release at a constant rate at the instant the application is completed. The accuracy of values predicted for the mass remaining and for the mass released using the time-dependent release rate increases with decreasing size of area assumed to be instantaneously coated. For the purpose of assessing consumer exposure to chemical substances volatilizing from coatings applied to surfaces, the surface area determined to be painted in one minute can probably be assumed to be coated instantaneously.

(2) Equations. The following equation is used to estimate the release rate of a chemical substance for those scenarios in which the assumption of a continuous rate of release is applicable.

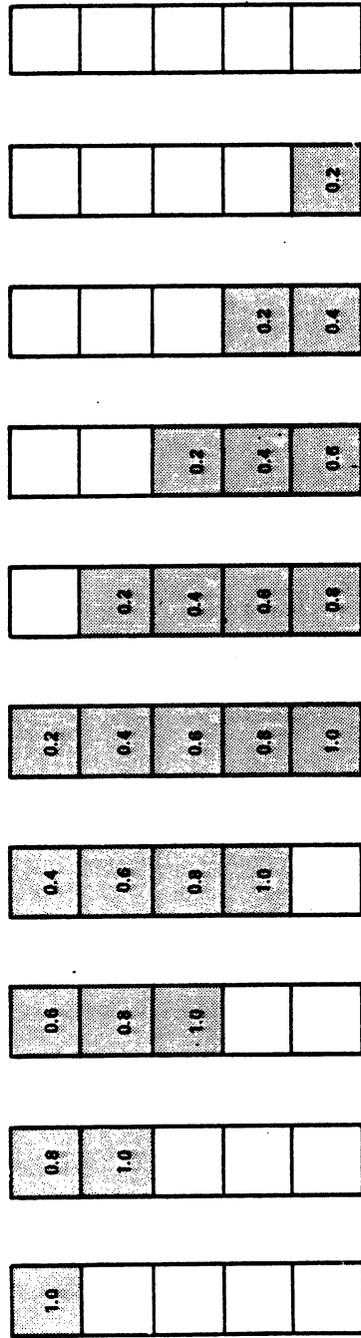
$$G = N \times SA \times MW \times 3600 \quad (4-2)$$

where

- G = release rate of chemical substance (grams/hr)
- N = molar flux of pure chemical substance (mole/cm²-sec)
- SA = surface area covered by liquid film (cm²)
- MW = molecular weight of chemical substance (g/mole).

Equation (4-5) is used to estimate the release rate of a chemical substance for those scenarios in which the assumption of a time-dependent

TIME - DEPENDENT RELEASE



TIME ELAPSED AFTER PAINTING IS INITIATED (MINUTES)	1	2	3	4	5	6	7	8	9	10
CUMULATIVE MASS APPLIED (GRAMS)	1.0	2.0	3.0	4.0	5.0					
CUMULATIVE MASS REMAINING ON SURFACE (GRAMS)	1.0	1.8	2.4	2.8	3.0	2.0	1.2	0.6	0.2	0
CUMULATIVE MASS RELEASED TO AIR (GRAMS)	0.0	0.2	0.6	1.2	2.0	3.0	3.8	4.4	4.8	5.0
MASS RELEASED TO AIR DURING EACH MINUTE (GRAMS)		0.2	0.4	0.6	0.8	1.0	0.8	0.6	0.4	0.2

 - SHADED BLOCK DENOTES VOLATILE SUBSTANCE REMAINING ON SURFACE

FIGURE 1. MASS OF VOLATILE CHEMICAL SUBSTANCE REMAINING ON SURFACE OF EACH SQUARE FOOT OF BOARD AS A FUNCTION OF TIME

rate of release is applicable. Equation (4-5) is the product of equations (4-3) and (4-4).

$$G_N = N \times MW \times 3600 \quad (4-3)$$

where

$$G_N = \text{Mass flux (g/cm}^2\text{-hr)}.$$

Equation (4-4) is as follows:

$$A_R = \frac{SA}{t_a} \quad (4-4)$$

where

A_R = rate of application of film to the surface (cm²/hr)

SA = surface area covered (cm²)

t_a = duration of application (hours).

The resulting equation, (4-5), is expressed below:

$$G_{NAR} = N \times MW \times 3600 \times (SA/t_a) \quad (4-5)$$

where

G_{NAR} = time-dependent release rate (g/hr²)

and the other variables in equation (4-5) are as defined previously.

The rate is expressed in units of mass/hr² because the mass released is changing with time. When this release rate is used in equations to calculate indoor air concentrations resulting from a time-dependent release situation, the resulting units of concentration are expressed in the correct units (e.g., mass/volume).

Both the continuous and time-dependent release rates are a function of the rate or molar flux of diffusion of a chemical substance, N , expressed in moles/time-area. This rate is essentially the average flow of the diffusing molecules per unit area (during diffusion) per unit time. It depends not only on the concentration gradient, but also on the characteristics of the diffusing compounds and on environmental parameters (temperature, pressure, etc.). The following equation is used to calculate the molar flux of a chemical substance.

$$N = \frac{-P \times D_{AB} \times (P_{B2} - P_{B1})}{L \times R \times T \times (P_A)_{lm}} \quad (4-6)$$

where

- N = molar flux (mole/cm²-sec)
- P = atmospheric pressure (atm)
- D_{AB} = diffusion coefficient of chemical substance in air at 25°C and 1 atmosphere (cm²/sec)
- P_{B1} = partial pressure of chemical substance at interface of liquid and gas film (atm)
- P_{B2} = partial pressure of chemical substance at interface of gas film and main air stream (atm)
- L = gas film thickness (cm); (A value of 2.54 cm or 1 inch can be assumed if no other information is available.)
- R = gas constant, 82.05 atm-cm³/mole-°K
- T = temperature (°K); (A value of 298°K or 25°C is usually assumed to represent ambient conditions.).

Equation (4-7) is used to calculate the parameter, $(P_A)_{lm}$, in equation (4-6).

$$(P_A)_{lm} = \frac{P_{A2} - P_{A1}}{\ln(P_{A2}/P_{A1})} \quad (4-7)$$

where

- P_{A2} = partial pressure of air at interface of gas film and main air stream (atm)
- P_{A1} = partial pressure of air at interface of liquid and gas film (atm).

The variables P_{A1}, P_{A2}, P_{B1}, and P_{B2} must be determined prior to calculating $(P_A)_{lm}$ and N. The partial pressures of a two-component system form an integral part of the molar flux calculations. In computing the partial pressures, one has to consider the two interfaces involved in the diffusion process. Diffusion is controlled by the concentration gradient of B in a stagnant gas film on the surface of the liquid film. Considering the liquid and air as the two components of a system, the interfaces could be defined as (1) the interface between the liquid and the gas film and (2) interface between the gas film and the main air stream (Versar 1984b). A value of 1 atm can be assumed for P_{A2}. The value of P_{B2}, usually assumed to be zero, is calculated as follows:

$$P_{B2} = 1 - P_{A2} \quad (4-8)$$

where these variables are as previously defined. The value of P_{A1} is calculated as follows:

$$P_{A1} = 1 - P_{B1} \quad (4-9)$$

where these variables are as previously defined.

The following equation is used to calculate P_{B1} .

$$P_{B1} = \frac{VP}{P} \quad (4-10)$$

where

- VP = the vapor pressure of the chemical substance at the desired room temperature (mm Hg)
- P = atmospheric pressure at the desired altitude (mm Hg); (e.g., P = 760 mm Hg at sea level).

The values R and T are as defined previously.

To calculate the molar flux, N, a value for the diffusion coefficient, D_{AB} , of the chemical substance in air under the appropriate environmental conditions must be obtained. Use of experimentally determined values is preferred if they are available for the chemical substance being examined under the specific environmental conditions under which exposure is occurring. In the absence of such data, the Fuller, Schettler, and Giddings (FSG) method or the Wilke and Lee (WL) method can be used to estimate the diffusion coefficients (Lyman et al. 1982). The FSG method is reportedly applicable to nonpolar gases at low to moderate temperatures, and the WL method is applicable to a wide range of compounds over a fairly wide temperature range. The WL method, presented here, is preferred because the average number of errors obtained with this method is considerably less than obtained with the FSG method.

$$D_{AB} = \frac{\left(0.00217 - 0.00050 \sqrt{1/M_A + 1/M_B}\right) T^{3/2} \sqrt{1/M_A + 1/M_B}}{P \sigma_{AB}^2 \Omega} \quad (4-11)$$

where

- D_{AB} = diffusion coefficient (cm²/sec)
- T = absolute temperature (°K)
- M_A, M_B = molecular weight of air and chemical substance, respectively
- P = absolute pressure (atm).
- σ_{AB} = characteristic length, Å (Angstrom units)
- Ω = collision integral.

The collision integral, Ω , is a function of the molecular energy of attraction, ϵ , and the Boltzmann Constant, k_B , as given below:

$$\Omega = \frac{a}{(T^*)^b} + \frac{c}{\exp(T^*d)} + \frac{e}{\exp(T^*f)} + \frac{g}{\exp(T^*h)} \quad (4-12)$$

where

the values a-h are as given in Chapter 17, Lyman et al. (1982), and

$$T^* = \frac{T}{\sqrt{(\epsilon/k_B)_A (\epsilon/k_B)_B}} \quad (4-13)$$

Values of ϵ/k_B are given in Treybal (1968) for some of the more common gases. Values for other gases can be approximated using the following formula (Lyman et al. 1982):

$$\epsilon/k_B = 1.15T_b \quad (4-14)$$

where

T_b = normal boiling point ($^{\circ}$ K).

The characteristic length, σ_{AB} , can be calculated using the following relationship:

$$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} \quad (4-15)$$

where

$$\sigma_A = 3.711 \text{ \AA} \quad (\text{angstrom units})$$

$$\sigma_B = 1.18V'_B{}^{1/3} \quad (4-16)$$

V'_B = molar volume of the chemical substance at its normal boiling point (cm^3/mole). (See Treybal (1968) or Lyman et al. (1982) for atomic and molecular volumes.)

Fuller, Schettler, and Giddings (FSG) (1966) present a simplified approach for calculating the diffusion coefficient, D_{AB} . The method is applicable for nonpolar gases in air at low to moderate temperatures:

$$D_{AB} = \frac{10^{-3} T^{1.75} \sqrt{M_r}}{P (V_A^{1/3} + V_B^{1/3})} \quad (4-17)$$

where

D_{AB} = diffusion coefficient in air
 $M_r = (M_A + M_B)/M_{AMB}$
 M_A = molecular weight of air; (28.979 g/mole)
 M_B = molecular weight of chemical substance
 T = temperature ($^{\circ}K$)
 V_A = molar volume of air; (20.1 cm^3 /mole)
 V_B = molar volume of chemical substance
 P = pressure (atm).

Both the WL and the FSG methods are subject to errors of from 5 to 15 percent when used for the applicable situations indicated above. Experimentally determined diffusion coefficients for selected organic chemical substances in air are presented in Table 20.

The method presented in this section for calculating molar flux and resulting release rate of a chemical substance does not account for the effect of absorption of a chemical substance into surfaces onto which the coating is applied. In addition, the effect of humidity, a factor which may be especially important in determining the rate of release of chemical substances from water-based paints, is not considered in this method. Still another factor not taken into account is the effect on release rate that results from the gradual transition from a wet to a dry film.

Most of the factors not taken into consideration with this method for calculating molar flux and resulting release rate of a chemical substance are expected to tend to decrease the release rate of the chemical substance. Consequently, use of this method in equations for calculating concentrations of chemical substances to which consumers are expected to be exposed will, under most circumstances, result in overestimation of consumer exposure.

(3) Correction Factor for Mixtures. It must be noted that the method for estimating the rate of release of a chemical substance from a liquid film assumes that the film from which the chemical substance is being released behaves as an ideal solution. To behave as an ideal solution, the film must consist of only the pure chemical substance or a combination of chemical substances that have similar molecular sizes and structures. Most liquid films, however, are a mixture of a number of different solvents, resins, and pigments having a vast range of molecular sizes and structures and, therefore, do not behave as ideal solutions. In a non-ideal mixture, an individual volatile chemical substance will

Table 20. Diffusion Coefficients (@ 25°C and 1 atm)
for Selected Organic Chemicals in Air

Chemical	Molecular weight	Diffusion coefficient (cm ² /sec)
Hexane	86.17	0.0732
Benzene	78.11	0.0932
Toluene	92.13	0.0849
Benzyl alcohol	108.13	0.0712
Chlorobenzene	112.56	0.0747
Nitrobenzene	123.11	0.0721
Benzyl chloride	126.58	0.0713
o-Chlorotoluene	126.58	0.0688
m-Chlorotoluene	126.58	0.0645
p-Chlorotoluene	126.58	0.0621
Diethyl phthalate	222.23	0.0497
Dibutyl phthalate	278.34	0.0421
Diisooctyl phthalate	390.56	0.0377
Chloroform	119.39	0.0888
Carbon tetrachloride	153.84	0.0828
1,1-Dichloroethane	98.97	0.0919
1,2-Dichloroethane	98.97	0.0907
1,1-Dichloroethylene	96.95	0.1144
Vinyl chloride	62.50	0.1225
1,1,1-Trichloroethane	133.42	0.0794
1,1,2-Trichloroethane	133.42	0.0792
1,1,2,2-Tetrachloroethane	167.86	0.0722
Trichloroethylene	131.40	0.0875
Tetrachloroethylene	165.85	0.0797
Pentachloroethane	202.31	0.0673
Hexachlorobenzene	284.80	0.12

Source: Schwope et al. (1985).

exhibit a rate of evaporation different from that which it exhibits in the pure state.

To adjust the release rate of the pure chemical to account for non-ideal behavior as a result of interactions among mixture components and to account for the effects of dilution of the mixture in water or other solvents, the release rate of the pure chemical must be multiplied by a correction factor. The correction factor can be, in order of preference, the activity coefficient, the mole fraction, or the weight fraction of the chemical in the mixture from which it is evaporating.

Methods for estimating activity coefficients for two-component systems are presented in the Handbook of Chemical Property Estimation Methods (Lyman et al. 1982). Although the activity coefficient is the most accurate correction factor, the detailed data required regarding components of the mixture and the length of time required to complete the calculations are major disadvantages. The weight fraction of each component of the mixture must be known. In addition, the activity coefficient for each component with each of the other components of the mixture must be obtained.

A simpler approach for obtaining the correction factor is to use the mole fraction of the chemical in the mixture as a substitute for the activity coefficient. The mole fraction, although less accurate than the activity coefficient as a correction factor, is easier to calculate. To calculate the mole fraction, the weight fraction and the molecular weight of each component of the mixture must be known.

In the absence of data on the weight fraction and/or molecular weight of each component of a mixture, it is suggested that the weight fraction of the chemical substance in the mixture be used as a correction factor. Use of the weight fraction as a correction factor provides the lowest degree of accuracy of the three variables suggested. The major advantage, however, is the ease with which a value for correction factor can be obtained.

4.3.3 Chemical Release from Bulk Liquids and Solids

This method can be used to calculate release rates of chemical substances migrating through bulk liquids and solids. Applicable scenarios include dermal contact with solid objects, contaminant release from containers to food or liquids intended for consumption, release from open containers of bulk liquids to air, and release from dry coatings and solid objects to air.

The optimal way to determine the diffusion coefficient of a migrant in a liquid or solid is experimentation. Schwope et al. (1985) present experimentally determined diffusion coefficients for the diffusion of

migrants through selected polymers as a function of the molecular weight of the migrant. The diffusion coefficient through a specific polymer can vary by several orders of magnitude depending on the molecular weight of the migrant. The values of these diffusion coefficients range from 10^{-7} to 10^{-4} cm^2/sec for migrant in silicone rubber, the most flexible material discussed in Schwope et al. (1985), and from 10^{-17} to 10^{-7} cm^2/sec for migrant in unplasticized PVC, the most rigid material discussed in this study. By comparison, the corresponding diffusion coefficients through air range from 10^{-2} cm^2/sec to 10^{-1} cm^2/sec (Schwope et al. 1985). Diffusion through the polymer is usually the rate controlling step for migrant release.

Experimental data are not available for most migrant/polymer pairs. Schwope et al. (1985) present an empirical approach to estimating the diffusion coefficient of a migrant through a polymer, knowing only the molecular weight of the migrant and the general type of polymer involved.

Diffusion coefficients for migrants in a water solution can be estimated by the Wilke-Chang method (Reid et al. 1977) using the following equation:

$$D_w = (7.4 \times 10^{-8} (\phi M)^{1/2} T) / n_w V_B^{0.6} \quad (4-18)$$

where

- ϕ = solution association constant (2.26)
- M = molecular weight of migrant
- T = temperature ($^{\circ}\text{K}$)
- n_w = viscosity of water in cp (1.002 at 20°C and 0.8904 at 25°C)
- V_B = molar volume of migrant at boiling point ($\text{cm}^3/\text{g-mole}$).

At 20°C , diffusion coefficients for inorganic and organic migrants in water typically range from 0.4×10^{-5} to 5×10^{-5} cm^2/sec . A listing of experimentally determined diffusion coefficients for selected migrants in water is presented in Table 21.

Schwope et al. (1985) have developed a method for estimating the fraction of total migrants released over a given time period when diffusion through a polymer is the rate controlling step. The most simplified version of the method is shown here; it assumes that the external phase is well mixed and that it provides no resistance to migrant release from the polymer. The method requires calculating two dimensionless parameters, ψ and α , using equations (4-19) and (4-20), respectively.

$$\psi = Dt/L^2 \quad (4-19)$$

Table 21. Diffusion Coefficients in Aqueous Solutions at Infinite Dilution

Chemical	Temperature (°C)	Diffusion coefficient in water ($\times 10^{-5}$) (cm^2/s)
Hydrogen	25	4.8
Oxygen	25	2.41
	29.6	3.49
Nitrogen	29.6	3.47
Nitrous oxide	25	2.67
Carbon dioxide	25	2.00
Ammonia	12	1.64
Methane	2	0.85
	20	1.49
	60	3.55
n-Butane	4	0.50
	20	0.89
	60	2.51
Propylene	25	1.44
Methylcyclopentane	2	0.48
	10	0.59
	20	0.85
	60	1.92
Benzene	2	0.58
	10	0.75
	20	1.02
	60	2.55
Ethylbenzene	2	0.44
	10	0.61
	20	0.81
	60	1.95
Methyl alcohol	15	1.26
Ethyl alcohol	10	0.84
	15	1.00
	25	1.24

Table 21. (continued)

Chemical	Temperature (°C)	Diffusion coefficient in water ($\times 10^{-5}$) (cm^2/s)
n-Propyl alcohol	15	0.87
Isoamyl alcohol	15	0.69
Allyl alcohol	15	0.90
Benzyl alcohol	20	0.82
Ethylene glycol	20	1.04
	25	1.16
	40	1.71
	55	2.26
	70	2.75
Glycerol	15	0.72
Acetic acid	20	1.19
Oxalic acid	20	1.53
Benzoic acid	25	1.21
Ethyl acetate	20	1.00
Urea	20	1.20
	25	1.38
Diethylamine	20	0.97
Acetonitrile	15	1.26
Aniline	20	0.92
Furfural	20	1.04
Pyridine	15	0.58
Vinyl chloride	25	1.34
	50	2.42
	75	3.67

Source: Schwope et al. (1985).

where

D = diffusion coefficient of the migrant through the polymer
(cm²/sec)
t = time of release (seconds)
L = thickness of source (cm) in cases of one-sided exposure; in
cases of two-sided exposure use a value for L corresponding
to half the thickness of the source.

$$\alpha = aK/L \quad (4-20)$$

where

a = external phase volume divided by surface area of source (cm)
K = partition coefficient (dimensionless ratio of concentration
in external phase volume to the concentration in source).

The calculated values of ϕ and α can be used with Figure 2 to determine the fraction, F, of migrant which has been released from the polymer at time, t. The fraction of migrant released at time, t, can then be multiplied by the original concentration in the polymer and the polymer volume to find the total mass of migrant released as follows:

$$M_t = F C_{s0} V_s \quad (4-21)$$

where

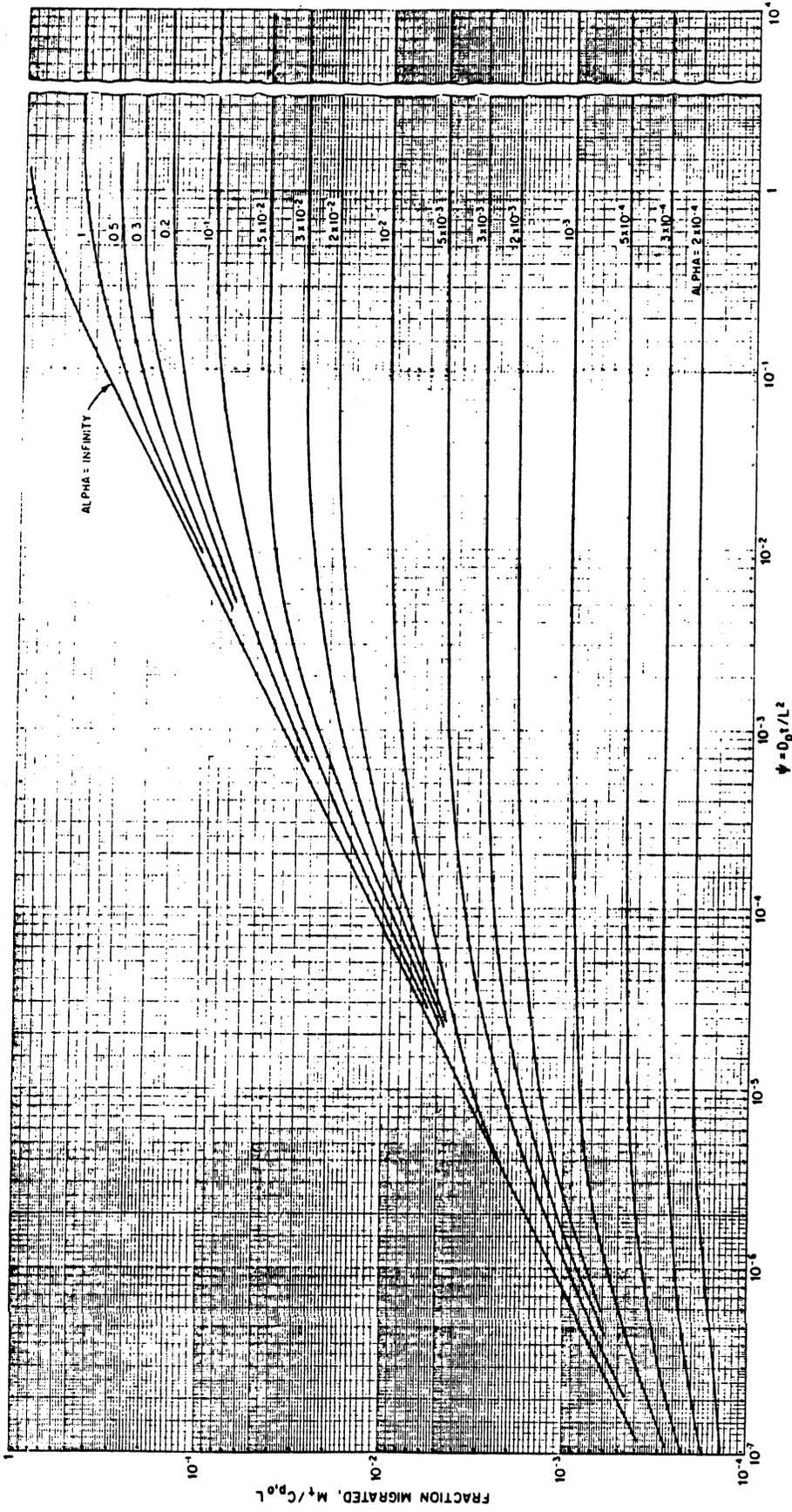
M_t = mass of migrant released (g)
F = fraction of migrant released
 C_{s0} = original concentration in polymer (g/cm³)
 V_s = volume of polymer (cm³).

The mass, M_t , should be divided by the time to get the average release rate during the period. This release rate can be used in the appropriate equations presented in Section 4.4.2 to calculate average concentrations resulting from continuous releases.

Other methods of estimating release rates can also be found in Schwoppe et al. (1985), including methods for estimating the rate of migrant release from one phase to another, where diffusion through the external phase or diffusion through a boundary layer is rate-controlling or where partitioning between the polymer and external phase affects the migration rate.

4.4 Methods for Estimating Concentrations in Indoor Air

The following subsections present equations used to estimate concentrations of chemical substances to which consumers may be exposed



Source: Schwoppe et al. (1985).

Figure 2. Fraction migrated as a function of ψ for well-mixed domains.

as a result of releases of chemical substances from consumer products to room air. The equations presented for estimating the concentration at any specified time during exposure and for estimating the average concentration during the period of exposure are those used in the Computerized Consumer Exposure Model (CCEM). These equations are applicable to any situation in which release of the chemical substance from the consumer product is to a volume of air that may be considered a single compartment. Consequently, these equations are designed to estimate concentrations in a single room containing a consumer product that releases a chemical substance. These equations include no parameters to account for the flow of air from one indoor compartment to another. They are, therefore, not intended to be applied to estimate concentrations of chemical substances in rooms other than the room containing the consumer product from which the chemical is released. These equations are also not intended to be used to estimate average concentrations of chemical substances in entire residences. Multi-compartment models that take into account air flow patterns from one indoor air compartment to another and for specific configurations of the types of residences being considered (e.g., split-level home, two-story home, rambler, office building) in addition to other applicable parameters are more suitable for this purpose.

Releases of chemical substances from consumer products are characterized in this methodology as instantaneous releases, continuous releases, or time-dependent releases. Appropriate equations for estimating concentrations in indoor air are shown for each type of release. The equations for estimating concentrations of chemical substances in indoor air as a result of continuous and time-dependent releases are derived from equations for estimating concentrations resulting from instantaneous releases. A brief discussion of concentrations resulting from instantaneous releases of chemical substances is presented in Section 4.4.1. For details on the derivation of equations for all types of releases, refer to Volume 12 of Methods for Assessing Exposure to Chemical Substances. Equations presented for estimating concentrations resulting from continuous releases of chemical substances are used in the continuous release - aerosol and the continuous release - film modules of CCEM. The continuous release - aerosol module estimates concentrations for instantaneous and continuous discharges from aerosol consumer products. Equations for estimating concentrations resulting from time-dependent releases of chemical substances are used in the time-dependent release module of CCEM. Uniform distribution of the releases throughout the room is assumed for instantaneous, continuous, and time-dependent releases.

In all three modules of CCEM, average concentrations can be calculated for any interval of time after release of the chemical occurs. The time at the beginning of exposure, t_b , and the time at the end of exposure, t_e , are used to specify the interval. If the time at

the beginning of exposure is not specified, the time at the beginning of exposure is assumed to be the time at the beginning of release, t_0 . The time at the beginning of release is always zero. When specifying the time at the beginning of exposure, a time cannot be selected that occurs before release of the chemical begins (i.e., t_b must be greater than or equal to $t = 0$, or t_0). The time at the beginning of exposure must also be less than the time at the end of exposure (e.g., t_b must be less than t_e).

In all three modules of CCEM, the duration of exposure does not have to correspond to the interval of time for which the average concentration is estimated. For example, a chemical is released continuously from a film on a surface for a period of 30 days. The receptor, however, is only exposed to the chemical for a period of 8 hours per day. This corresponds to one exposure event. In this case, the average concentration would be estimated for the interval from $t = 0$ to $t = 720$ hours (24 hours/day x 30 days). To calculate exposure, the duration of exposure would be set equal to 8 hours per event and the annual frequency of exposure would be set equal to 30 events per year.

4.4.1 Concentrations Resulting from Instantaneous Releases of Chemical Substances

These methods are most applicable to exposure scenarios in which a short-term release of a chemical substance occurs (e.g., on the order of a few seconds). Examples include release of a chemical substance due to a single discharge of product from an aerosol spray container or a spill of a volatile liquid or fine powder. The basic criterion for classifying a release as instantaneous is that the initial concentration, C_0 , is the maximum concentration to which an individual is exposed and that the concentration decreases and approaches zero as time progresses.

The following equation is used to estimate the concentration resulting from an instantaneous release to indoor air at any time, t , during a period of exposure (Porter 1983).

$$C = C_0 e^{-m(Q/V)t} \quad (4-22)$$

where

- C = concentration of chemical substance at any time, t , during exposure (mg/m^3)
- C_0 = initial concentration of chemical substance (mg/m^3)
- m = mixing factor (unitless)
- Q = ventilation flow rate (m^3/hr)
- V = room volume (m^3)
- t = time during exposure period (hrs).

The initial concentration, C_0 , can be estimated for chemical substances discharged from aerosol containers using the following equation.

$$C_0 = \frac{WF \times M \times FA}{V} \quad (4-23)$$

where

WF = weight fraction of chemical substance in product (unitless)
M = mass of product released (mass)
OV = fraction of product released that is overspray (unitless)
V = room volume (m^3).

For products that are spilled, the following equation can be used:

$$C_0 = \frac{WF \times M \times FA}{V} \quad (4-24)$$

where

FA = fraction of spilled material entrained in air (unitless) and the other variables are as defined previously. Methods for estimating WF, M, FA, and OV are presented in Section 3 of this volume.

The equations used to estimate concentrations resulting from continuous and time-dependent releases are derived from equations for estimating concentrations resulting from instantaneous releases. It must be noted that any type of release requires some amount of time to occur and, by definition, cannot be truly instantaneous. For increased accuracy, it is suggested that equations for estimating concentrations resulting from continuous releases be used for those situations in which a release might be characterized as instantaneous.

The mixing factor, m , is an empirical number that accounts for room-specific effects on transport of chemical substances (Repace and Lowrey 1980). Removal of chemical substances is more rapid in a well-mixed atmosphere than in a poorly mixed, stable one. Factors that affect the mixing factor include type and placement of ventilation grills, ventilation flow rates, inhomogeneous distribution of a chemical substance in a room, physical barriers, circulation fans, and room traffic (Repace and Lowrey 1980). A mixing factor of 1.0 implies ideal mixing. If the environmental conditions are such that the air throughout the room is continuously and vigorously mixed, then mixing of air in the room is considered ideal. Table 22 presents values for mixing factors recommended for several common air supply system configurations. According to Repace and Lowrey (1980), the best standard condition is the perforated ceiling

Table 22. Values for Mixing Factor Recommended for Several Common Air Supply System Configurations

Configuration of air supply system	Mixing factor
Perforated ceiling*	1/2
Trunk system with amenostats	1/3
Trunk system with diffusers	1/4
Natural draft and ceiling exhaust fans	1/6
Infiltration and natural draft	1/10

* This is the best standard condition.

Source: Repace and Lowrey (1980).

air supply system configuration, which has a recommended value of 1/2 for mixing factor. The air supply system configurations presented in Table 22 are listed in order of most to least thorough mixing of room air.

The ventilation flow rate, Q, is the product obtained from multiplying the room volume by the air exchange rate. Table 23 presents values for typical volumes of rooms in houses and apartments. According to figures from the Bureau of the Census, the average floor area of new houses in 1983 was 1780 square feet.* The average ceiling height is eight feet. The average volume of a new house is, therefore, estimated to be 14,240 cubic feet, or approximately 403 cubic meters. The main living space, including living room, dining room, kitchen, one bedroom, and one bath is estimated to be from 110 to 131 m³. The actual values for room volume are based on professional judgment. Typical air exchange rates in residences are presented in Table 24.

The average concentration following an instantaneous release can be estimated by integrating equation (4-22) from the time of instantaneous release to any point in time after the instantaneous release occurs. The following equation is used to estimate the average concentration following an instantaneous release.

$$C_{ave} = \frac{\left(\frac{-C_0V}{mQ}\right) e^{-m(Q/V)t} + \frac{C_0V}{mQ}}{t_u - t_0} \Bigg|_{t_0}^{t_u} \quad (4-25)$$

where

t_0 = time at which instantaneous release occurs (hours)
 t_u = any point in time after the instantaneous release occurs (hours)

and all other variables in equation (4-25) are as defined previously. It should be noted that equation (4-25) will overestimate average concentrations resulting from instantaneous releases of aerosols because it does not include a factor to account for gravitational settling of particulates. The derivations of equations (4-22) and (4-25) are presented in Volume 12 of Methods for Assessing Exposure to Chemical Substances.

It must be noted that the time at the beginning of exposure and the time at the end of exposure can be specified at any time after release begins. The only stipulation is that the time at the beginning of

* Stan Rollock, Bureau of the Census, Annual Housing Survey, personal communication with Peggy Redmond of Versar Inc., April 5, 1985.

Table 23. Typical Room Volumes

Location	Volume* (m ³)
<u>Typical House</u>	
Master bedroom	41
Standard bedrooms (2)	40
Baths (2)	18
Living room	41
Dining room	20
Kitchen	20
Basement (partial)	125
Garage (1 car)	60
Foyer/hallways	<u>15</u>
Total	380 [†]
<u>Typical Apartment</u>	
Master bedroom	41
2nd bedroom or den	20
Bath	9
Living/dining room	61
Kitchen	20
Foyer/hallways	<u>15</u>
Total	166

*All values for room volume are Versar estimates.

[†]Total volume is less than the value of 403 cubic meters estimated from Annual Housing Survey data; the difference between these totals can be attributed to the exclusion of closets in the total volume for typical house presented in this table.

Table 24. Air Changes Occurring Under Average Conditions in Residences
Exclusive of Air Provided for Ventilation^a

Kind of room	No. air changes/hour (ACH)
Rooms with no windows or exterior doors	0.5
Rooms with windows or exterior doors on one side	1
Rooms with windows or exterior doors on two sides	1.5
Rooms with windows or exterior doors on three sides	2
Entrance halls	2

^aFor rooms with weatherstripped windows or with storm sash, use two-thirds of these values.

Source: American Society of Heating, Refrigerating, and Air-Conditioning Engineers, Inc. (1977).

exposure must occur before the time at the end of exposure. The average concentration during exposure is calculated using equation (4-25). The variable, t_b , is substituted for t_0 , and the variable, t_e , is substituted for t_u in equation (4-25).

4.4.2 Concentrations Resulting from Continuous Releases of Chemical Substances

Continuous release scenarios are characterized by a chemical substance that is released at a constant rate until the period of exposure ends or the source ceases to emit the chemical substance, whichever comes first. If the exposure continues after the source ceases to emit the chemical substance, equation (4-22) for calculating room air concentrations during instantaneous releases is used. The value for C_0 used in equation (4-22) would be the value of C at the time at which the solvent ceased to be emitted. Examples of scenarios in which the rate of release is continuous include (1) single releases of chemical substances from pressurized aerosol products for time periods of more than a few seconds; (2) multiple discharges of chemical substances from pressurized aerosol products in which each discharge occurs within a short time of the other; (3) releases of chemical substances from films formed when products are spilled or sprayed instantaneously onto surfaces; and (4) releases of migrants from solid matrices or bulk liquids. Equation (4-26) is used to calculate the concentration in the room at any time, t , prior to cessation of release of the chemical substance. The initial concentration is assumed to be zero.

$$C = \frac{G}{mQ} - \frac{G}{mQ} e^{-m(Q/V)t} \quad (4-26)$$

If the initial concentration is not equal to zero,

$$C = \frac{G}{mQ} + C_0 - \frac{G}{mQ} e^{-m(Q/V)t} \quad (4-27)$$

where

- G = release rate of the chemical substance calculated using the appropriate method (see Section 4.3) (mg/hr)
- m = mixing factor (unitless)
- Q = ventilation flow rate (m^3/hr)
- V = room volume (m^3).

Equation (4-28), the integrated form of equation (4-26), is used to calculate the average concentration in the room during release of the chemical substance.

$$C_{ave} = \frac{\left(\frac{G}{mQ}\right) t + \left(\frac{GV}{m^2Q^2}\right) e^{-m(Q/V)t} \Big|_{t_0}^{t_g}}{t_g - t_0} \quad (4-29)$$

where

t_g = time at which release of the chemical substance ceases (hours),

and the other variables of equation (4-28) are as defined previously. The room air concentration at the time at which the chemical substance is no longer released, C_{tg} , is calculated by substituting t_g into equation (4-26). For continuous releases, the parameter, t_g , is calculated using the following equation:

$$t_g = \frac{M}{G} \quad (4-29)$$

where

M = mass of chemical substance released from aerosol product, or mass applied, sprayed, or spilled onto a surface

G = release rate of the chemical substance calculated using the appropriate method (see Section 4-3) (mass/hour).

Equation (4-30), a variation of equation (4-22), is used to calculate the room air concentration at any time, t , after release of chemical substance from the source has ceased.

$$C = C_{tg} e^{-m(Q/V)(t-t_g)} \quad (4-30)$$

Equation (4-31) is used to calculate the average concentration from the time the release of chemical substance has ceased until any point in time greater than the time at which release of the chemical ceases.

$$C_{ave} = \frac{\left(\frac{-C_{tg} V}{mQ}\right) e^{-m(Q/V)(t-t_g)} \Big|_{t_g}^{t_u}}{t_u - t_g} \quad (4-31)$$

where

t_u = any point in time greater than the time at which release of the chemical ceases (hours).

If average concentrations are desired for a period starting before release ceases and ending after release of the chemical substance from the source has ceased, the average concentration during this period can

be estimated by calculating a time-weighted average of the average concentration during release and the average concentration after release has ceased:

C_{ave} (during period that starts before release ceases, but ends after release ceases) =

$$C_{ave} \text{ (during release)} \times \left(\frac{(t_g - t_o)}{(t_u - t_o)} \right) + C_{ave} \text{ (after release)} \times \left(\frac{(t_u - t_o)}{(t_u - t_o)} \right) \quad (4-32)$$

The derivations of equations (4-26) through (4-31) are presented in Volume 12 of Methods for Assessing Exposure to Chemical Substances.

In estimating average concentrations during exposure, it must be noted that the time at the beginning of exposure and the time at the end of exposure can be specified at any time after release begins. The only stipulation is that the time at the beginning of exposure must occur before the time at the end of exposure. Three possible cases for the time at the beginning of exposure and the time at the end of exposure are the following:

- Case 1: The time at the beginning of exposure and the time at the end of exposure are less than the time at the end of release. In this case, the average concentration during exposure is calculated using equation (4-28). The variable, t_b , is substituted for t_o and the variable, t_e , is substituted for t_g in Equation (4-28).
- Case 2: The time at the beginning of exposure is less than the time at the end of release and the time at the end of exposure is greater than the time at the end of release. In this case, the average concentration during exposure is calculated using equations (4-28), (4-31), and (4-32). The variable, t_b , is substituted for t_o in equation (4-28). The variable, t_e , is substituted for t_u in equation (4-31). The average concentration during release obtained from equation (4-28) and the average concentration after release obtained from equation (4-31) are used in equation (4-32) to obtain the average concentration during exposure. In addition, t_b is substituted for t_o and t_e is substituted for t_u in equation (4-32).
- Case 3: The time at the beginning of exposure and the time at the end of exposure are greater than the time at the end of release. In this case, the average concentration during exposure is calculated using equation (4-31). The variable, t_b , is substituted for t_g , and the variable, t_e , is substituted for t_u in equation (4-31).

4.4.3 Concentrations Resulting from Time-Dependent Releases of Chemical Substances

The following equations are applicable for estimating concentrations that occur when the rate of release of a chemical substance is time-dependent. These equations are applicable to scenarios in which a coating or film containing the chemical substance for which exposure is being assessed is applied to a surface and the time required for application is more than a few minutes. To use this method, the assessor must first ascertain whether the time for evaporation of the chemical substance from the film, once it is applied to the surface (t_g), is less than, greater than, or equal to the time required to apply the film to the surface (t_a). A method for estimating the time required to apply a film to a surface is presented in Section 3.1 of this volume. The following expression is used to estimate t_g for a time-dependent release.

$$t_g = M/t_a/G_{NA_R} \quad (4-33)$$

where M is the total mass of chemical substance in the film applied to the surface and G_{NA_R} is calculated using the method cited in Section 4.3.

This method for estimating t_g assumes that evaporation occurs at a constant rate. Because of the effect that drying of the coating or film may have on the release rate and because some chemical substances do not evaporate completely from the film or coating before the coating dries (Newman et al. 1975; Newman and Nunn 1975), the assumption of constant release until the entire mass of chemical substance is released may not be true. It is recommended that the value of t_g obtained using equation (4-33) be used only to estimate concentrations during release up to the time reported for the specific coating to form a dry film, if this time is known.

Four equations are used to calculate concentrations in indoor air resulting from time-dependent releases of chemical substances. These equations mathematically describe four physical situations that occur at specific intervals that characterize a time-dependent release. For the case in which the time for evaporation of the chemical substance from the film once it is applied to the surface is less than the time to apply the film to the surface (Case 1), a description of the physical situation during each of the four intervals follows:

- (1) $t_0 < t \leq t_g$: Mass of chemical substance released is increasing and concentration at any time, t , is increasing during this interval. The mass of chemical substance released is increasing because of the additional mass being applied to the surface.

- (2) $t_g < t \leq t_a$: The mass of chemical substance released remains constant and the concentration is increasing. The additional mass applied to the surface is balanced equally by the portion of the surface from which the chemical has already evaporated.
- (3) $t_a < t \leq t_r$: The variable t_r denotes the time at which the very last bit of chemical substance has been released from the surface. During this interval, the film is no longer being applied but chemical substance is still being released. Therefore, the mass of chemical substance released is decreasing. Whether the concentration at any time, t , during this interval is increasing or is decreasing is determined by the air exchange rate.
- (4) $t_r < t \leq t_u$: The mass released is zero. The concentration is decreasing with time as ventilation air flows out of the room.

For the case in which the time for evaporation of the chemical substance from the film once it is applied to the surface is greater than, or equal to the time to apply the film to the surface (Case 2), a description of the physical situation during each of the four intervals follows:

- (1) $t_0 < t \leq t_a$: Mass of chemical substance released is increasing, and concentration at any time, t , is increasing during this interval. The mass of chemical substance released is increasing because of the additional mass being applied to the surface.
- (2) $t_a < t \leq t_g$: Mass of chemical substance released remains constant, and the concentration at anytime, t , continues to increase during this interval.
- (3) $t_g < t \leq t_r$: The mass of chemical substance released is decreasing.
- (4) $t_r < t \leq t_u$: The mass of chemical substance released is zero, and the concentration is decreasing with time.

By making appropriate substitutions, one set of equations can be used to determine concentrations for both of the cases described previously. For Case 1, let t_g equal t_1 and t_a equal t_2 . For Case 2, let t_a equal t_1 , and t_g equal t_2 . The following equations are used to determine the concentration of chemical substance at any time, t , during each interval and the average concentration during each interval.

The average concentration during the exposure period is determined by calculating a time-weighted average based on the average concentration calculated during each interval. Note that $k = mQ/v$.

(1) From t_0 to t_1 :

$$C = \frac{G_{NAR}}{Vk} \left[t - \frac{1}{k} + \frac{e^{-kt}}{k} \right] \quad (4-34)$$

$$C_{ave} = \frac{\frac{G_{NAR}}{Vk} \left[\frac{t^2}{2} - \frac{t}{k} - \frac{e^{-kt}}{k^2} \right]_{t_0}^{t_1}}{t_1 - t_0} \quad (4-35)$$

(2) From $t_1 < t \leq t_2$

$$C = \frac{G_{NAR}}{Vk} \left[t_1 - \frac{1}{k} \left(e^{-k(t-t_1)} - e^{-kt} \right) \right] \quad (4-36)$$

$$C_{ave} = \frac{\frac{G_{NAR}}{Vk} \left[t_1 t + \frac{1}{k^2} \left(e^{-k(t-t_1)} - e^{-kt} \right) \right]_{t_1}^{t_2}}{t_2 - t_1} \quad (4-37)$$

(3) From $t_2 < t \leq t_r$

$$C = -e^{-k(t-t_2)} \left[\frac{G_{NAR}}{Vk} \left(\frac{1}{k} + t_r - t_2 \right) - C_{t_2} \right] + \left[\frac{G_{NAR}}{Vk} \left(\frac{1}{k} + t_r - t \right) \right] \quad (4-38)$$

$$C_{ave} = \frac{\frac{e^{-k(t-t_2)}}{k} \left[\frac{G_{NAR}}{Vk} \left(\frac{1}{k} + t_r - t_2 \right) - C_{t_2} \right] + \left[\frac{G_{NAR}}{Vk} t \left(\frac{1}{k} + t_r - \frac{t}{2} \right) \right]_{t_2}^{t_r}}{t_r - t_2} \quad (4-39)$$

where

C_{t_2} = concentration at the time, t_2 , calculated using equation (4-36).

(4) From $t_r < t \leq t_u$

$$C = C_{t_r} \left[e^{-k(t-t_r)} \right] \quad (4-40)$$

$$C = \frac{C_{t_r} \left[\frac{-e^{-k(t-t_r)}}{k^2} \right]_{t_r}^{t_u}}{t_u - t_r} \quad (4-41)$$

where

C_{t_r} = concentration at the time at which release ends calculated using equation (4-38) (mass/volume).

It must be noted that the time at the beginning of exposure and the time at the end of exposure can be specified at any time after release begins. The only requirement is that the time at the beginning of exposure must occur before the time at the end of exposure. To delineate the possible cases that can occur, the convention that t_1 corresponds to t_a or t_g , whichever is smaller, and that t_2 corresponds to t_a or t_g , whichever is larger, is used. Possible cases for the time at the beginning of exposure and the time at the end of exposure in relation to t_1 , t_2 , t_r , and t_u include the following:

- Case 1: The time at the beginning of exposure and the time at the end of exposure are less than or equal to t_1 . In this case, the average concentration during exposure is calculated using equation (4-35). The variable, t_b , is substituted for t_0 and the variable, t_e , is substituted for t_1 , in equation (4-35).
- Case 2: The time at the beginning of exposure is less than or equal to t_1 , and the time at the end of exposure is greater than t_1 , but less than or equal to t_2 . In this case, the average concentration during exposure is the weighted average of average concentrations calculated using equations (4-35) and (4-37). The variable, t_b , is substituted for t_0 in equation (4-35). The variable, t_e , is substituted for t_2 in equation (4-37).
- Case 3: The time at the beginning of exposure is less than or equal to t_1 , and the time at the end of exposure is greater than t_2 , but less than or equal to t_r . In this case, the average concentration during exposure is the weighted average of average concentrations calculated

using equations (4-35), (4-37), and (4-39). The variable, t_b , is substituted for t_0 in equation (4-35). The variable, t_e , is substituted for t_r in equation (4-39).

- Case 4: The time at the beginning of exposure is less than or equal to t_1 , and the time at the end of exposure is greater than t_r . In this case, the average concentration during exposure is the weighted average of average concentrations calculated using equations (4-35), (4-37), (4-39), and (4-41). The variable, t_b , is substituted for t_0 in equation (4-35). The variable, t_e , is substituted for t_u in equation (4-41).
- Case 5: The time at the beginning of exposure and the time at the end of exposure are greater than t_1 but less than or equal to t_2 . In this case, the average concentration during exposure is calculated using equation (4-37). The variable, t_b , is substituted for t_1 , and the variable, t_e , is substituted for t_2 in equation (4-37).
- Case 6: The time at the beginning of exposure is greater than t_1 , but less than or equal to t_2 . The time at the end of exposure is greater than t_2 , but less than or equal to t_r . In this case, the average concentration during exposure is the weighted average of average concentrations calculated using equations (4-37) and (4-39). The variable, t_b , is substituted for t_1 in equation (4-37). The variable, t_e , is substituted for t_r in equation (4-39).
- Case 7: The time at the beginning of exposure is greater than t_1 , but less than or equal to t_2 . The time at the end of exposure is greater than t_r . In this case, the average concentration during exposure is the weighted average of average concentrations calculated using equations (4-37), (4-39), and (4-41). The variable, t_b , is substituted for t_1 in equation (4-37). The variable, t_e , is substituted for t_u in equation (4-41).
- Case 8: The time at the beginning of exposure and the time at the end of exposure are greater than t_2 , but less than or equal to t_r . In this case, the average concentration during exposure is calculated using equation (4-39). The variable, t_b , is substituted for t_2 , and the variable, t_e , is substituted for t_r in equation (4-39). The concentration at the time at the beginning of exposure, Ct_b , is substituted for Ct_2 in equation (4-39). Ct_b is calculated by substituting t_b for t in equation (4-36).

- Case 9: The time at the beginning of exposure is greater than t_2 , but less than or equal to t_r . The time at the end of exposure is greater than t_r . In this case, the average concentration during exposure is the weighted average of average concentrations calculated using equations (4-39) and (4-41). The variable, t_b , is substituted for t_2 in equation (4-39). The variable t_e , is substituted for t_u in equation (4-41). The concentration at the time at the beginning of exposure, Ct_b , is substituted for Ct_2 in equation (4-39). Ct_b is calculated by substituting t_b for t in equation (4-36).
- Case 10: The time at the beginning of exposure and the time at the end of exposure are greater than t_r . In this case, the average concentration during exposure is calculated using equation (4-41). The variable, t_b , is substituted for t_r and the variable, t_e , is substituted for t_u in equation (4-41). The concentration at the time at the beginning of exposure, Ct_b , is substituted for Ct_r in equation (4-41). Ct_r is calculated by substituting t_b for t in equation (4-38).

It must be noted that the physical situations described for the intervals comprising these two cases are generally applicable under environmental conditions considered most likely to occur indoors. If, however, the ventilation air flow rate is sufficiently high to offset the rate at which the chemical substance is released, the physical situations that occur during each interval will vary from those previously described. Additional data are required to determine the combination of release rate of chemical substance and air exchange rate that would cause the actual physical situation to deviate. The derivations of equations (4-34) through (4-41) are presented in detail in Appendix E of this volume.

Under some circumstances, the concentrations predicted using these methods may exceed the saturation concentration of the chemical substance under the environmental conditions for which it is being modeled. Such circumstances are most likely to be encountered in scenarios in which a large mass of a chemical substance with a relatively low vapor pressure is available for release from surfaces to which a film containing the chemical substance is applied.

A reason for predicted concentrations' exceeding the saturation concentration is the underlying assumption of the methods presented in this section that release occurs at a constant rate. Release at a constant rate can only be assumed if the kinetics of mass transfer are slow enough that the concentration of the chemical substance in the room

never reaches a level that is high enough to have an appreciable effect on the rate of release. If the kinetics of mass transfer are fast enough that equilibrium is approached before the film or coating dries, the rate of release will decrease exponentially; a numerical method of solution must instead be used to provide estimates of concentrations occurring during exposure. To implement a numerical method of solution, a computer program must be used because of the extensive calculations that must be carried out.

In the event that the average concentration predicted using the equations described previously exceeds the saturation concentration of the chemical substance in any of the four intervals during exposure, it is suggested that the assessor substitute the saturation concentration for the value of the average concentration during that interval. The average concentration during the exposure period is then determined by calculating a time-weighted average from the average concentration used during each applicable interval.

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5. EXPOSED POPULATIONS

Studies of populations exposed to chemical substances in consumer products comprise three basic elements:

- Identification of exposed populations
- Enumeration of exposed populations
- Characterization of the population according to age and/or sex.

Identification of the exposed populations relies on identification of consumer products containing the chemical substance of concern. The users of the products (i.e., those who actively use and those who are present during use) are the exposed population. Once the users are identified, the exposed population can be enumerated and characterized by the methods described in Volume 4 of this series, Methods for Enumerating and Characterizing Populations Exposed to Chemical Substances, EPA 560/5-85-004 (Dixon et al. 1985). This section will summarize the population enumeration report and indicate how it applies to consumer exposure assessment.

5.1 Identification of Exposed Populations

The steps required for identifying the population exposed to a chemical substance in consumer products can be summarized as follows:

1. Use the data sources discussed in Section 3, or for a new chemical substance consult the Premanufacture Notice (PMN), to compile a list of the consumer products known to or thought to contain the chemical substance of interest.
2. Determine whether all or a portion of the consumer product class contains the chemical substances; if possible, identify the product by brand name to expedite enumeration.
3. Identify products obviously intended for use by males or females or specific age groups.
4. Evaluate each product to determine whether passive exposure is of concern. Consumer product use patterns and chemical release patterns will identify the passively exposed population (i.e., family or household members).

5.2 Enumeration of the Exposed Population

Enumeration of the population exposed to a chemical substance in consumer products depends on two factors: (1) the availability of use data specific to the products and (2) whether both active and passive exposure to the chemical substance is involved. The following subsections

briefly review the sources of available data and the methods for their use. Volume 4 of the series, Methods for Assessing Exposure to Chemical Substances presents methods for enumerating populations exposed to chemical substances.

5.2.1 Enumeration of Exposed Populations via Simmons Market Research Bureau Reports

The Simmons Market Research Bureau (SMRB) reports are described in detail in Volume 4 of this series; they are also discussed in Section 6.2 and Appendix D of this volume. Briefly, SMRB is a market research corporation that collects information on the buying habits of the U.S. population. SMRB collects this information for over 1,000 consumer products. For each consumer product, SMRB also collects data on the specific product type (e.g., aerosol rug shampoo versus liquid rug shampoo) as well as the brand name (e.g., Bissell Shampoo versus Johnson's Shampoo). For each type and brand name product, SMRB collects information on the frequency of use (described in greater detail in Section 6.2 of this report), the total number of buyers as well as the number of buyers in each use category, and the demographics (e.g., age, race, employment, economic level, geographic location) for the buying population. All this information is presented in a series of 29 volumes organized according to major product categories. The 29 volumes of SMRB data collected in 1982 have been purchased by EPA-OTS and are included in the Exposure Evaluation Division library.

Enumeration of populations exposed to a chemical substance in a consumer product is, therefore, a straightforward process with the use of the SMRB reports. It should be noted, however, that SMRB presents the consumer product data according to the "buyer" and not necessarily according to the user (i.e., actively exposed individuals). It may be necessary to adjust the data to reflect potential uses in a household. The investigator must judge on a case-by-case basis how to use the data to accurately represent the user or actively exposed population. Populations that are passively exposed as a result of their proximity to the product both during and following its active use may also be estimated via SMRB data. For product buyers, SMRB reveals the frequency distribution of household size. For example, SMRB may present 1,000 female homemakers (i.e., the actively exposed population) as purchasers of rug shampoo. For the 1,000 female homemakers, SMRB depicts the number of households having 1, 2, 3 or 4, or 5 or more persons; these households would also total 1,000. To approximate the number of persons living in the 1,000 households and potentially passively exposed to the chemical substance in rug shampoo, the investigator can apply the frequency distribution and household size. Ranges can be used to accurately estimate the exposed population; use of the high end of the ranges generates a conservative estimate of exposed persons.

The SMRB data are clearly intended to describe the market variability of existing products. Consequently, the data are generally more applicable to existing chemicals and product formulations currently on the market than to new chemical substances. The SMRB data may, however, prove useful to assessments of PMN substances when the new chemical is intended for use as a substitute for an existing chemical. If use information included in a PMN submittal is sufficiently detailed, the SMRB data can be used to predict the number of exposed consumers.

Finally, as part of the investigation and development of this methods report, considerable population data have already been extracted and recorded for many of the consumer products under investigation (as listed in Section 1.3).

5.2.2 Enumeration of Exposed Populations via Production and Sales Data

For consumer products not covered by SMRB, the users can be enumerated by applying a number of assumptions and estimation techniques to economic data such as chemical production volume, Census of Manufacturers output, and retail sales information. To enumerate the users of a consumer product, the investigator must estimate the number of units of a product bought by consumers, and then apply such data on use patterns to determine the average number of consumers. This method can be summarized in the following steps.

1. Determine the number of units of the product sold or produced annually according to one of the following options:
 - Consult the Census of Manufacturers (Bureau of the Census 1980b) to obtain production in unit quantities.
 - Estimate the number of units produced by dividing the amount of the chemical destined for that use by the formulation percent and the total mass of product per unit. (Note: This information must be derived from the materials balance for the chemical substance of concern.)
2. Determine the use patterns for the product. SMRB reports provide data on frequency of use of consumer products. Based on product similarities, the investigator can estimate use patterns (e.g., number of units used per year).
3. Calculate the exposed population by dividing the production volume units by the units used per person per year.

The results of this approach will be an estimate, but a fairly valid one; the parameters used in the calculation are from reliable sources.

5.2.3 Enumeration of Exposed Populations via Chemical-Specific Information

Various sources of chemical-specific information can also be used to enumerate exposed populations in lieu of SMRB or production and sales data. The information sources include the following:

- Consumer product associations as listed in the Encyclopedia of Associations.
- Government agencies (e.g., Food and Drug Administration (FDA), Consumer Product Safety Commission (CPSC), Bureau of the Census (see Section 3.4 for additional information)).
- Publications of the Bureau of the Census (e.g., Annual Housing Survey, The Statistical Abstract of the United States).

The published literature can also provide valuable information on the users of consumer products.

5.3 Characterization of Exposed Populations

Consumer inhalation and ingestion rates and surface areas for potential dermal contact are a function of the individual's age and sex. Accurate estimates of exposure distributions, therefore, require characterization of the exposed population according to age and sex. If the chemical substance of concern has special effects on particular age classes such as the elderly or children, further characterization of the population is required. Another example would be a chemical substance that has been determined to be teratogenic; enumeration of women of child-bearing age may then be required.

Data sources for characterizing the exposed population include the SMRB reports and the general age and sex distribution of the U.S. population. Procedures for characterizing exposed populations can be summarized as follows:

1. If the consumer population was enumerated by the use of SMRB data, use the demographic characteristics reported for buyers/users to characterize the actively exposed population by age and sex. Populations enumerated by other methods can also be characterized by consulting the SMRB reports for the product(s) most similar to that being assessed.

2. Consult Volume 4 (Table 12) of the exposure assessment methods series to derive generic age and sex distribution for:

- Consumer populations under the age of 18 .
- Passively exposed household members
- The entire U.S. population.

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6. EXPOSURE ANALYSIS

Before discussing exposure, it is necessary to differentiate between the concepts of "exposure" and "dose." Dose is the amount absorbed by the receptor; exposure refers to the quantity contacting the receptor and available for absorption. To be absorbed, a substance must pass a barrier: the gastrointestinal (or oral) epithelium in the case of ingestion exposure, the pulmonary epithelium for respired substances, or the epidermis in the case of dermal contact. Whether the results of an assessment are to be expressed as exposure or as absorbed dose depends on what use is to be made of the exposure assessment (see Volume 1 of this series). If results in terms of absorbed dose are desired, units are often expressed as mass of chemical / kilogram of body weight / day. A table of average body weights, in kilograms, for humans is presented in Appendix D. Average body weight values in this table are presented by age group. In actual practice, experimental data measuring absorption of chemical substances is limited to a few specific chemical substances and conditions. Although methods for estimating absorption will be discussed, the emphasis in this volume will be on exposure.

Section 6 is divided into three subsections. Section 6.1 defines exposure pathways and explains their relevance to exposure analysis. Section 6.2 discusses methods for calculating exposure. Current knowledge of absorption parameters is summarized in Section 6.3. Emphasis is on pathways and scenarios of interest to OTS and on sources of chronic low-level (rather than acute) exposure. A detailed discussion of key factors governing deposition of particles in regions of the respiratory tract and of methods for estimating inhalation exposure to aerosols is presented in Appendix A.

6.1 Exposure Pathways and Routes

An exposure route is the means by which a pollutant in a given medium contacts or enters the receptor. A pathway is the history of the flow of a pollutant from the source to receptor, including qualitative description of emission type, transport, medium, and route. This section will discuss significant pathways of exposure from consumer products. All of these pathways are not covered in this volume. They are all listed here so they can be put in perspective.

6.1.1 Inhalation Pathways

Although inhalation exposure is probably more significant in the ambient and occupational settings, it may reach levels of grams per year in the consumer setting. Consideration of odor thresholds suggests that inhalation exposures from volatile household chemicals may reach levels of grams per person (Becker et al. 1979). Reports of acute inhalation toxicity from consumer products are largely restricted to cases of carbon

monoxide poisoning. Reports of subacute toxicity are fairly common, e.g., pneumonitis from household pyrethrum use (Carlson and Villaveces 1977), epistaxis and liver-function abnormalities associated with consumer use of butyl caulk (NIOSH 1982b), and systemic toxicity from mothballs (Stricof et al. 1983). There is also increasing awareness of the fact that household solvents and pesticides may be associated with various subclinical, delayed, or otherwise overlooked chronic effects such as altered mental states and behavioral manifestations (Levin et al. 1976, Clark 1971). Finally there is a small, but significant, subpopulation of hypersensitive persons who display symptoms at substance concentrations harmless to most people (Sandifer et al. 1972).

Inhalation pathways are the most complex to analyze and quantify, since they always involve transport through a medium (air) and associated emission, fate, and other parameters, which are only occasionally involved in dermal and ingestion pathways.

The physical state of the inhaled substance may be gaseous or aerosol (i.e., a suspension of liquid or solid particles in air). Significant pathways can be summarized as follows:

- Inhalation of an aerosol resulting from the spray application of a product. The spray may be directed onto the user's person, onto a surface to be treated, or into the air itself (as in a room deodorant or pesticide space spray). Exposure may also result from the aerosolization of a poured liquid.
- Inhalation of gas evaporating from a liquid surface. This surface may be a film on an object to which the liquid has been sprayed or otherwise applied; the liquid may also be evaporating from a container left open during use of the product.
- Inhalation of a gas diffusing from a solid matrix, e.g., from plastics, dry paint films.
- Inhalation of solid particles resulting from (a) application or pouring of dusts or powders; (b) use or modification of a solid product, e.g., by sawing; or (c) re-entrainment during sweeping, dusting, etc.
- Inhalation of gas or particles resulting from the indoor or outdoor combustion of fuels or other products, e.g., candles, matches, or firelogs.

Methods for all of the above, except the last item and (b) and (c) of the fourth item, are delineated in this methods report.

6.1.2 Dermal Pathways

Acute poisoning via dermal exposure is infrequent in the consumer setting, although cases have been reported, e.g., fatalities from aniline in canvas shoes and laundry markers (Becker et al. 1979). Local irritation and sensitization are more commonly reported, e.g., contact dermatitis from chemicals in paper (Marks 1981) and in home dyes (NIOSH 1982a).

The most common pathways involve direct contact with a liquid or powdered product. These may be applied to the body directly or contacted during use or application; the product may also be contacted accidentally when one touches the surface to which it has been applied.

Additional dermal exposure pathways include the following:

- Exposure to aerosol droplets or dust particles suspended in the air. The relevant variables are difficult to quantify and include such parameters as motion of the receptor through the room.
- Dermal exposure to gases.
- Exposure to solid products.

No scenarios have been developed for the first two pathways listed above. Contact with solids can be further broken down as follows:

- Exposure to ingredients leached, diffused, or dissolved out of a solid matrix; e.g., plasticizers in plastic products or pesticides in pressure-treated wood. Such exposure is of particular concern when the receptor is hypersensitive to the substance; in such a case, the slightest contact with the solid object itself may cause a toxic reaction, even though the absorbed dose may be below the limits of accurate quantification. No scenario has been developed for this pathway.
- Exposure to chemical substances in clothing. These substances may be ingredients of the fabric (e.g., dyes) or contaminants (e.g., detergent residues). This pathway is separated from the above because opportunities for exposure to a chemical used on fabric are much higher. Fabric used to make clothing is in contact with the skin for many hours per day. Systemic toxicity has been reported in a series of cases involving inadvertent contamination of a shipment of clothing as the result of a pesticide spill (Roueche 1971).
- Exposure to fragments or fibers which have become embedded in the skin (e.g., steel wool, glass wool, insulation). Such exposure is

beyond the scope of this volume, since resulting symptoms are more likely due to physical irritation than to chemical toxicity per se (although subsequent chemical absorption via leaching or dissolution is possible). In any case, this is not a true dermal pathway but a subcutaneous injection pathway (see Section 6.1.4).

- Exposure from rub-off of surface material which subsequently adheres to the skin as a powder (e.g., dried ink on printed matter; dust from cat box filler, charcoal briquets, or insulation).
- Contact with dust generated or released during installation, machining, or removal/demolition of a solid product (e.g., wallboard, roofing, tile, lumber).

The last two pathways mentioned are considered identical to dust exposure, and methods are delineated accordingly.

6.1.3 Ingestion Pathways

Ingestion is the most significant route of exposure to toxic substances when incidents of acute toxicity are considered. Data compiled by the National Center for Health Statistics (NCHS) suggest that at least 1,200 people yearly receive oral doses of between 5 and 30 grams of single chemicals in paints, cleaning agents, disinfectants, and petroleum products, based on the number of fatalities reported and the toxicities of the relevant ingredients (Becker et al. 1979). There are insufficient data to present typical ranges for cumulative annual ingestion of individual chemicals resulting from chronic, rather than acute, exposure to consumer products. Exposure resulting from ingestion of contaminated food and drinking water will not be considered in this volume. Exposure via food is covered by Volume 8, and exposure via drinking water is covered in Volume 5 of the exposure assessment methods series.

The following pathways may result in significant exposure:

- Deliberate ingestion of a product not meant to be ingested (see below).
- Accidental transfer to the mouth of a chemical that has contaminated or settled on the hands or face during use. There is currently no reliable method for assessing such exposure.
- Contamination of food in the home, e.g., during preparation, storage, or serving. In this case, the subject chemical is an extraneous household pollutant rather than a food ingredient or additive; examples include detergent residues, plasticizers in

film wrap, and leachable/soluble constituents of vessels, dishes, or silverware. This pathway can be significant for chronic exposure. Occasional cases of acute toxicity occurring by this pathway have been reported, e.g., from lead in pottery and in cocktail glasses (Bird et al. 1982). Exposure may also occur via settling onto food of airborne particles or aerosol droplets. Such infrequent events lack predictable common characteristics and do not lend themselves to analysis via standardized scenarios.

- Ordinary use of objects designed to be used in the mouth. This category is basically restricted to infants' toys such as teethingers and pacifiers and to such unusual items as athletic mouthguards. It may also apply to dental fillings and prostheses. In this pathway, the subject chemical must be leached or dissolved out of the solid matrix.
- Liquids normally used in the mouth but not intended to be swallowed. Examples include toothpaste and mouthwash; some of this may be swallowed, and some absorbed by the oral mucosa.
- Ingestion as a subset of inhalation, i.e., swallowing of inhaled particles too large to be respired.

Methods are delineated in this volume for the last three pathways.

Methods for estimating exposure from deliberate ingestion of products will not be delineated in this volume, despite the frequency and seriousness of clinical poisoning via this pathway, for several reasons. Deliberate ingestion of inedible substances may be either purposeful (e.g., pica, suicide) or not (e.g., product mistaken for something edible). Exposure may involve the ingestion of a chemical substance per se, usually in liquid form, or the swallowing of a solid object, e.g., a pill bottle desiccant (Muhletaler et al. 1980). The swallowing of objects is essentially a product safety consideration and is beyond the scope of OTS responsibility. (However, it should be noted that the body may absorb toxic substances released from the ingested object during gastrointestinal retention (Litovitz 1983).) Deliberate ingestion of liquids will not be considered. Quantifying acute threats requires a different approach from that used to predict isolated incidents of negligence or misuse.

It should be noted that some unusual forms of exposure may fall into more than one setting. An example is a reported case of drinking water contamination from phenol originating from the tank liner of a solar water heater (Trincher and Rissing 1983). Volume 5 of this series describes the framework for calculating exposure to chemicals contaminating drinking water, and presents data on such required input parameters as daily drinking water intake. However, the water heater in

question is purchased and operated by consumers; therefore, other parameters (e.g., exposed population, chemical release, and ultimate concentration) must be calculated by methods discussed in this volume. Such "hybrid" exposures are relatively uncommon and should be handled on a case-by-case basis.

6.1.4 Other Pathways

Chemicals may be absorbed from consumer products via routes other than the three most common ones discussed above. No scenarios will be developed for these; however, they will be listed for completeness. Three examples that may occasionally be significant include: (1) direct ocular absorption, e.g., of pesticide vapors (Morgan and Roan 1974); (2) use of rectal and vaginal suppositories or devices; and (3) injection (subcutaneous or other).

The last two categories are restricted to use of medical products, at least under ordinary circumstances, and are therefore beyond the jurisdiction of EPA. Exceptions include penetration of the skin by fibers (e.g., asbestos) and trauma (e.g., the accidental injection into the hand via spray-gun of lead-containing paint) (Lilis et al. 1981). Such incidents are unpredictable and not amenable to quantification.

Medical implants and prostheses are also excluded from consideration. Note that contact with oral mucosa is included under "ingestion" and with the upper respiratory epithelium under "inhalation."

6.2 Exposure Calculation

This section presents methods and data needed to estimate exposure. Frequency of use is a parameter required to estimate annual exposure to consumer products for inhalation, dermal, and ingestion pathways. Section 6.2.1 provides information to aid the assessor in determining frequency of use. Methods for estimating inhalation exposure are found in Section 6.2.2. Section 6.2.3 presents methods for estimating dermal exposure, while Section 6.2.4 cites methods for estimating ingestion exposure. Methods for estimating inhalation exposure to particulates discharged from consumer products are presented in Appendix A.

6.2.1 Frequency of Use

Market research reports are a very useful source of data on product use frequency. One readily available series of market research reports is the Simmons Market Research Bureau (SMRB) reports. SMRB is a market research corporation that collects information on the buying habits of the population through questionnaires administered to a nationwide panel of consumers. This study, The Simmons Media and Market Report (SMRB

1982), is designed to serve retailers, advertising agencies, and the media by providing up-to-date, comprehensive information on current and potential sales markets for consumer products.

Appendix B lists products covered in SMRB by volume. For each product category, section 1B of SMRB usually indicates how many households buy or use the product. If the product requires installation, SMRB often indicates the number of persons installing it themselves. Products are often broken down by type, e.g., aerosol, liquid, powder.

Populations are reported for heavy, medium, and light use categories (H, M, L). These are defined separately for each product, and a table is provided. This permits calculation of a distribution of frequency of use.

In many instances, SMRB reports the number of containers, cans, or bottles purchased per time period instead of the number of uses. To translate these data into uses per year, it is necessary to know how much product is consumed per use, and how much is contained in a single container. This information can be obtained from a number of sources, including product labels, or contact with trade associations, industry, users' (e.g., hobby) associations, and government agencies such as CPSC or FDA. These same sources can also be consulted when a particular product is not listed in SMRB.

6.2.2 Inhalation Exposure

Inhalation exposure is defined for the purpose of this report as the quantity of a chemical substance that is taken into the body via the inhalation route during a given period of time. Exposure is to be distinguished from absorbed dose, which refers to the quantity of chemical absorbed across biological membranes as a result of exposure. Background information on the inhalation route of exposure is provided in (1), followed by a discussion of the method used to estimate inhalation exposure to gases and vapors in (2).

(1) Background. Chemical substances present in ambient air as gases or vapors may be inhaled, thus contributing to exposure via the lungs. Although a significant fraction of the inhaled chemical may be exhaled, this fraction is chemical-specific and thus not easily predicted. For this reason, exposure estimates for gases and vapors are based on the entire quantity of inhaled chemical. Aerosols (i.e., suspensions of small liquid or solid particles in air), however, are subject to differential deposition in various regions of the respiratory tract. Particle deposition patterns can be roughly predicted based on knowledge of the particle size distribution of inhaled aerosols. Particle sizes are usually measured as particle aerodynamic diameter, defined as the diameter (in μm) of a sphere of unit density having the

same terminal velocity as the particle in question, regardless of its shape and density (Marple and Rubow 1980). Exposure calculations for inhaled aerosols can be refined by incorporating information on particle size distribution and knowledge of the relationship between particle size and respiratory tract deposition patterns. A detailed discussion of key factors governing deposition of particles and of methods for estimating inhalation exposure as a function of regional deposition of particles in the respiratory tract is presented in Appendix A of this volume.

(2) Exposure Calculation. Assessment of inhalation exposure to consumer products involves finding a simple or complex solution to the following equation:

$$E_I = I \int C(t)dt \quad (6-1)$$

where

E_I = inhalation exposure (mass/time)
 I = inhalation rate (volume/time)
 t = duration of exposure (time)
 $C(t)$ = concentration of chemical in air as a function of time (mass/volume).

In practice, the algorithm used to calculate inhalation exposure is usually an integrated and simplified version of equation (6-1), often incorporating simplifying assumptions about the change in concentration with time. (See Section 4 for a detailed discussion of methods for calculating concentration.) In many cases, exposures can be calculated using an average concentration for a given period of time; exposures from several such consecutive time periods can be summed to estimate total inhalation exposure to a given product. The simplified version of equation (6-1) is presented below.

$$IHX = IR \times DU \times FQ \times CN \quad (6-2)$$

where

IHX = inhalation exposure (mg/yr)
 IR = inhalation rate (m^3/hr)
 DU = duration of exposure event (hours)
 FQ = frequency of exposure (events per year)
 CN = average indoor air concentration of a given constituent (mg/m^3).

The variables of equation (6-2) are determined as follows:

(a) Inhalation rate. Inhalation rate (IR) is expressed in m^3/hr . The factors that have the most influence on human lung

ventilation rates include tidal volume of the lung and breathing frequency. Tidal volume (i.e., volume of gas inhaled or exhaled per respiration cycle) is dependent upon individual characteristics, including size, age, and sex. The breathing frequency is based on the degree of exertion, which can be related to general types of activities.

Data on ventilation rates as a function of these factors are provided in Development of Statistical Distributions or Ranges of Standard Factors Used in Exposure Assessments (Anderson et al. 1984). The data presented include ventilation values for adult males, adult females, and children during resting and during light, moderate, and heavy exertion. Representative values for each activity category are presented in Table 25. Values of inhalation rates presented in this table represent the midpoint of ranges of values reported for each activity level in Anderson et al. (1984). Resting is characterized by activities such as watching television, reading, or sleeping. Light activity includes meal cleanup; care of laundry and clothes; domestic work and other miscellaneous household chores; attending to personal needs and care; photography; hobbies; and conducting minor indoor repairs and home improvements. Heavy activity includes heavy indoor cleanup (e.g., scrubbing surfaces), and performing major indoor repairs and alterations (e.g., remodeling). Maximal activity consists of vigorous physical exercise, such as weight lifting, dancing, or riding an exercise bike. Light activity is the level that occurs most frequently during the use of consumer products.

Additional factors that influence inhalation rates include altitude and body temperature. The respiratory rate increases 5 to 6 breaths per minute per each degree Celsius rise in body temperature (ICRP 1974); likewise, inhalation rate increases with increasing altitude. Knowledge of the effect of these parameters on inhalation is not likely to enhance the quality of most exposure assessments, however.

(b) Duration of exposure. Inhalation exposure to many consumer products can be divided into several stages, each of which may have a different duration. For example, exposure to an aerosol product during active use of that product may last for only seconds or minutes. Passive exposure to direct release of that product may last for hours. And, if the aerosol product is a coating (e.g., paint) applied to a surface indoors, a third inhalation exposure stage, consisting of the period during which the chemical release rate is controlled by diffusion from the solid coating, may last for weeks or months. Duration of exposure during application of coatings to surfaces can be estimated from information on labor production (e.g., surface area covered per unit of time) and on the surface area to be covered. For some exposure scenarios involving the use of pressurized aerosol products, in the absence of better information, it may be necessary to assume that duration of exposure is equal to the duration of active release. For aerosol products in which direct release occurs intermittently over the course of

Table 25. Summary of Human Inhalation Rates for Men, Women, and Children by Activity Level (m³/hour)^a

	Resting ^b	Light ^c	Moderate ^d	Heavy ^e
Adult male	0.6	1.3	2.8	7.1
Adult female	0.6	1.3	2.4	4.9
Average adult ^f	0.6	1.3	2.6	6.0
Child, age 6	0.4	1.4	2.1	2.4
Child, age 10	0.4	1.7	3.3	4.2

^aValues of inhalation rates for males, females, and children presented in this table represent the midpoint of ranges of values reported for each activity level in Anderson et al. (1984).

^bIncludes watching television, reading, and sleeping.

^cIncludes most domestic work, attending to personal needs and care, hobbies, and conducting minor indoor repairs and home improvements.

^dIncludes heavy indoor cleanup, performance of major indoor repairs and alterations, and climbing stairs.

^eIncludes vigorous physical exercise and climbing stairs carrying a load.

^fDerived by taking the mean of the adult male and adult female values for each activity level. A representative 24-hour breathing rate for an average adult is 1.1. This value is based on the assumption that the average adult spends 93.2 percent of the time at the light/resting level of activity, 5.8 percent at a moderate level of activity, and 0.9 percent at a heavy level of activity. Values for the percent of time spent at each activity level are from Methods for Assessing Exposure to Chemical Substances in the Ambient Environment, Volume 2 of Methods for Assessing Exposure to Chemical Substances.

several minutes, professional judgment must be used to estimate the duration of active use.

Most long-term passive inhalation scenarios involve exposure to a chemical substance being released from a solid matrix. One possible approach for estimating duration of passive inhalation exposure to chemical substances released from solid matrices is to assume that release of a chemical substance will occur continuously at a constant rate throughout the lifetime of a product. One can then also assume that the duration of exposure is equivalent to the lifetime of the product. Information regarding product lifetimes can sometimes be obtained from the industry that manufactures the product or the trade association that represents the industry that manufactures the product.

(c) Frequency of exposure. Frequency of exposure, expressed in number of exposure events per year, is discussed in Section 6.2.1.

(d) Concentration of the chemical substance in indoor air. The concentration of chemical substance in indoor air is expressed in units of mass of chemical substance per cubic meter of air. The method for calculating the concentration of a chemical substance in indoor air is determined by whether the chemical substance is released instantaneously, continuously, or in a time-dependent manner. Examples of instantaneous releases include releases of volatile chemical substances from spills of products and short-term releases of chemical substances from aerosol containers. Examples of continuous releases include volatilization of chemical substances from liquids spilled instantaneously and migration of chemical substances from solids, such as dry paint films and plastics. Time-dependent releases include volatilization of chemical substances from films or coatings applied to surfaces. Usually products such as coatings are not applied instantaneously to surfaces. As a result, a method is needed to account for the fact that a chemical substance may have almost completely volatilized from the portion of the surface coated at the beginning of the period of application, while it has only begun to volatilize from the portion of the surface coated at the end of the period of application. Such differences in the change of concentration with time are accounted for in the equations used to calculate indoor air concentrations of chemical substances as a result of time-dependent releases. Equations for calculating concentrations of chemical substances in indoor air as a result of instantaneous, continuous, and time-dependent releases are presented in detail in Section 4.4.

Generally, the equations for calculating the average concentration of chemical substance in air for a given set of exposure conditions are used to estimate the value of CN to be used in the equations to estimate inhalation exposure.

6.2.3 Dermal Exposure

Despite the relative simplicity of most dermal exposure calculations, dermal exposure presents some conceptual difficulties that are not associated with inhalation or ingestion exposure. Exposure has been defined earlier as the amount of substance contacting the receptor and available for absorption. Absorption occurs when the substance crosses a physical barrier to penetrate the tissues of the receptor. "Contact" merely implies that the substance has touched the body of the receptor. "Availability" indicates that the substance has reached (but not crossed) the absorptive barrier. In the case of inhalation and ingestion, the substance is taken into a body cavity (mouth, lungs) prior to absorption. Therefore, the substance is made available by swallowing or inhaling, and the quantity to which the receptor is exposed is equivalent to the quantity inhaled or swallowed. In the case of dermal exposure, the substance contacts only the outer surface (skin) of the receptor and is not taken into the body until it has penetrated the skin (i.e., after it has been absorbed). In addition, the substance may contact the skin but be removed before it can be absorbed. This makes it difficult to define "exposure" when the receptor is in contact with large ambient volumes of liquids or gases or with a small portion of a large solid surface.

The sections that follow delineate methods that can be used to estimate dermal exposure that has occurred via three pathways: (1) exposure to a film of liquid deposited on the skin; (2) exposure to dusts and powders deposited on the skin; and (3) exposure of skin to chemical substances contained in or adhering to solid matrices. A method for assessing exposure during immersion of skin in liquids is not presented. A method for estimating absorbed dose resulting from this pathway, however, is delineated in Section 6.3.2. The major problem with attempting to assess exposure during immersion of skin in liquids is that the portion of the entire mass of the chemical substance in the solution that is in contact with the receptor is not known. Obviously, the skin of the receptor is not in contact with the entire volume of the solution. A method for determining the exact thickness of the film, or solution, in contact with the skin during the period of exposure, however, cannot be readily determined because the physical state of the solution in contact with the skin is exactly the same as the physical state of the solution that is not in contact with the skin. Any attempt to assess exposure for this pathway without taking into consideration parameters needed to estimate absorbed dose is not very meaningful.

(1) Exposure to a Film of Liquid Deposited on the Skin. Most significant, quantifiable dermal consumer exposure scenarios involve liquid films on the skin. Exposure is generally expressed as mass per year. For each use of the product, the assessor determines the mass of liquid deposited on the skin by multiplying (1) the estimated volume of

liquid deposited by (2) the estimated concentration of the subject chemical substance in the liquid deposited on the skin. This, multiplied by the number of annual exposures, yields total mass per year. Since exposure is by direct physical contact, there are no fate or transport-related parameters involved.

The product obtained by multiplying (1) the area of skin likely to be exposed during ordinary use by (2) the film thickness is an estimate of the volume of liquid deposited on the skin. The film thickness of a liquid can be determined using the following equation:

$$\text{Film thickness (cm)} = \frac{\text{amount of liquid retained on skin (mg/cm}^2\text{)}}{\text{density of liquid (g/cm}^3\text{)} \times 1000 \text{ (mg/g)}}$$

Experimentally determined values of the amount of liquid retained on hands are presented in Methods for Estimating the Retention of Chemical Liquids on Hands, Volume 13 of Methods for Assessing Exposure to Chemical Substances (Versar 1984a). In this study, the retention of selected liquids on the hands of human volunteers was measured under five conditions of exposure: (1) uptake by dry skin (initial uptake); (2) uptake by skin previously exposed to the liquid and still wet (secondary uptake); (3) uptake from handling a rag; (4) uptake from spill cleanup; and (5) uptake from immersion of a hand in a liquid.

Initial uptake, secondary uptake, and uptake from handling a rag all involved contact with a cloth saturated with the liquid. The method for determining liquid retained on the hands for each of the five experimental conditions is as follows:

- Initial uptake - A cloth saturated with liquid was rubbed over the front and back of both clean, dry hands for the first time during an exposure event.
- Secondary uptake - As much as possible of the liquid that adhered to the skin during initial uptake was removed using a clean cloth. A cloth saturated with the liquid was then rubbed over the front and back of both hands for the second time during an exposure event.
- Uptake from handling a cloth - A cloth saturated with liquid was rubbed over the palms of both hands for the first time during an exposure event in a manner simulating handling of a wet cloth.
- Uptake from immersion - An individual immersed one hand in a container of liquid, removed the hand, then allowed the liquid to drip from the hand back into the container for 30 seconds (one minute for cooking oil).

- Uptake from spill cleanup - An individual used a clean cloth to wipe up 50 milliliters (ml) of liquid poured onto a plastic laminate countertop.

For each exposure condition, the quantity of liquid retained on the hands was determined: (1) immediately following the exposure condition; (2) after a partial wipe; and (3) after a full wipe (except in the case of uptake by immersion and uptake from spill cleanup). A partial wipe refers to a light, quick wipe with a clean cloth. A full wipe refers to a thorough, complete wipe with a clean cloth.

The method for determining the quantity of liquid remaining on the exposed area of the hands, presented in mg/cm^2 , was the same for all tests involving use of a cloth saturated with liquid. The quantity of liquid remaining on the exposed area of the hands immediately following exposure (the initial quantity) was determined by subtracting the weight of the cloth saturated with liquid after exposure from the weight of the cloth saturated with liquid before exposure, and dividing this difference by the exposed skin surface area. The quantity of liquid remaining on the exposed area of the hands after a partial wipe was determined by subtracting the quantity removed by a partial wipe from the initial quantity, and dividing this difference by the exposed surface area. The quantity remaining after a full wipe was determined by subtracting the quotient of the quantity removed by the full wipe divided by the exposed surface area from the quantity remaining after a partial wipe.

The quantity of liquid remaining on the exposed area of the hands immediately following immersion and spill cleanup was determined by, first, summing the quantities of liquid removed by a partial wipe and a full wipe. This sum was then divided by the exposed surface area. The resulting quotient was added to the value for quantity in mg/cm^2 remaining on the skin after a full wipe as determined in the initial uptake test. To give an estimate of the total quantity of liquid deposited by immersion or spill cleanup, the quantity of liquid remaining after a partial wipe was determined by dividing the quantity removed by a full wipe by the exposed surface area and adding this quotient to the value for quantity remaining on the skin after a full wipe as determined in the initial uptake test.

Initially six liquids were selected in this study to represent a broad range of kinematic viscosities. The liquids used were (1) mineral oil, (2) cooking oil, (3) water-soluble oil (bath oil), (4) oil/water emulsion (50:50, water:water-soluble oil), (5) water, and (6) water/ethanol (50:50). (Efforts to include additional liquids in this study are on-going). Table 26 presents values of film thickness for these six liquids under each of the five exposure conditions immediately following exposure, after a partial wipe, and after a full wipe. The

Table 26. Film Thickness Values of Selected Liquids
Under Various Experimental Conditions (10^{-3} cm)

	Mineral oil	Cooking oil	Bath oil	Oil/ water	Water	Water/ ethanol
<u>Initial uptake</u>						
Initial film thickness of liquid on hands	1.62	1.63	1.99	2.03	2.34	3.25
Film thickness after partial wipe	0.69	0.68	0.76	1.55	1.83	2.93
Film thickness after full wipe	0.21	0.16	0.21	1.38	1.97	3.12
<u>Secondary uptake</u>						
Initial film thickness of liquids on hands	1.43	1.51	1.80	1.60	2.05	2.95
Film thickness after partial wipe	0.47	0.53	0.51	1.19	1.39	2.67
Film thickness after full wipe	0.14	0.11	0.12	0.92	1.32	2.60
<u>Uptake from handling a rag</u>						
Initial film thickness of liquid on palms	1.64	1.50	2.04	1.88	2.10	4.17
Film thickness after partial wipe	0.44	0.34	0.53	1.21	1.48	3.70
Film thickness after full wipe	0.13	0.01	0.21	0.96	1.37	3.58

Table 26. (Continued)

	Mineral oil	Cooking oil	Bath oil	Oil/ water	Water	Water/ ethanol
<u>Uptake from immersion</u>						
Estimated initial film thickness of liquid on hand	15.88	11.28	12.06	9.81	4.99	6.55
Estimated film thickness of liquid remaining after partial wipe	1.49	1.59	1.51	2.42	2.14	2.93
<u>Uptake from spill cleanup</u>						
Estimated initial film thickness of liquid on hand	1.23	0.73	0.89	1.19		
Estimated film thickness of liquid remaining after partial wipe	0.55	0.51	0.48	1.36		

Source: Versar (1984a)

values for film thickness presented in this table were derived from the experimental data on (1) amounts of liquid retained on the hands and (2) densities of liquids from the study to assess exposure resulting from retention of chemical liquids on hands (Versar 1985a).

The volume of liquid deposited on the skin cannot be estimated reliably by calculations involving quantity of product consumed per use except in cases when the total amount consumed per use is applied directly to the skin (e.g., cosmetic products). For example, exposure to substances spilled on the skin has occasionally been estimated by predicting (arbitrarily) the amount likely to be spilled (e.g., 1 ml) or the percent of product likely to be spilled (e.g., 10 percent). This may yield an unrealistically high level of exposure, since measured film thicknesses of liquids on the skin are on the order of magnitude of 10^{-3} cm (Versar 1984a). Therefore, most of a quantity of liquid spilled on the skin would probably drip off immediately and not constitute genuine exposure.

An estimate of the concentration of the subject chemical substance on the skin is derived by multiplying together: (1) the weight fraction (WF) of the chemical substance in the product, (2) the density (DSY) of the formulation, and (3) the dilution factor (DIL), or fraction of formulation present as used by the consumer during the exposure event.

The basic equation for estimating annual dermal exposure via a liquid film is as follows:

$$\text{DEX} = \text{WF} \times \text{DSY} \times \text{DIL} \times \text{T} \times \text{AV} \times \text{FQ} \quad (6-3)$$

where

DEX = annual dermal exposure (mg/yr)
WF = weight fraction of chemical substance in product (unitless)
DSY = density of formulation (mg/cm³)
DIL = dilution fraction (unitless)
T = film thickness of liquid on the skin surface (cm)
AV = skin surface area exposed per event (cm²/event)
FQ = frequency of events per year (events/yr).

The variables of equation (6-3) are determined as follows:

- The weight fraction (WF) of a chemical substance in a formulation can sometimes be obtained from the product label. Other sources of information that may be needed to determine the weight fraction of chemical substances in products are discussed in Section 3. A

generic approach for determining the weight fraction of a chemical substance based on knowledge of its function in a product can also be used. This generic approach and values for the weight fraction of functional components in select consumer products are presented in Section 3.

- The density (DSY) of a formulation can sometimes be obtained from the product label. It can also be easily determined experimentally if the product is available. Table 11 of Section 3 presents experimentally determined values for the density of select consumer products. For products not included in Table 11 it is suggested that the density of the chemical substance making up the largest weight fraction in the formulation be used as a default value for the density of the product. Densities for specific chemical substances can be obtained from references listed in Table 9 of Section 2.
- The dilution fraction (DIL) is the quotient obtained from dividing the mass of product by the mass of substance in which this mass of product is diluted. The dilution fraction can sometimes be determined from information on the product label. Products that are used undiluted are assigned a value of 1.0 for dilution fraction.
- The film thickness of a liquid on the skin (T) is the quotient obtained by dividing the mass of liquid retained per square centimeter (cm^2) of skin surface by the density of the liquid as used by the consumer. Table 26 presents values for film thickness of selected liquids under various experimental conditions based on data from Methods for Estimating the Retention of Chemical Liquids on Hands (Versar 1984a). For assessing dermal exposure to liquids listed in Table 26, the values presented in this table for film thickness can be used without adjustment. To assess dermal exposure to liquids that are not listed in this table, one can use data for the liquid that most closely resembles the liquid for which one is trying to assess exposure. Two physical properties that can be used to compare liquids are kinematic viscosity and density. Values for kinematic viscosity and density can be obtained from references listed in Table 9 of Section 2. The experimentally determined values for density and kinematic viscosity for the six liquids used in the study to assess exposure from retention of liquids on hands are presented in Table 27. However, the error from using default values as values of film thickness for liquids not listed in Table 26 may be considerable. In the study to assess exposure from retention of liquids on hands, the relationship between kinematic viscosity and mass of liquid retained per cm^2 of skin was examined. Although liquid

Table 27. Experimentally Determined Values for Density and Kinematic Viscosity of Six Selected Liquids

Liquid	Density (g/cm ³)	Kinematic viscosity (cSt ^a)
Mineral oil	0.8720	183.0
Cooking oil	0.9161	65.4
Bath oil	0.8660	67.2
Bath oil/water	0.9357	4.19
Water	0.9989	1.02
Water/ethanol	0.9297	2.55

Source: Versar (1984a).

^acentistokes.

retention was found to increase with kinematic viscosity, the data did not support a functional relationship between these two parameters. Additional liquids must be examined to determine whether a functional relationship exists between these two parameters.

- The exposed skin surface area (AV) can be ascertained from judgment as to regions of the body likely to be exposed during use of the product and from generic values for skin surface area presented in Table 28.

(2) Exposure to Dusts and Powders Deposited on the Skin. Exposure to dusts and powders is similar to exposure to liquid films, since it involves the deposition of a limited, quantifiable amount of product on the skin. The parameter, dust adherence (DA), however, replaces the film thickness (T) and density (DSY) parameters required in equation (6-3) for estimating dermal exposure to liquid films. The dust adherence parameter is expressed in units of mass per unit of skin surface area and unlike liquid films, does not require a density factor to convert volume to mass.

The basic equation for estimating annual dermal exposure to dusts and powders deposited on skin is as follows:

$$\text{DEX} = \text{WF} \times \text{AV} \times \text{DA} \times \text{FQ} \quad (6-4)$$

- DEX = annual dermal exposure (mg/year)
WF = weight fraction of chemical substance in product (unitless)
AV = skin surface area exposed per event (cm²/event)
DA = dust adherence (mg/cm²)
FQ = frequency of events per year (events/year).

Methods for determining the variables, WF, AV, and FQ, were delineated in Section 6.2.3(1). Data on dust adherence to skin (DA) are limited. The following experimental values for dust adherence were reported by the Toxic Substances Control Commission of the State of Michigan (Harger 1979):

- Vacuum cleaner dust sieved through an 80-mesh screen adheres to human hands at 3.44 mg/cm².
- Dust of the clay mineral kaolin adheres to hands at 2.77 mg/cm².
- Commercial potting soil adheres to hands at 1.45 mg/cm².

Table 28. Surface Area of Body Regions^a

Body region	Percent of total surface area		Generic surface area (cm ²)		
	Male	Female	Male	Female	Average adult
Total adults ^c	100	100	19,400	16,900	18,150
Head and neck	7.8	7.1	1,180	1,100	1,140
Face ^d	2.6	2.4	390	370	380
Neck ^d	2.6	2.4	390	370	380
Scalp ^d	2.6	2.4	390	370	380
Upper extremities ^e	18.8	17.9	3,190	2,760	2,975
Arms (both, excluding hands)	14.1	14.0	2,280	2,100	2,190
Upper arms ^f	7.4	7.4	1,430	1,250	1,340
Forearms ^f	5.9	5.9	1,140	1,000	1,070
Hands	5.2	5.1	840	750	795
Outstretched palm and fingers ^g	2.6	2.6	420	375	400
Lower extremities ^h	37.5	40.3	6,360	6,260	6,310
Legs	31.2	32.4	5,050	4,880	4,970
Thighs	18.4	19.5	1,980	2,950	2,470
Lower legs	12.8	12.8	2,070	1,940	2,005
Feet	7.0	6.5	1,120	975	1,050
Trunk	35.9	34.8	5,690	5,420	5,555
Total, 3-6 year-old child ^c	100	100	7,280	7,110	7,200
Total, 6-9 year-old child ^c	100	100	9,310	9,190	9,250
Total, 9-12 year-old child ^c	100	100	11,600	11,600	11,600

^aUnless otherwise noted, values for surface area presented in this table are mean values reported in Anderson et al. (1984).

^bValues presented in this table for average surface area are the average of values reported or derived for males and females.

^cThe values for surface area of the total body presented in this table for adults and children are based on values of surface area, reported for the 50th percentile group in Anderson et al. (1984).

^dValues presented for surface area of this body region are based on the assumption that this body region comprises one-third of the surface area of the head and neck.

^eIncludes arms and hands.

^fAnderson et al. (1984) do not report values for females for these body regions; values presented were obtained by applying the percentage of total body surface area reported for males for these body regions to the total body surface area value for females presented in this table.

^gA value of one-half the surface area of the hands is assumed.

^hIncludes legs and feet.

The conditions of the experiment were not reported. Since the research was performed to support predictions of occupational exposure to the chemical, 4, 4' - methylenebis (2-chloroaniline) (MBOCA), and since occupational contact is likely to yield maximum saturation of the skin, it is assumed that the experimental conditions were designed to encourage maximum dust adherence (Versar 1982). It is not known, however, which physical or chemical properties of a powdered substance determine the extent of its adherence to skin; therefore, it is not possible to predict the extent to which the three substances tested may represent commonly encountered household products (e.g., powdered detergent).

Until more data become available, the value for vacuum cleaner dust can be used as an upper limit. Substances that are lipophilic or surfactant, or that tend to clump in the presence of skin moisture, may adhere to a greater extent. However, since maximum adherence is probably rare in most household exposure scenarios, the value for vacuum cleaner dust probably represents dust adherence under reasonable worst case conditions.

(3) Exposure of Skin to Chemical Substances Contained in or Adhering to Solid Matrices. The primary application for assessing exposure of skin to chemical substances contained in or adhering to solid matrices is the assessment of dermal exposure to substances in clothing. Exposure to substances in clothing can be divided into substances contaminating clothing, such as detergent residues, and substances that are ingredients of clothing, such as dyes. In the case of both dyes and residues, the fraction transferred to the skin must be known to accurately assess exposure. The tendency for chemical substances to transfer to skin varies with the quantity of residue or dye on the fabric, the specific chemical substance being transferred from the fabric to the skin, physical and chemical properties of the skin surface being contacted, and duration of contact of skin with the substance being transferred. No experimental data regarding transfer of residues or dyes to skin have been found. As a result of a lack of data for this parameter, arbitrary values for percent transfer during exposure must be used.

In an assessment of consumer exposure to sodium LAS (Linear alkanesulfonate surfactant) in detergent products, Procter and Gamble (1981 as cited in JRB 1982b) calculated dermal absorption of sodium LAS in detergent residues on clothing using an arbitrary transfer factor for detergent residue of ten percent (.10) (JRB 1982b). Equation (6-5) is suggested for estimating annual dermal exposure to chemical substances in residues or to dyes and other chemicals on clothing in cases where the amount of chemical substance deposited on the fabric surface is known or can be estimated. This equation is adapted from an equation used by Procter and Gamble to determine dermal absorption of sodium LAS present in detergent residues on clothing.

$$\text{DEX} = \text{ADF} \times \text{TF} \times \text{AV} \times \text{FQ} \times \text{WF} \quad (6-5)$$

where

- DEX = annual dermal exposure (mg/year)
- ADF = amount of product or residue deposited on the fabric surface (mg/cm²)
- TF = fraction of residue transferred to the skin per exposure event (event⁻¹)
- AV = area of skin surface exposed (cm²)
- FQ = frequency of events per year (events/year)
- WF = weight fraction of chemical substance of interest in product or residue. (This value is equal to 1 where the product or residue is the chemical of interest.)

Note that for substances formulated to adhere to fabric, such as dyes, an arbitrary transfer factor of ten percent for a given exposure event would probably yield a vast overestimate of dermal exposure under most conditions. It is suggested that the assessor arbitrarily assume the percent of dye that would be lost during a lifetime of wearings. The assessor can then assume that a major portion of the dye would be lost when the fabric is washed. The remaining fraction of dye could then be assumed to be lost during fabric wear. Information regarding the typical lifetime of the cloth item and on the number of times that an individual would contact or wear the item could be used to estimate the fraction of dye transferred to the skin per event. Some of this information can be found in The Generic PMN Report on Surfactants (JRB 1982b) prepared for the Exposure Evaluation Division of the Office of Pesticides and Toxic Substances of the U.S. Environmental Protection Agency. Trade associations representing the textile industry may also be a source for this information.

6.2.4 Ingestion Exposure

Methods for assessing exposure resulting from ingestion are delineated in this section for two pathways: Exposure due to ingestion of chemical substances leached out of objects used in the mouth and exposure resulting from unintentionally swallowing liquids used in the mouth. A method for estimating ingestion exposure as a result of swallowing inhaled particles too large to be respired is described in Appendix A.

(1) Ingestion Exposure to Chemical Substances Leached Out of Objects Designed to Be Used in the Mouth. Athletic mouth guards, pacifiers, and teethers can serve as sources of chemical substances that can be ingested. For example, children place teethers and/or pacifiers in their mouths and suck or chew on them. In the process, chemical substances may

leach or diffuse from the object into saliva and may subsequently be swallowed. Exposure from this pathway can be estimated if experimental data on the rate of leaching of the chemical substance from the object into saliva are available. The basic equation for estimating annual ingestion exposure to a chemical substance that has leached out of an object used in the mouth is as follows:

$$\text{ING} = \text{LR} \times \text{SAO} \times \text{D} \times \text{F} \quad (6-6)$$

where

- ING = annual ingestion exposure (mass/year)
- LR = experimentally determined leaching rate of the chemical substance from the object into saliva (mass/hr/cm²)
- SAO = surface area of the object being placed in mouth (cm²)
- D = duration of exposure (hours/event)
- F = annual frequency of exposure events (events/year).

A major limitation of this method is the necessity of using experimental data on rate of leaching of the specific chemical substance from the object.

(2) Ingestion Exposure from Unintentionally Swallowing Liquids Used in the Mouth. Toothpaste and mouthwash are examples of consumer products intended to be used in the mouth but not intended to be consumed. The basic equation for estimating annual ingestion exposure to chemical substances present in liquids used in the mouth that are swallowed unintentionally is as follows:

$$\text{ING} = \text{WF} \times \text{M} \times \text{LUS} \times \text{F} \quad (6-7)$$

where

- ING = annual ingestion exposure (mass/year)
- WF = weight fraction of chemical substance in liquid (unitless)
- M = mass of liquid used per exposure (mass/event)
- LUS = fraction of liquid used in the mouth that is swallowed unintentionally (unitless)
- F = annual frequency of exposure events (events/year).

A major limitation of this method is that there are no data to support any generalization regarding the proportion of liquids used in the mouth that may be swallowed unintentionally. Consequently, an arbitrary value must be selected for this parameter.

6.3 Absorbed Dose

6.3.1 Inhalation

Absorption from the lung of toxicants that are gases, volatilized liquids, or liquid aerosols is usually rapid and complete, since the lung surface is large (50 to 100 square meters) and blood flow to the lung is high and in proximity to the alveolar air (10 μm) (Casarett and Doull 1975). Absorption of liquids in aerosols probably occurs by diffusion; therefore, lipid-soluble compounds are absorbed most readily.

Particulate matter reaching the alveoli can be removed by three major routes: (1) direct translocation of the toxicant from the alveoli into the blood, (2) removal via the bronchi to the gastrointestinal tract, and (3) migration via the lymphatic system (Casarett and Doull 1975). Removal of particulate matter via direct translocation of the toxicant from the alveoli into the blood is an important route for soluble compounds. Removal via the bronchi to the intestinal tract appears to be composed of a relatively rapid clearance phase (1 day) that is not affected by the nature of the toxicant and a much slower phase (days to years) that is dependent on the nature of the toxicant. Particles can penetrate the interstitial tissue of the lung and migrate via the lymphatic system as free particles or engulfed in cells that consume debris and foreign bodies (phagocytes). Particulate material can remain in the lymphatic tissue for long periods of time. Some particulates may remain in the alveolus indefinitely, however, in cases where lung tissue proliferates to form a plaque or nodule around the particle.

6.3.2 Dermal

In order to be absorbed through the skin, a substance must pass through epidermal cells, the cells of the sweat or sebaceous glands, or hair follicles. Most substances pass through epidermal cells. Chemicals must pass through a large number of cells: the outer densely packed layer of horny, keratinized epidermal cells; the germinal layer of the epidermis; the corium; and the systemic circulation. For lung or gastrointestinal absorption, on the other hand, a substance need pass through only two cells.

The first phase of percutaneous absorption is diffusion through the epidermis, which is rate-limiting. The stratum corneum is much thicker in some areas than others. The stratum corneum conjunctivum area is the least permeable. Polar and nonpolar substances diffuse by different molecular mechanisms. Polar substances diffuse through the outer surface of the protein filaments of the hydrated stratum corneum, while nonpolar molecules probably dissolve in and diffuse through the nonaqueous lipid matrix between the protein filaments. The rate of diffusion of nonpolar

substances is related to the lipid solubility and inversely related to the molecular weight. The second phase is clearance of substance from dermis, which is much less compact than epidermis, and passage into circulation. The latter phase depends on blood flow, interstitial fluid movement, lymphatics, and other factors (Casarett and Doull 1975).

Brown et al. (1984) present a comprehensive list of variables that influence rate and amount of skin absorption. Variables such as amount of skin surface area exposed, duration of exposure, and type of skin exposed are acknowledged by Brown et al. (1984) to influence absorption. Other variables reported by Brown et al. (1984) to influence absorption are discussed below.

- Hydration - Absorption is reported to increase with increasing hydration of the skin. If the skin is hydrated (covered with perspiration, immersed in water) or the chemical substance being absorbed is in solution, diffusion and penetration will be enhanced. A pure liquid solvent, on the other hand, will dehydrate skin and elicit compaction of the stratum corneum, which will act to slow absorption of the chemical.
- Temperature - Increased skin or solute (water) temperature is reported to enhance skin absorption capacity proportionately.
- Skin Condition - Any damage (sunburn, cuts, wounds, abrasions) to the stratum corneum is reported to compromise its ability to act as a barrier against foreign substances.
- Regional Variability - The epidermis of the hand is reported to represent a greater barrier to penetration than the epidermis of many other parts of the body; penetration through the scrotum is estimated to be 100 percent.
- Individual Variability - Absorption rates are reported to vary among individuals, and even for the same individual over time. Variables such as age, sex, ratio of body fat to total weight, previous exposure, nutrition, type and amount of skin exposed, and the specific conditions of exposure are all reported to affect actual absorption.

- Physical and Chemical Properties of the Chemical Substance - Factors affecting absorption are reported to include lipophilicity, polarity, volatility, molecular weight, carbon number, and solubility of the chemical substance in the stratum corneum. The pH of a solution is also reported to affect absorption of the solution.
- Vehicles and Accelerants - Various compounds such as alcohols, solvents, and chloroform are reported to demonstrate permeability-enhancing effects. Soaps and surfactants are also reported to increase skin permeability significantly.
- Synergistic Effects - Combinations of compounds are reported to have greater effects on the stratum corneum and to be absorbed more readily.

Brown et al. (1984) also reported findings from a review of the existing literature on absorption rates of volatile solvents in aqueous solutions having direct contact with skin. According to this review, for dilute aqueous solutions, absorption of solute is directly proportional to concentration in accordance with Fick's law; for pure or highly concentrated liquids, however, this relationship is not necessarily true. In fact, much experimental evidence exists indicating that permeation rates are actually increased with dilute aqueous solutions as compared to pure liquids. Investigators reportedly attribute this effect to the compaction and dehydration of the stratum corneum when in contact with pure liquids, in addition to other factors. The implication of the findings from this literature review is that the use of absorption rates obtained from experiments with pure chemicals may considerably underestimate absorption of chemical substances in dilute aqueous solutions.

The following subsections present equations and describe methods that can be used to estimate dermal absorption of chemical substances via three exposure pathways : (1) dermal absorption from exposure to a film of liquid deposited on the skin; (2) dermal absorption from exposure during immersion of skin in liquids; and (3) dermal absorption during exposure of skin to chemical substances contained in or adhering to solid matrices. The equation for estimating dermal absorbed dose is the same for exposure to a film of liquid on the skin and for exposure during immersion of skin in liquids. For purposes of estimating dermal absorbed dose, these two exposure pathways are grouped together. The method used is referred to as the method for estimating absorbed dose resulting from dermal contact with liquids. This method is presented in section (1). The method for estimating dermal absorption during exposure of skin to chemical substances contained in or adhering to solid matrices is presented in section (2). A method for estimating absorbed dose for

solids not in solution (i.e., dusts and powders) is not delineated. No information was found in a limited information search to predict dermal absorbed dose for solids not in solution.

(1) Method for Estimating Dose Absorbed as a Result of Dermal Contact with Liquids. The parameters required to estimate dermal absorption are the same for contact with liquids via any exposure pathway. The following equation can be used to estimate dermal absorption resulting from contact with liquids.

$$ADD = C \times D \times AV \times K_p \times FQ \quad (6-8)$$

where

ADD = annual dermal dose (mg/year)
C = concentration of chemical substance in the liquid medium (mg/l)
D = duration of dermal exposure (hours/event)
 K_p = permeability constant (liters/cm² x hours)
FQ = frequency of exposure events per year (events/year).

The permeability constant (K_p) is influenced by such factors as the absorption rate and concentration of the chemical substance. The absorption rate is, in turn, determined by factors such as skin condition, chemical and physical properties of the chemical substance, and other factors discussed previously in Section 6.3.2. Where skin absorption rate and concentration are known, for dilute aqueous solutions, the permeability constant can be calculated using Fick's law. The following equation expresses Fick's law.

$$J_s = K_p \Delta C_s \quad (6-9)$$

where

J_s = permeation rate (flux) of the solute (mg/cm² - hr)
 K_p = permeability constant (liters/cm² - hr)
 ΔC_s = concentration difference of the solute across specified tissue (mg/liter).

Additional experimental data are needed, however, to determine the relationship between skin absorption rate and concentration for highly concentrated or pure chemicals. Furthermore, more experimental data are needed to determine at what concentration of a chemical substance the assumption of linearity (proportionality) no longer holds true.

(2) Method for Estimating Dermal Absorption During Exposure of Skin to Chemical Substances Contained in or Adhering to Solid Matrices. The following equation has been used by Procter and Gamble (JRB 1982b) to estimate dermal absorption of sodium LAS present in residues on clothing surfaces.

$$ADD = ADF \times TF \times AV \times FA \times FQ \times WF \quad (6-10)$$

where

- ADF = amount of product or residue deposited on the fabric surface (mg/cm²)
- TF = fraction of residue transferred to the skin per exposure event (unitless)
- AV = area of skin surface exposed (cm²)
- FA = fraction of chemical substance absorbed (unitless)
- FQ = frequency of exposure events (events/year)
- WF = weight fraction of chemical substance of interest in product or residue; (This value is equal to 1 where the product or residue is the chemical of interest.)

Because of a general lack of data on the tendency for substances to transfer to skin, an arbitrary factor must be used. In the assessment of consumer exposure to sodium LAS in detergent residues on clothing, Procter and Gamble used an arbitrary value of .10 to represent the fraction of detergent residue transferred to the skin per exposure event (JRB 1982b). No information has been found regarding arbitrary values used in consumer exposure assessments to represent the fraction of dyes transferred to skin per exposure event. The qualitative method based on estimates of the percent of dye that would be lost during a lifetime of wearings, described in Section 6.2.3(3), can be used in the absence of quantitative data for this parameter. Another limitation of this method is that the fraction of chemical substance absorbed over the period of exposure must be known. This requires experimental data on dermal absorption of chemical substances for which absorption is being estimated. If such data are lacking for the specific chemical substance for which absorption is being estimated, absorption data for analogues of the chemical substance must be used, if available. Even if experimental data on absorption are available, such data must be used with the understanding that absorption measured during the experimental condition may not necessarily be applicable to factors contributing to absorption during the exposure event.

6.3.3 Ingestion

Absorption from the gastrointestinal tract can occur anywhere along its length, from the mouth to the rectum. For example, some drugs are administered sublingually (e.g., nitroglycerine) where they are absorbed rapidly; also, when substances are absorbed via oral mucosa, passage through the liver is minimized, retarding metabolism of the substance (Goodman and Gilman 1975).

If a substance is a weak organic acid or base, it will tend to be absorbed by diffusion in the part of the gastrointestinal tract in which it exists in the most lipid-soluble form. Since the gastric juice is very acid and the intestinal contents are nearly neutral, the lipid solubility of a substance can be very different in these two areas. For example, a weak organic acid (e.g., benzoic acid) is in the nonionized lipid-soluble form in the stomach and therefore tends to be absorbed by the stomach. However, a weak organic base (e.g., aniline) is not in the lipid-soluble form in the stomach but is lipid soluble in the intestine, so it tends to be absorbed in the intestine. Because of their large surface area, however, the intestines will continue to absorb nonionized chemicals present as long as the equilibrium maintains a finite concentration of them available for absorption (Casarett and Doull 1975).

Specialized transport systems occur in the gastrointestinal tract for the absorption of nutrients and electrolytes. For example, there are a number of carrier systems for the absorption of certain sugars, amino acids, and pyrimidines, as well as for iron, calcium, and sodium. Pollutants can often be absorbed by these systems, e.g., 5-fluorasil by the pyrimidine transport system, thallium by the system that normally absorbs iron, and lead by the system that normally transports calcium. Some metals are absorbed by a two-step process. For example, iron first diffuses into intestinal cells and then is actively transported into the blood; cobalt and manganese compete for this transport system (Casarett and Doull 1975).

Particles can be absorbed by the gastrointestinal epithelium, including azo dyes of nearly 100 μm diameter, and polystyrene latex particles from an emulsion, up to 220 μm in diameter.

The following are some of the factors that influence gastrointestinal absorption (Casarett and Doull 1975):

- Stability of substance to the acids, enzymes, and flora of the gastrointestinal system.
- Presence of compounds that increase absorption; e.g., EDTA alters the state of membranes by removing calcium, thus increasing permeability to bases, acids, and neutral compounds alike.

- Alteration of gastrointestinal motility.
- Dissolution rate if substance is insoluble.
- Size of particles.
- Bulk content of food mass.

Also, complexes with other substances in food may decrease absorption (Goodman and Gilman 1975).

The complexity of the above factors makes it difficult to predict absorption. For example, the fully ionized quaternary ammonium compound, pralidoxime (2-PAM), is not expected to be absorbed on the basis of the pH-partition hypothesis described earlier. Nevertheless, experimental results show that it is almost completely absorbed from the gastrointestinal tract (Casarett and Doull 1975). Because the factors that determine gastrointestinal absorption are highly situation-specific and lack common quantifiable parameters, no methods for estimating gastrointestinal absorption are delineated herein.

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APPENDIX A

**Method for Estimating Inhalation Exposure to Particulates
Discharged from Consumer Products**

(1) Introduction. Airborne particulates in the volume of inhaled air have several possible fates. Particles originally in the volume of inhaled air may not even enter the respiratory system. The aspiration efficiency (the fraction of particles originally in the volume of inhaled air that enters the nose or mouth) depends on particle size, air velocity, inhalation flow rate, and whether nose or mouth breathing is used. When averaged over all wind directions for winds ranging from 0.75 m/sec to 2.75 m/sec (typical conditions), the maximum aspiration efficiencies for particle sizes of 1 μm , 5 μm , and 10 μm are 100 percent, 85 percent, and 70 percent, respectively. Aspiration efficiency drops slowly for particle sizes larger than 10 μm ; aspiration efficiencies for particles 30 μm and 60 μm in diameter are 50 percent and 35 percent, respectively (Hinds 1982).

Once inhaled, particles may undergo respiratory tract deposition or they may be exhaled without deposition. Total deposition, as the term is used here, is defined as the average probability of an inspired particle touching a surface of the respiratory tract and thereby being deposited (Heyder et al. 1980b). The respiratory tract may be divided into three deposition regions, based on the physical processes governing deposition and the ultimate fate of deposited particles. Deposition in the head region (i.e., nose, mouth, pharynx, and larynx) is the result of sedimentation and impaction (Hinds 1982). This region effectively filters out all inhaled particles greater than 10 μm in diameter, and a large number of particles in the 1 μm to 10 μm range. The tracheobronchial region, which comprises the airways from pharynx to terminal bronchioles, traps many smaller particles in the 0.01 μm to 10 μm size range by impaction and sedimentation (Meyer 1983, Hinds 1982). Particles 0.01 μm to 10 μm in diameter that pass through the bronchioles are available for deposition via diffusion and sedimentation in the alveolar region of the lungs. Particles deposited in the head and tracheobronchial regions are either cleared to pharynx and swallowed, thus available for indirect ingestion exposure via the gastrointestinal tract, or are expelled with sputum. Thus, of the mass of inhaled particulates, only the respirable particles (i.e., particles small enough to reach the alveolar region) are available for exposure via the lungs.

Most exposure assessments have neglected to distinguish between inhaled chemicals destined for the lungs and inhaled chemicals destined for the gastrointestinal tract. Equation (A-1) below represents the traditional approach to assessment of inhalation exposure.

$$E_I = I \int C(t) dt \quad (A-1)$$

where

- E_I = inhalation exposure (mass/time)
- I = inhalation rate (volume/time)
- t = duration of exposure (time)
- C_t = concentration of chemical in air as a function of time (mass/volume).

While the traditional approach is suitable for chemicals in gaseous or vapor form and as a model for "worst case" exposure to chemicals in particulate form, a more refined approach, which distinguishes between pulmonary and gastrointestinal exposure to particulates, will enhance the precision of both exposure and risk assessments. Therefore, the methods presented in this Appendix will depart from the traditional approach by providing algorithms that allow for separate estimates of the pulmonary and gastrointestinal tract components of inhalation exposure for inhaled particulates, to be used at the discretion of the exposure assessor. It should be stressed that, despite the distinction made here between pulmonary exposure and gastrointestinal exposure, these methods do not include calculation of absorbed dose. The factors that govern the extent to which inhaled substances are absorbed are largely chemical-specific; therefore, the prediction of absorbed dose is not currently amenable to the generic approach that is the foundation of this report.

(2) Exposure Calculation. Assessment of inhalation exposure to consumer products involves finding a simple or complex solution to equation (A-1) and identifying appropriate parameter values. In practice, the algorithm used to calculate inhalation exposure is usually an integrated and simplified version of equation (A-1), often incorporating simplifying assumptions about the change in concentration with time. (See Section 4 for a detailed discussion of methods for calculating concentration.) In many cases, exposures can be calculated using an average concentration for a given period of time; exposures from several such consecutive time periods can be summed to estimate total inhalation exposure to a given product. The simplified version of equation (A-1) is presented below.

$$IHX = IR \times DU \times FQ \times CN \quad (A-2)$$

where

IHX = quantity inhaled (mg/yr)
IR = inhalation rate (m³/hr)
DU = duration of exposure event (hours)
FQ = frequency of exposure (events per year)
CN = indoor air concentration of a given constituent (mg/m³).

If precise estimates of exposure are desired, modifications of the above equation can be made for chemicals present in air as particulates, to account for the previously mentioned variation in both total and regional deposition as a function of particle size. In this case, the total exposure to inhaled particulates is calculated using equation (A-3), which includes a term (TDF) that accounts for the fraction of inhaled particulates deposited in the respiratory tract. (Note that aspiration efficiency is assumed to be 100 percent, a worst case assumption.)

$$\text{IHx} = \text{IR} \times \text{DU} \times \text{FQ} \times \text{CN} \times \text{TDF} \quad (\text{A-3})$$

where

IHX, IR, DU, and FQ are as used in equation (A-2).

TDF = total deposition fraction, which is the weight fraction of inhaled particles deposited in the respiratory tract.

The total exposure to particulates calculated in equation (A-3) can be divided into the pulmonary region exposure (IHXP) and the gastrointestinal tract exposure (IHxG), using equations (A-4) and (A-5), respectively. This partitioning of inhalation exposure is an option that may be worthwhile for chemicals whose effects depend on the mode of entry into the body.

$$\text{IHx}_p = \text{IR} \times \text{DU} \times \text{FQ} \times \text{CN} \times \text{RF} \quad (\text{A-4})$$

$$\text{IHx}_G = \text{IR} \times \text{DU} \times \text{FQ} \times \text{CN} \times \text{NRF} \quad (\text{A-5})$$

where

RF = respirable fraction, which is the weight fraction of all inhaled particles deposited in the pulmonary airspaces

NRF = nonrespirable fraction, which is the weight fraction of all inhaled particles deposited in the head or tracheobronchial regions.

For the purpose of this analysis, it is assumed that all of the inhaled particulates that are deposited in the respiratory tract are destined for either the lungs or the gastrointestinal tract, as shown in equation (A-6). (No information was available on the fraction of material initially deposited in the head or tracheobronchial region that might be subsequently expelled with sputum.)

$$\text{IHx} = \text{IHx}_p + \text{IHx}_G \quad (\text{A-6})$$

(3) Inhalation Exposure Parameters. Information on the parameters included in equations (A-2) through (A-6) above is presented in this subsection. Parameters are listed in alphabetical order.

(a) CN. Chemical concentration in the air, expressed in mg/m³, can be calculated in a number of ways, as discussed in Section 4. Depending on the particular exposure scenario, the concentration may be taken as constant or as changing over the period of exposure. Among the variables that affect concentration are total quantity of chemical released, release rate of the chemical, room size, ventilation rates, and time lapse.

(b) DU. Duration of exposure is discussed in general in Section 6.2. An inhalation exposure event can be measured in seconds, minutes, or hours. Inhalation exposure to many consumer products can be divided into several stages, each of which may have a different duration. For example, exposure to an aerosol product during active use may last for only seconds or minutes. Passive exposure to direct release of that product may last for hours. And, if the aerosol product is a coating (e.g., spray paint) applied to an object that remains indoors, a third inhalation exposure stage, consisting of the period during which the chemical release rate is controlled by diffusion from the solid coating, may last for weeks or months.

There are several ways to obtain estimates of duration for inhalation exposure scenarios. Methods used for estimating the duration for an inhalation exposure scenario are determined by whether the assessor is concerned primarily with exposure during active use of the product or with exposure during passive use, or both. A method for estimating duration of active exposure during the application of coatings to surfaces is presented in detail in Section 3.1 of this volume. In some cases, estimates of duration can be made based on literature values or professional judgment. Additional general guidelines to follow for estimating duration are presented in Section 6.2.1 of this volume.

(c) FQ. Frequency of exposure, expressed in exposure events per year, is discussed in Section 6.2.1.

(d) IHX. Total individual inhalation exposure, expressed in mg/year, refers specifically to the quantity of inhaled particulates that are likely to be deposited in the respiratory tract. Depending on the particle size distribution of the inhaled aerosol, this quantity may be equal to or significantly less than the quantity inhaled. In practice, there may not be sufficient data on particle size distribution to estimate the quantity deposited in the respiratory tract; in such cases, 100 percent deposition can be assumed as a worst case.

(e) IHX_p. Pulmonary inhalation exposure, measured in terms of mg/year, is the quantity of inhaled particulate material that is available for alveolar absorption. (This is to be distinguished from the quantity that is absorbed across the alveolar membrane, which is not addressed in this report.) IHX_p depends on the respirable fraction RF (see (i) below), which in turn depends on the particle size distribution of the inhaled aerosol.

(f) IHX_G. Gastrointestinal inhalation exposure, measured as mg/year, is the quantity of inhaled particulate material that is initially deposited in the head or tracheobronchial region, thus subject to gastrointestinal rather than pulmonary exposure. As with IHX_p, IHX_G depends on the particle size distribution of the inhaled aerosol

via a deposition factor, NRF (see below). The portion of IHX_G that is expelled from the body via nose-blowing or expectoration, and thus not available for exposure, is assumed to be insignificant for the purpose of these exposure calculations.

(g) IR. Inhalation rate, expressed in m^3/hr , is discussed in Section 6.2.2.

(h) NRF. The nonrespirable fraction is a unitless parameter, ranging from 0 to 1, that represents the weight fraction of inhaled particulates initially deposited in the head and tracheobronchial regions of the respiratory tract, and thus not available for exposure via the lung. Particles deposited in these areas are cleared to the gastrointestinal tract. Values for NRF of particulates discharged from select consumer products are presented in Table 29 at the end of Appendix A. NRF is calculated by using equation (A-7), provided that the supporting data on particle size distribution are available.* If there are insufficient data for equation (A-7) but the mass median diameter is known, a less reliable estimate of NRF can be made using the ICRP model in Figure 3 (see discussion of TDE below).

$$NRF = \sum_{i=1}^n [(TDE_i - PDE_i) \times WF_i] \quad (A-7)$$

TDE_i = total respiratory tract deposition rate for particles within aerodynamic diameter size class i (a unitless fraction varying from 0 to 1)

PDE_i = pulmonary deposition rate for particles within aerodynamic particle diameter size class i (a unitless fraction)

WF_i = the weight fraction of particles in aerodynamic diameter size class i (a unitless fraction).

Detailed information on the applications and data sources for each of the parameters in equation (A-7) is provided below:

- TDE. The fraction of inhaled particles in a given size range that is deposited in the respiratory tract has been studied both theoretically and experimentally. Theoretical models such as the International Commission on Radiological Protection's (ICRP) Task

*Note: Equation (A-7) could just as easily be written as:

$$NRF = TDF - RF$$

See (j) for a discussion of TDF and (i) for a discussion of RF.

Group on Lung Dynamics Model, presented as Figure 3, have been used in the past to determine deposition. There are discrepancies, however, between the ICRP model, which relates deposition to particle mass median diameter (i.e., the diameter below which lies 50 percent of the mass of the particles), and more recent experimental data relating deposition to aerodynamic diameter. For this reason, exposure estimates should be based on the experimental data rather than the ICRP model in cases where sufficient data on particle size distribution are available. Total deposition in the respiratory tract is the sum total of deposition in the head, tracheobronchial, and pulmonary regions. Total deposition depends on particle diameter, particle density, total volume, breathing rate, and type of breathing used (nose or mouth) (Heyder et al. 1980b). As discussed in Section (1), particles ranging from 1 μm to 100 μm are retained in the head region, and particles in the 0.01 μm to 10 μm range are absorbed in the tracheobronchial tract or proceed into the pulmonary cavity.

The relationship between total respiratory tract deposition and aerodynamic particle size is given in Figure 4, based on information or data reported in Heyder et al. (1974), Heyder et al. (1980a), Heyder et al. (1980b), Hinds (1982), Stahlhofen et al. (1980), and Meyer (1983). It should be noted that some of the information reported in these sources is conflicting; Figure 5 represents a synthesis of the information in all of these sources. Two graphs are given in Figure 4, one representing deposition under "typical" breathing conditions (i.e., normal nose breathing during rest or light activity), the other representing "maximum" deposition (i.e., maximum values reported in the reviewed literature). Information on deposition for particles smaller than 0.1 μm is sparse and conflicting. Deposition of these small particles occurs largely by diffusion; thus, it cannot be clearly expressed as a function of aerodynamic particle diameter (Heyder et al. 1980a). A comparison of Figure 4 with Figure 5 indicates that tracheobronchial deposition accounts for the majority of the total deposition of smaller particles in this size range; this enhancement of tracheobronchial deposition can be attributed to the rapid Brownian motion (Hinds 1982). A large fraction of particles smaller than 0.05 μm may be exhaled unless they dissolve or react with or on the surface (Meyer 1983). Total deposition of particles in the 0.1 μm to 1 μm size range, where sedimentation becomes important in addition to diffusion, is lower than for smaller particles. Deposition via impaction in the head region becomes increasingly important for particles in the 1 μm to 10 μm size range; total deposition approaches 100 percent for particles larger than about 3 μm .

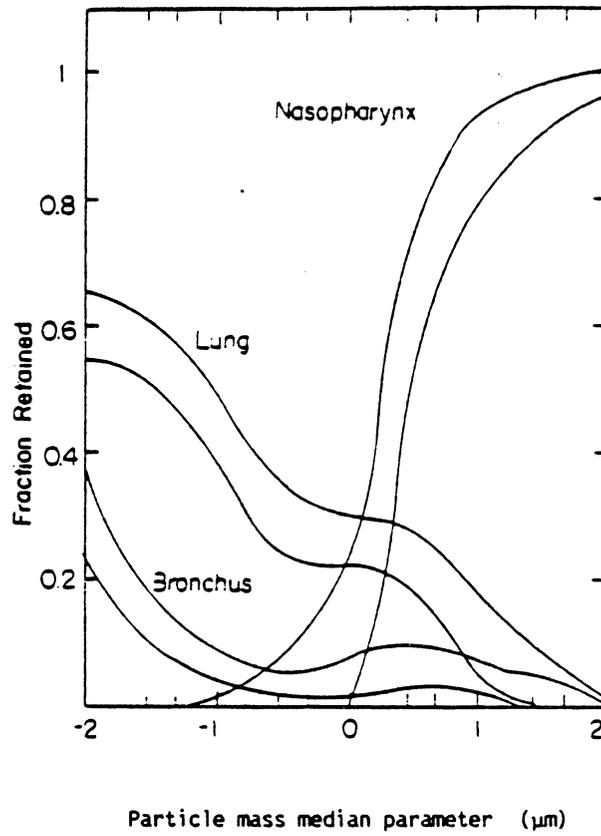


Figure 3. ICRP Model of Regional Respiratory Tract Deposition as a Function of Particle Size.

Source: Meyer 1983.

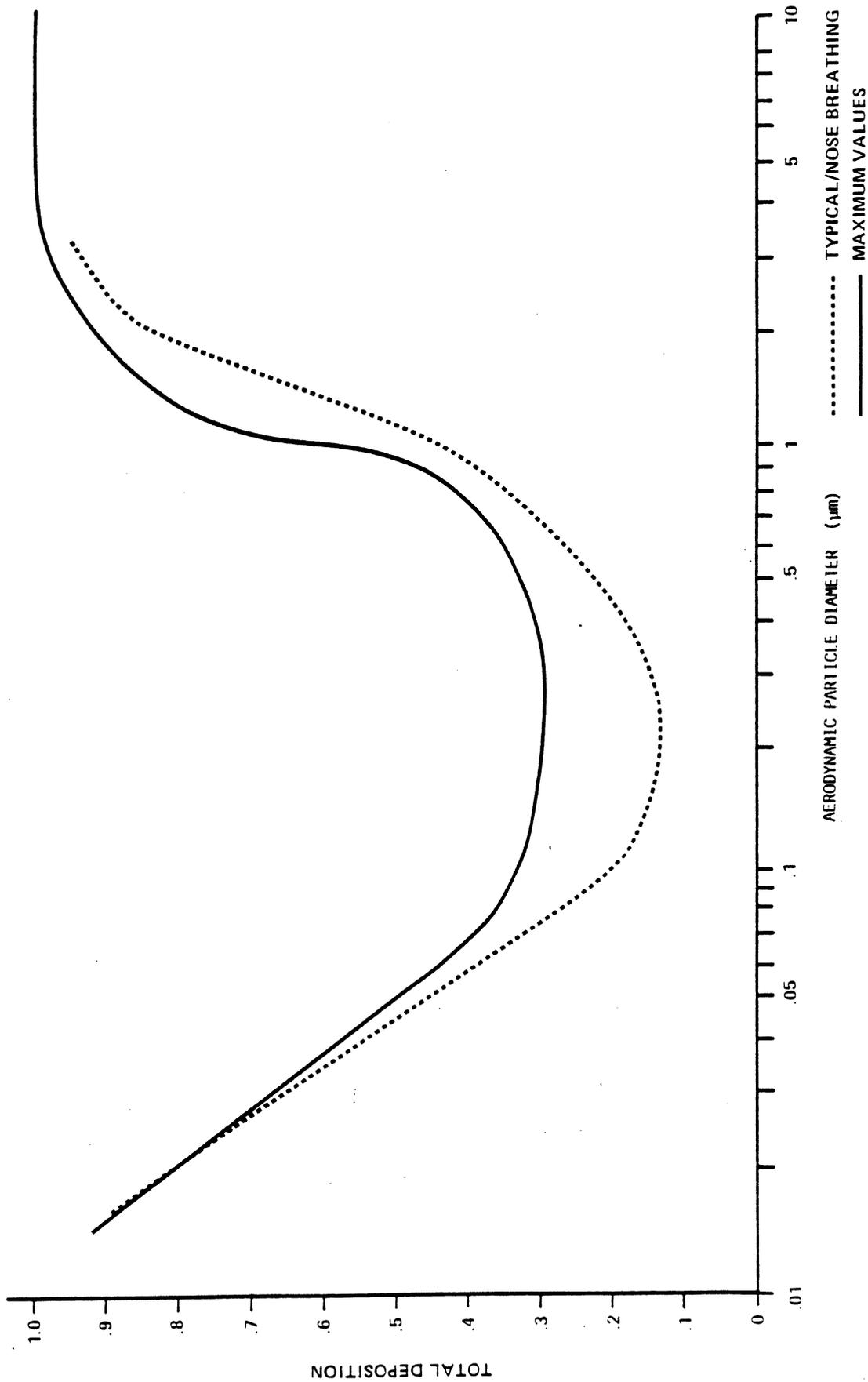


FIGURE 4 . TOTAL DEPOSITION OF PARTICULATES IN THE RESPIRATORY TRACT AS A FUNCTION OF PARTICLE SIZE

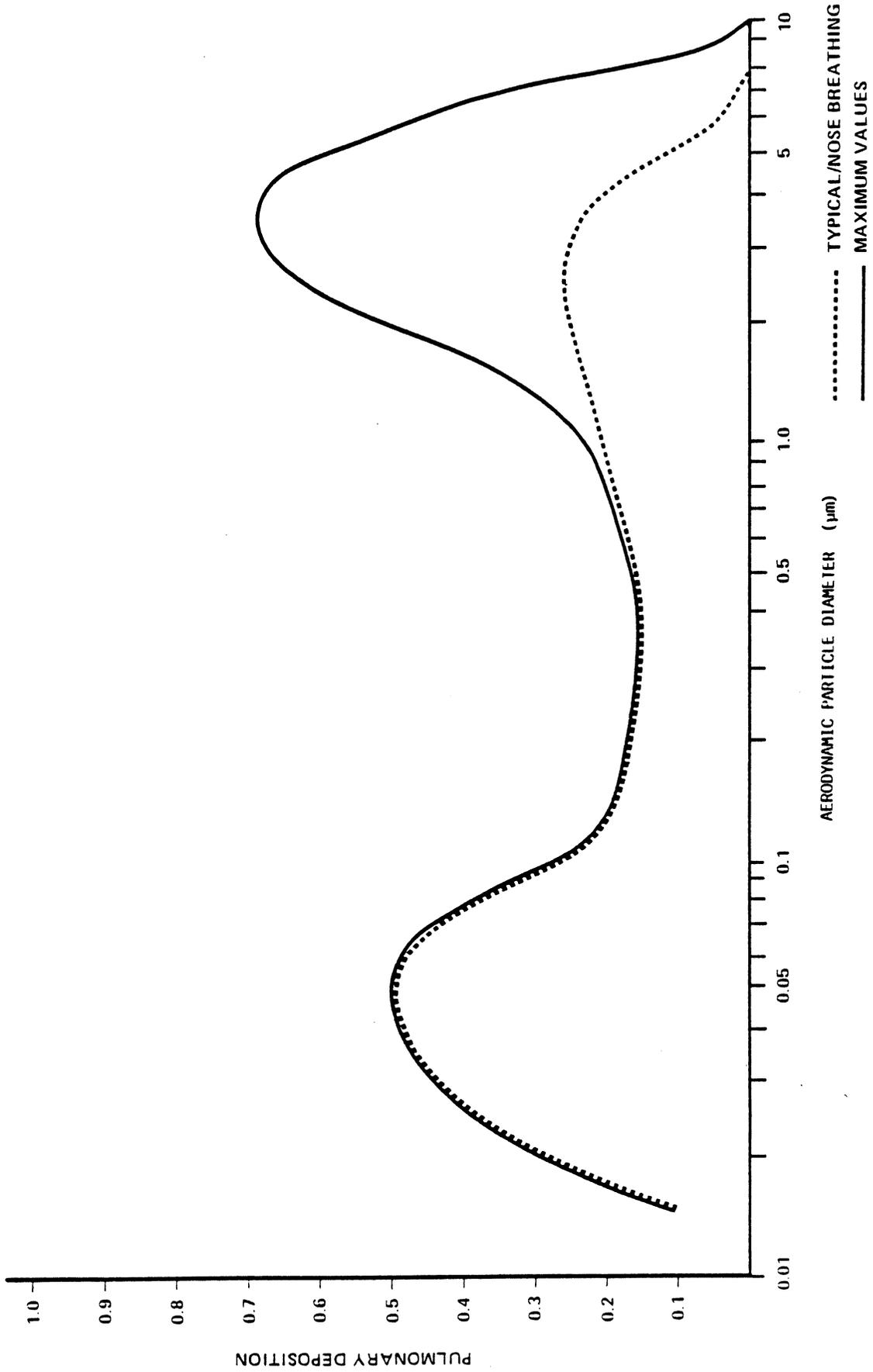


FIGURE 5. PULMONARY DEPOSITION OF PARTICULATES AS A FUNCTION OF PARTICULATE SIZE

- PDE. The fraction of inhaled particles in a given size range subject to pulmonary deposition has been studied both theoretically and experimentally. The discussion of discrepancies between the ICRP model (Figure 3) and experimental data in relation to estimates of the parameter TDE applies equally well to the parameter PDE. A summary of the relationship between particle size and pulmonary deposition is given in Figure 5 based on data or information reported in Heyder et al. (1974), Heyder et al. (1980a), Heyder et al. (1980b), Hinds (1982), Stahlhofen et al. (1980), and Meyer (1983). The reader should be aware that other factors in addition to particle size affect alveolar deposition; these include breathing characteristics, such as type of breathing (nose vs. mouth), breathing rate, and tidal volume. Under constant breathing conditions, however, there is a clear relationship between aerodynamic particle diameter and pulmonary deposition for particles larger than about 0.1 μm . The data summarized in Figure 5 are discussed in more detail below.

Figure 5 includes two graphs, one representing deposition to be expected under typical conditions (i.e., nose breathing during light activity) and the other representing the highest deposition values reported in the reviewed literature. No distinction between "typical" and "maximum" is provided for particles less than about 0.3 μm , because the information on deposition in this size range is sparse. The PDE values corresponding to aerodynamic particle diameters less than 0.1 μm in Figure 5 were taken from Heyder et al. (1980a) who did not specify the origin of the data. The trend in decreasing pulmonary deposition with decreasing particle size in the 0.05 μm to 0.01 μm range is presumably related to enhanced tracheobronchial deposition for this size range (see TDE, above). Pulmonary deposition between 0.1 μm and 1 μm is about 20 percent, independent of particle size (Hinds 1982). Pulmonary deposition peaks again around 2.5 μm to 3 μm and approaches 0 around 6 to 7 μm . Particles larger than 1 μm are increasingly filtered out by the head region. This explains the decrease in pulmonary deposition with increasing particle size for particles larger than about 3 μm . Figure 5 suggests that 0.75 might be used as a worst case estimate of PDE in cases where detailed particle size distribution data are not available.

- WF. The weight fraction of aerosol particles in a given aerodynamic diameter size range i , must be known or estimated in order to estimate regional deposition in the respiratory tract. Because of the limited availability of particle size distribution information, WF will often be the stumbling block in exposure calculations involving inhaled particulates. Particle size distribution information is available for a number of aerosol can products and can be found in various trade association journals.

Typical particle size distributions for other types of particulates (e.g., asbestos fibers, household dust, cigarette smoke) generated during the use of consumer products have, in some cases, been measured in health-related studies. A complete particle size distribution may not be necessary for crude worst reasonable case exposure calculations. Considerable professional judgment will be needed by the exposure assessor in converting available information on particle size distribution to WF in equation (A-7). In cases where the only information available is the mass median diameter, this parameter can be used in conjunction with data in Figure 3 to estimate respiratory tract deposition.

(i) RF. The respirable fraction is the fraction of inhaled aerosol particles likely to be deposited in the pulmonary airspaces. This parameter, which ranges from 0 to about 0.7, is a function of the particle size distribution of the inhaled aerosol and can be calculated using equation (A-8), providing that sufficient data are available. A less accurate estimate of RF can be made using the model given in Figure 3 in conjunction with the mass median diameter (see discussion under TDE in (h), above).

$$RF = \sum_{i=1}^n (PDE_i \times WF_i) \quad (A-8)$$

A detailed explanation of the parameters used in equation (A-8) can be found under NRF (see (i)). It should be obvious that the data provided in Figure 5 are essential in calculating RF. Values of RF of particulates discharged from selected consumer products are presented in the Table at the end of Appendix A.

(j) TDF. The total deposition fraction is the weight fraction of all inhaled particles deposited in the respiratory tract. This parameter can be calculated using equation (A-9), providing that the particle size distribution is known. A cruder estimate of TDF can be made using the model given in Figure 3 in conjunction with the mass median diameter (see discussion under TDE in (h), above).

$$TDF = \sum_{i=1}^n (TDE_i \times WF_i) \quad (A-9)$$

A detailed discussion of these parameters is included in the discussion of NRF (see (i), above). It must be noted that data on TDF particulates discharged from selected consumer products are not presented in the table at the end of Appendix A. In all cases where nonrespirable and respirable fractions of particulates were calculated or estimated, a

maximum value for TDF of 1.0 was used. The total deposition, or average probability that an inspired particle may undergo respiratory tract deposition, was not considered in this analysis. Precise data on aspiration efficiency according to particle size are needed to accurately quantify the TDF of particulates. Aspiration efficiency, or the fraction of particles originally in the volume of inhaled air that enters the nose or mouth, is dependent on a number of factors. These include particle size, air velocity, inhalation flow rate, and whether nose or mouth breathing is used. To circumvent the difficulties involved in attempting to quantify each of these factors, as a worst case, the aspiration efficiency was assumed to be 100 percent. As a result, a maximum value for TDF of 1.0 is suggested for use in all calculations requiring this parameter. The value of 1.0 for TDF, however, represents a worst case assumption.

Table 29. Values of Respirable and Nonrespirable Fraction of Particulates for Selected Consumer Products (continued)

Aerosol product	Nonrespirable fraction			Respirable fraction			Comments
	Minimum	Typical	Maximum	Minimum	Typical	Maximum	
Deodorant/antiperspirant	0.66	0.88	0.96	0.04	0.12	0.34	Calculated using typical and maximum pulmonary deposition factors presented in Figures 4 and 5 and available data on particle size distribution of particulates discharged from deodorants/antiperspirants. ^a
Hairspray	0.66	0.88	0.97	0.03	0.12	0.34	Calculated using typical and maximum pulmonary deposition factors presented in Figures 4 and 5 and available data on particle size distribution of particulates discharged from hairspray. ^b
Furniture polish	0.5	0.82	1.0	7.6x10 ⁻⁵	0.18	0.50	Calculated using typical and maximum pulmonary deposition factors presented in Figures 4 and 5 and available data on particle size distribution of particulates discharged from aerosol furniture polish. ^c
General cleaner/ disinfectant	---	0.87	0.97	0.03	0.13	---	Calculated using typical and maximum pulmonary deposition factors presented in Figures 4 and 5 and available data on particle size distribution of particulates discharged from aerosol disinfectant. ^d
Insecticide, home and garden	---	0.92	0.98	0.02	0.08	---	Calculated using typical and maximum pulmonary deposition factors presented in Figures 4 and 5 and available data on particle size distribution of particulates discharged from products designed for use on flying insects. ^e
Insect repellent	0.5	---	1.0	0	---	0.5	Values are estimates based on ranges of values calculated for other aerosol products.

Table 29. Values of Respirable and Nonrespirable Fraction of Particulates for Selected Consumer Products

Aerosol product	Nonrespirable fraction		Respirable fraction		Comments	
	Minimum	Typical	Minimum	Typical		
Lubricant	--	--	0.5	0.5	0.5	Values are estimates based on ranges of values calculated for other aerosol products.
Oven cleaner	0.5	--	--	--	0.5	Values are estimates based on ranges of values calculated for other aerosol products.
Pet pesticide	0.5	--	0	--	0.5	Values are estimates based on ranges of values calculated for other aerosol products.
Room deodorizer	0.64	--	0.08	--	0.36	Calculated using typical and maximum pulmonary deposition factors presented in Figures 4 and 5 and available data on particle size distribution of particulates discharged from aerosol room deodorizer. f
Spray starch	--	--	6×10^{-4}	--	--	Calculated using typical and maximum pulmonary deposition factors presented in Figures 4 and 5 and available data on particle size distribution of particulates discharged from spray starch. g
Suede cleaner/polish	0.5	--	0.06	--	0.5	Values are estimates based on ranges of values calculated for other aerosol products.
Fabric protector	--	0.52	0.17	0.48	--	Calculated using typical and maximum pulmonary deposition factors presented in Figures 4 and 5 and available data on particle size distribution of particulates discharged from aerosol fabric protector. h
Home spray paint	0.78	0.92	--	0.08	0.22	Calculated using typical and maximum pulmonary deposition factors presented in Figures A-2 and A-3 and available data on particle size distribution of particulates discharged from spray paints. i
Automotive touch-up paint	0.78	0.92	--	0.08	0.22	Values are assumed to be the same as those for home spray paint.

f-h

10-10

APPENDIX A - REFERENCES

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APPENDIX B

Simmons Market Research Bureau (SMRB) Reports

APPENDIX B - SIMMONS MARKET RESEARCH BUREAU (SMRB) REPORTS

The tables included in this Appendix are a guide to the individual SMRB reports (volumes) and the products covered by each volume. The following are the tables included in this Appendix:

Table 30. SMRB reports (1983) by Volume

Table 31. Products Listed in SMRB Reports (1983) by Product Category

Table 30. SMRB Reports (1983) by Volume

Volume	Title
P-1	Automobiles
P-2	Cycles, Trucks, Vans & Tires
P-3	Automotive Products and Services
P-4	Travel
P-5	Banking, Investments, Memberships, Public Activities & Contribution
P-6	Insurance & Credit Cards
P-7	Books, Records, Tapes, Stereo & TV
P-8	Appliances, Sewing & Garden Care
P-9	Home Furnishings & Home Improvements
P-10	Sports & Leisure
P-11	Restaurants, Stores & Grocery Shopping
P-12	At Home Shopping, Yellow Pages, Florists & Telegrams
P-13	Jewelry, Wristwatches, Luggage, Binoculars, Pens & Pencils and Men's Apparel
P-14	Women's Apparel
P-15	Tobacco Products & Photography
P-16	Distilled Spirits & Mixes
P-17	Malt Beverages & Wine
P-18	Coffee, Tea, Milk, Soft Drinks, Juices & Bottled Water
P-19	Dairy Products, Spreads, Cookies, Desserts, Baking & Bread Products
P-20	Cereals, Rice, Pasta, Pizza, Mexican Foods, Fruits & Vegetables
P-21	Soup, Meat, Fish, Poultry, Condiments & Dressings
P-22	Chewing Gum, Candy & Snacks
P-23	Soap, Laundry & Paper Products & Kitchen Wraps
P-24	Household Cleaners, Room Deodorizers & Pet Foods
P-25	Health Care Products & Remedies
P-26	Oral Hygiene Products, Skin Care & Deodorants
P-27	Hair Care & Shaving Products
P-28	Women's Beauty Aids, Cosmetics & Personal Products & Beauty Salons
P-29	Games & Toys, Children's & Babies' Apparel & Specialty Products
P-30	Relative Volume of Consumption

Table 31. Products Listed in SMRB Reports (1983)
by Product Category

Product Category	Volume	Product
APPAREL - CHILDREN'S & BABIES'	(P-29)	Clothing Diapers/Cloth, Disposable Jeans or Dungarees Outerwear Shoes Sleepwear Suitwear Underwear
APPAREL - MEN	(P-13)	Clothing Bought for a Woman Coats Jackets Jeans & Slacks Shirts Shoes, Boots & Sneakers Sports Apparel Suits Sunglasses Sweaters
APPAREL - WOMEN	(P-14)	Blouses & Shirts Clothing Bought for a Man Coats Dresses Hosiery Jeans & Slacks Lingerie Shoes, Boots & Sneakers Ski & Tennis Clothes Skirts Suits Sunglasses Sweaters Swimsuits Warm-up Suits

Table 31. (Continued)

Product Category	Volume	Product
APPLIANCES & DURABLES:		
<u>Calculators/Typewriters</u>	(P-8)	Bought in Last 12 Months/For Whom/Amount Spent Desk Top Calculator Pocket or Hand-Held Electronic Calculator Typewriter, Electric Portable
<u>Household Appliances & Durables</u>	(P-8)	Bought in Last 12 Months/Decision Maker Air Conditioner, Separate Room Burglar Alarm System Ceiling Fan Electric Air Purifier Electric Broom Electric Clothes Dryer Gas Clothes Dryer Grills: Gas, Electric, Charcoal Home Computers, Brands and Use Room Heater, Portable Room Heating System, Separate Room Dehumidifier, Separate Room Humidifier, Separate Sewing Machine Smoke/Fire Detector Stationary Bicycle Videocamera Washing Machine, Automatic Water Purifier or Filter
<u>Kitchen Appliances & Durables</u>	(P-8)	Bought in Last 12 Months/Decision Maker Automatic Dishwasher Blender, Electric Canning Jars & Lids Coffee Maker Food Processor, Electric Food Dehydrator Fry Pan, Electric

Table 31. (Continued)

Product Category	Volume	Product
APPLIANCES & DURABLES:		
<u>Kitchen Appliances & Durables (cont')</u>	(P-8)	Garbage Disposal Home Freezer, Separate Juicer, Electric Metal Cookware Set Mixer, Electric Oven: Microwave Self-Cleaning/Continuous -Cleaning Pressure Cooker Refrigerator, Electric Steam Cooker, Electric Stove or Range, Electric or Gas Trash Compactor, Electric Woodburning Stove/Heater
<u>Personal Appliances</u>	(P-8)	Bought in Last 12 Months/For Whom/Amount Spent Hair Curler Set, Electric Hair Dryer, Bonnet-Type or Electric Hand-Held Hair Styling Comb, Electric Hot Lather Machine Lighted Makeup Mirror Shaver, Battery or Electric Toothbrush, Electric
<u>Power Equipment & Hand Tools</u>	(P-8)	Bought in Last 12 Months/Decision Maker Drill, Electric Electric Router Garden Tiller Hand Tool Outfit Portable Workbench Power Mower, Electric or Gas Power Yard Trimmer Sander, Electric Saw: Chain, Electric or Gas Circular Jig/Sabre Stationary Radial/Arm Snow Blower Tractor, Garden

Table 31. (Continued)

Product Category	Volume	Product
AT HOME SHOPPING, YELLOW PAGES, FLORISTS & TELEGRAMS:	(P-12)	Door-to-Door Sales Florists Telegrams & Wires
<u>Mail & Phone Order</u>	(P-12)	Auto Accessories Recipe Cards Cook Books Books from Book Club Other Books Cosmetics Records Prerecorded Audio Cassette Tapes Prerecorded Audio Tape Cartridges Blank Audio Tapes or Cassettes Magazines Photo Processing Fruit, Cheese or Specialty Foods Shoes or Boots Clothing Needlecraft Kits & Supplies Camping Equipment Sporting Goods (Such as Fishing Tackle, Golf Balls, Ski Poles, etc.) Tools Coins (Numismatic) Medallions, Commemorative Plates (Such as Commemorative Medals, Ingots, Porcelain, etc.) Cookware & Kitchen Accessories Small Appliances Investment Information Insurance Real Estate Information Educational Programs Trees, Plants, Seeds Tupperware Parties Vitamins

Table 31. (Continued)

Product Category	Volume	Product
AUTOMOBILES	(P-1)	Air Conditioning Annual Miles Driven Automobile Club Bought New/Used Burglar Alarm in Car Car Leasing Car Rentals Current Auto Ownership Current Driver's License Decision Makers for One or More Cars How Purchased Where Purchased Insurance Makes & Models of Cars Owned/Domestic, Imported Model Type/Size Model Year Owned Next Car Purchase Radio/Tape Player Type of Car (Body Style) Type of Drive & Diesel Engine When Acquired
AUTOMOTIVE PRODUCTS & SERVICES	(P-3)	Air Filters Antifreeze Brake Linings/Pads Car Batteries Car Wax & Polish Gasoline & Diesel Fuel Gasoline Additives Motor Oil Motor Oil Additives Mufflers Oil Filters Rustproofing Shock Absorbers Spark Plugs Transmission Services

Table 31. (Continued)

Product Category	Volume	Product
BANKING, INVESTMENTS, MEMBERSHIPS, PUBLIC ACTIVITIES & CONTRIBUTIONS	(P-5)	Accounting Services Auto Loans Brokerage Account Checking Accounts Farm Ownership Gold/Silver I.R.A. or Keogh Plan Memberships Mortgages Now Accounts Personal Loans Public Activities Contributions to Public TV Retirement & Investment Property Safe Deposit Boxes Savings Accounts Savings Certificates Securities Treasury Bills Trust Agreements Vacation/Weekend Homes
BEAUTY AIDS, BEAUTY SALONS, COSMETICS & PERSONAL PRODUCTS - WOMEN	(P-28)	Bath & Shower Additives Beauty Salons Blusher Cotton Balls or Squares Eye Liner Eye Shadow Face Powder/Loose, Pressed Facial Moisturizers, Cleansing Creams & Lotions Feminine Hygiene Douches, Suppositories & Spray Deoderants

Table 31. (Continued)

Product Category	Volume	Product
DISTILLED SPIRITS & MIXES	(P-16)	Alcoholic Beverages Blended Whiskey or Rye Bourbon Whiskey Brand Influence of What Served in Home Brandy & Cognac Canadian Whiskey Cordials & Liqueurs Gin Irish Whiskey Prepared Cocktail Mixes with Liquor Purchase Distilled Spirits by the Case Rum Scotch Whiskey Tequila Vodka
FLOWER, VEGETABLE, LAWN SEED & FERTILIZER	(P-8)	Bought in Last 12 Months/Amount Spent Fertilizers House Plant Food, Lawn Vegetable Garden, Other Seed Flower, Lawn, Vegetable
GAMES & TOYS	(P-29)	Bought in Last 12 Months/Amount Spent Video & Non-Video Electronic Games

Table 31. (Continued)

Product Category	Volume	Product
HAIR CARE PRODUCTS	(P-27)	Creme Hair Rinses Hair Coloring Products Hair Conditioners Hair Sprays Hair Tonics or Dressings Home Permanents Shampoos
HEALTH CARE PRODUCTS & REMEDIES	(P-25)	Adhesive Bandages Asthma Relief Remedies Athlete's Foot Remedies Cold, Allergy & Sinus Remedies Cough Drops & Syrup Diet Control Products Eyeglasses & Contact Lenses Headache Remedies & Pain Relievers Illnesses & Ailments Indigestion Aids & Upset Stomach Remedies Laxatives Medicated Throat Lozenges Nasal Sprays Pain Relieving Rubs & Liquids Suntan & Sunscreen Products Throat Lozenges/Medicated Vitamins
HOME FURNISHINGS & HOME IMPROVEMENTS	(P-9)	Clocks: Wall, Mantle, Desk Standing Dinner & Tableware Glassware Crystalware Fine China Flatware Other Dinnerware Fluorescent & Incandescent Lighting Home Furnishings & Household Durables

Table 31. (Continued)

Product Category	Volume	Product
HOME FURNISHINGS & HOME IMPROVEMENTS (cont')	(P-9)	Beds/Other Bedroom Furniture Blankets, Electric/Other Comforters/Quilts Curtains & Draperies Dining Room Furniture Mattresses Pianos & Organs Telephones & Telephone Answering Machines Pillowcases Sheets Towels Home Improvements Bathroom Plumbing Carpeting Fixtures Flooring Flue Dampers Fireplaces Furnace Garage Door Opener Hot Tubs/Whirlpools Hot Water Heater House Plans Purchase Insulation for Ceiling, Floor or Wall Kitchen Cabinets & Sinks Outdoor & Indoor Lighting Outdoor Deck/Porch/Patio Roofing Siding Storm Doors or Windows Solar Heating/Solar Hot Water Thermostats Wall Paneling Wallpaper Weather Stripping Interior & Exterior Remodeling Paints & Stains Exterior Interior

Table 31. (Continued)

Product Category	Volume	Product
HOUSEHOLD CLEANERS & ROOM DEODORIZERS	(P-24)	Air Fresheners & Deodorizers All-Purpose Cleaners Bug Traps Drain Cleaners Floor Waxes Furniture Polishes Glue & Bonding Agents Insecticides Oven Cleaners Rug Cleaners & Shampoos Rug Deodorizers & Fresheners Scouring Pads & Sponges Scouring Powders Termite & Rodent Control Toilet Bowl Cleaners Window & Glass Cleaners
INSURANCE & CREDIT CARDS	(P-6)	Credit Cards 18 Credit Type Listings How Billed or Printed Used in Last 30 Days Home Owners/Personal Property Insurance Life Insurance Medical, Hospital, Health Insurance Other Types
JEWELRY, BINOCULARS, WRISTWATCHES, PENS & MECHANICAL PENCILS	(P-13)	Jewelry Costume Diamond Gold Other Jewelry and Gems Pens & Mechanical Pencils Bought for Self or Someone Else Wristwatches/Men Wristwatches/Women

Table 31. (Continued)

Product Category	Volume	Product
LUGGAGE	(P-13)	Luggage or Baggage
MALT BEVERAGES & WINES	(P-17)	Alcoholic Beverages Ale Beer Domestic Light/Low-Calorie Domestic Regular Draft Imported Malt Liquor Wine Aperitif & Specialty Champagne, Cold Duck & Sparkling Wines Light Domestic Dinner/Table Domestic Dinner/Table Imported Dinner/Table Port, Sherry & Dessert Sangria/Pop/Party Vermouth
MOTORCYCLES, SCOOTERS, MINICYCLES & BIKES, NOPEDS & MOPEDS	(P-2)	Minicycles, Minibikes, Mopeds, Nopeds, Motorscooters Any Owned in Household Decision Maker for Make Bought - Type Owned Most Recent Bought, New/Used Type Owned by Household Motorcycles Bought New/Used Decision Maker for One or More Motorcycles Engine Size Motorcycles Owned in Household Number Owned by Household Members Type Owned

Table 31. (Continued)

Product Category	Volume	Product
ORAL HYGIENE PRODUCTS, SKIN CARE & DEODORANTS	(P-26)	Breath Fresheners Denture Cleansers Deodorants & Antiperspirants Hand & Body Creams, Lotions, or Oils Medicated Skin Care Products Mouthwash Toothbrushes Toothpaste
PET FOODS, FLEA & TICK CARE PRODUCTS	(P-24)	Cat Ownership Cat Food Canned Packaged Dry Packaged Moist Dog Ownership Dog Food & Mixing Dog Food Types Canned Packaged Dry Packaged Moist Flea & Tick Care Products for Dogs & Cats Decision Makers for Brands of Dog & Cat Food (7 Different Types)

Table 31. (Continued)

Product Category	Volume	Product
PHOTOGRAPHY	(P-15)	Cameras/Movie, Still Film & Flash Equipment Film Processing Projectors, Movie, Slide
RESTAURANTS, STORES & GROCERY SHOPPING	(P-11)	Cents-Off-Coupons Catalogue Showroom, Department & Discount Stores Shopped in Last 3 Months/Amounts Spent in Last 30 Days Fast Food/Drive-In Family & Steak House Restaurants Gourmet & Health Food Specialty Stores Grocery Shopping Expenditures Supermarket & Food Shopping Supermarkets & Convenience Stores
SEWING	(P-8)	Finished Garments in Last 12 Months General Sewing or Mending in Last 12 Months Sewing Materials & Notions Sewing Patterns/Brands Sewing Offers from Magazines
SHAVING PRODUCTS	(P-27)	After Shave Lotion & Cologne, Use & Gift Purchases Depilatories Pre-Electric Shave Lotion Razor Blades Shavers/Disposable, Electric & Battery Shaving Cream or Gel

Table 31. (Continued)

Product Category	Volume	Product
SOAP, LAUNDRY & PAPER PRODUCTS/KITCHEN WRAPS	(P-23)	Aluminum Foil Automatic Dishwashing Detergent Bleach Dishwashing Liquid Disposable Cups & Dispenser Fabric Softeners Facial Tissues Laundry Pre-Soaks & Pre-Cleaners Laundry Washloads Liquid Toilet Soaps Paper Plates Paper Towels Plastic Garbage Bags & Trash Liners Plastic Sandwich or Food Bags Plastic Type Kitchen Wraps Reusable "Cloth" Towels (Non-Woven) Soaps & Detergents Toilet Paper Toilet Soap
SOUP, MEAT, FISH, POULTRY, CONDIMENTS & DRESSINGS	(P-21)	Bacon Barbecue & Seasoning Sauces Beef Bouillon Cubes Canned Chicken Canned Meat Spreads Canned Soup Canned Tuna Catsup Coating & Stuffing Products Cold Cuts Cooking Spray Corn Syrup Corned Beef

Table 31. (Continued)

Product Category	Volume	Product
SOUP, MEAT, FISH, POULTRY, CONDIMENTS & DRESSINGS (cont')	(P-21)	Corned Beef Hash Deviled Ham Dry Soup/Lunch Mix Cornish Game Hen (Fresh/Frozen) Frankfurters: Beef, Chicken & Turkey Fresh Fish/Shell Fish Fresh Breast of Turkey Other Fresh Turkey Frozen Dinners & Courses Frozen Fish/Shell Fish Frozen Prepared Seafood Fresh Chicken Frozen Breast of Turkey Frozen Pre-Stuffed Turkey Other Frozen Whole Turkey Frozen Fried Chicken Other Frozen Chicken Honey & Fructose Mayonnaise Mustard Meat Tenderizer Lamb Pancake & Table Syrup Pork Pork Sausage Salad & Cooking Oil Salad Dressings Sugar Veal Vienna Sausage Stews Canned Ham Roast Beef Hash

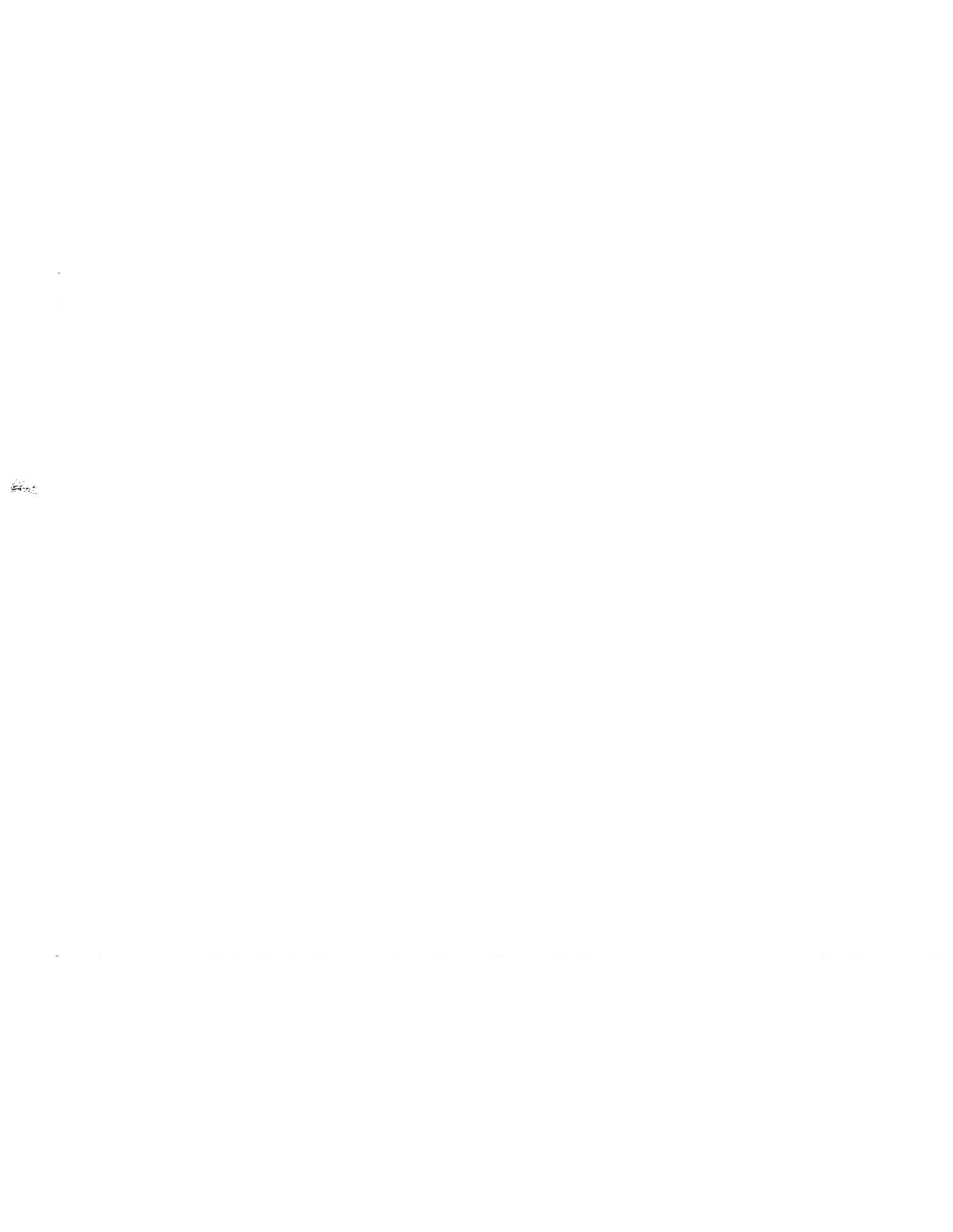


Table 31. (Continued)

Product Category	Volume	Product
TRUCKS, VANS & SPORT/ UTILITY VEHICLES	(P-2)	Any Owned in Household Bought to Replace Car/Truck Decision Maker for Make Bought - Type Owned Most Recent Bought New/Used by Type Model Year for Types Owned Most Recent Bought By 4-Wheel Drive & Diesel Engine By Type Primary Purpose Used for

APPENDIX C

An Alphabetical Listing of Variables Used
in This Volume

Table 32. An Alphabetical Listing of Variables Used in this Volume

Variable	Definition	Units
ADD	Annual dermal dose	mass/year
ADF	Amount of product or residue deposited on fabric surface	mass/area
A _R	Rate of application of film or coating to surface	area/time
AV	Area of skin surface exposed	area
C	Concentration of chemical substance in air at any point in time during exposure	mass/volume
C _{A1}	Concentration of air at liquid/gas film interface	moles/volume
C _{B1}	Concentration of chemical substance at liquid/gas film interface	moles/volume
C ₀	Initial concentration of chemical substance in air as a result of an instantaneous release	mass/volume
WC _S	Concentration difference of chemical substance across specified tissue	mass/volume
C _{SO}	Initial concentration of migrant in polymer	mass/volume
Ct _a	Concentration of the chemical substance at the time at the end of application of film or coating	mass/volume
Ct _g	Concentration of the chemical substance at the time at the end of its continuous release	mass/volume
Ct _r	Concentration of the chemical substance at the time at the end of release of all substance from the coating	mass/volume
D	Diffusion coefficient of migrant through polymer	mass
DA	Dust adherence to skin	mass/area
D _{AB}	Diffusion coefficient of chemical substance in air at 25°C and 1 atmosphere	area/time

Table 32. (continued)

Variable	Definition	Units
DEX	Annual dermal exposure	mass/year
DIL	Dilution fraction	unitless
DSY	Density of product	mass/volume
DU	Duration of exposure to consumer product	time
D_w	Diffusion coefficient in water	area/time
F	Fraction of migrant released from polymer	unitless
FA	Fraction of spilled material entrained in air	unitless
FA	Fraction of chemical substance absorbed	unitless
FQ	Frequency of exposure on an annual basis	unitless
G	Rate of release of chemical substance from consumer product	mass/time
G_N	Mass flux of chemical substance	mass/area-time
G_{NAR}	Time-dependent release rate	mass/time ²
IHX	Annual inhalation exposure	mass/year
IHX _G	Annual exposure to inhaled particulates that enter the gastrointestinal tract	mass/year
IHX _p	Annual exposure to inhaled particulates that enter the pulmonary region	mass/year
ING	Annual ingestion exposure	mass/year
IR	Inhalation rate	volume/time
J_S	Permeation rate (flux) of chemical substance	mass/area-time
k	A constant that is a product of the mixing factor, m, and the air exchange rate, Q/V	unitless

Table 32. (continued)

Variable	Definition	Units
K_p	Permeability constant	volume/area-time
L	Thickness of gas film or polymer	length
LR	Leaching rate of chemical substance from object placed in mouth to saliva	mass/time/area
LUS	Fraction of liquid used in the mouth that is swallowed unintentionally	unitless
M	Mass of consumer product spilled, sprayed, applied, or used in any other manner	mass
m	Mixing factor	unitless
M_A	Molecular weight of air	dimensionless
M_B	Molecular weight of chemical substance	dimensionless
M_t	Mass of migrant released from polymer	mass
MW	Molecular weight of chemical substance	dimensionless
N	Molar flux of pure chemical substance	moles/area-time
NRF	Nonrespirable fraction (e.g., weight fraction of all inhaled particles deposited in the head or tracheobronchial region)	unitless
OV	Fraction of product that is overspray (e.g., does not contact intended surface)	unitless
P	Vapor pressure of chemical substance at 25°C	atmospheres
P_{A1}	Partial pressure of air at interface of liquid and main air stream	atmospheres
P_{A2}	Partial pressure of air at interface of gas film and main air stream	atmospheres

Table 32. (continued)

Variable	Definition	Units
P _{B1}	Partial pressure of chemical substance at interface of liquid and main air stream	atmospheres
P _{B2}	Partial pressure of chemical substances at interface of gas film and main air stream	atmospheres
PDE	Fraction of inhaled particles subject to pulmonary deposition	unitless
Q	Ventilation air flow rate	volume/time
R	Universal gas constant	atm-cm ³ /mole-°K
RF	Respirable fraction (e.g., weight fraction of all inhaled particles deposited in the pulmonary air space)	unitless
SA	Surface area covered by film or coating	area
SAO	Surface area of object being place in mouth	area
T	Film thickness of liquid on skin surface	length
T	Temperature	degrees
t _a	Time at the end of application	time
TDE	Fraction of inhaled particles deposited in the respiratory tract	unitless
TDF	Total deposition fraction (e.g., weight fraction of inhaled particles deposited in the respiratory tract)	unitless
t _e	Time at the end of exposure	time
TF	Fraction of residue/dye transferred to the skin per exposure event	unitless
t _g	Time at the end of release of chemical substance	time

Table 32. (continued)

Variable	Definition	Units
t_0	Time at the beginning of exposure	time
t_r	Time at the end of release of all volatile chemical substance from a film or coating applied to a surface	time
V	Room volume	volume
V_A	Molar volume of air	volume/mole
V_B	Molar volume of chemical substance at its normal boiling point	volume/mole
V_S	Volume of polymer	volume
WF	Weight fraction of chemical substance in consumer product	unitless
WV	Workspace volume	volume

APPENDIX D

Average Body Weights of Humans by Age Group

Table 33. Average Body Weights of Humans by Age Group^a

Age Group	Body Weight (kilograms)
Adults, age 18-74	71.8
Adult males, age 18-74	78.1
Adult females, age 18-74	65.4
Child-bearing females, age 18-44	64.0
Child, less than 3 years old	11.6
Child, age 3-6	17.4
Child, age 6-9	25.0
Child, age 9-12	36.0
Child, age 12-15	50.6
Child, age 15-18	61.2

^a Average values adapted from Anderson et al. (1984).

- P. 100 on CCM

APPENDIX E

Derivation of Equations for Estimating
Concentrations of Chemical Substances
in Indoor Air

*1000
5000
10000*

APPENDIX E

The derivation of equations for estimating concentrations of chemical substances in indoor air at any point in time, t , as a result of a time-dependent release are presented for four intervals. These are:

- (1) $0 < t < t_1$;
- (2) $t_1 < t < t_2$;
- (3) $t_2 < t < t_r$; and
- (4) $t > t_r$.

The parameters, t_1 and t_2 , can represent the time to apply the liquid film to a surface from which a chemical substance volatilizes (t_a) or the time required for a chemical substance to evaporate from a liquid film once it has been applied to a surface (t_g). If t_a is smaller than t_g , then t_1 equals t_a and t_2 equals t_g . If t_g is smaller than t_a , then t_1 equals t_g and t_2 equals t_a . The parameter, t_r , is the sum of t_1 and t_2 .

(1) For $t < t_1$

The mass balance equation and the physical interpretation of each group of terms is

$$V \frac{dC}{dt} = G_{NAR} t - mQ C. \quad (E-1)$$

$$\left\{ \begin{array}{l} \text{The net mass of} \\ \text{chemical substance} \\ \text{in air in the room} \end{array} \right\} = \left\{ \begin{array}{l} \text{The mass of chemical} \\ \text{substance released} \\ \text{to air in the room} \end{array} \right\} - \left\{ \begin{array}{l} \text{The mass of chemical} \\ \text{substance removed by} \\ \text{air leaving the room} \end{array} \right\}.$$

Upon dividing Equation (E-1) by V , Equation (E-1) becomes

$$\frac{dC}{dt} = \frac{G_{NAR}}{V} t - \frac{mQ}{V} C. \quad (E-2)$$

By letting

$$k_1 = \frac{mQ}{V} \text{ and } k_2 = \frac{G_{NAR}}{V}$$

and substituting k_1 and k_2 as appropriate into Equation (E-2), the resulting expression is

$$\frac{dC}{dt} = k_2t - k_1C. \quad (E-3)$$

By letting

$$z = k_2t - k_1C, \quad (E-4)$$

and by differentiating with respect to time, the resulting expression is

$$\frac{dz}{dt} = k_2 - k_1 \frac{dC}{dt}. \quad (E-5)$$

By rearranging Equation (E-5), Equation (E-6) is

$$\frac{dC}{dt} = \frac{-1}{k_1} \left(\frac{dz}{dt} - k_2 \right). \quad (E-6)$$

When Equation (E-6) and Equation (E-4) are substituted into Equation (E-3), the resulting expression is

$$\frac{-1}{k_1} \left(\frac{dz}{dt} - k_2 \right) = z. \quad (E-7)$$

When Equation (E-7) is multiplied by k_1 and rearranged, the resulting expression is

$$\frac{dz}{dt} = -k_1z + k_2. \quad (E-8)$$

Equation (E-8) can be rearranged to

$$\frac{dz}{k_2 - k_1z} = dt. \quad (E-9)$$

Multiplying Equation (E-9) by k_2 yields

$$\frac{dz}{1 - (k_1/k_2)z} = k_2dt. \quad (E-10)$$

When Equation (E-10) is integrated, the resulting expression is

$$\frac{-k_2}{k_1} \ln \left(1 - \frac{k_1}{k_2} z \right) = k_2t + C^*. \quad (E-11)$$

When $C = 0$ at $t = 0$, this implies that $z = 0$ at $t = 0$ and that $C^* = 0$. Setting $C^* = 0$ and dividing Equation (E-11) by $(-k_2/k_1)$ yields

$$\ln \left(1 - \frac{k_1}{k_2} z \right) = -k_1 t. \quad (E-12)$$

Taking the antilog of Equation (E-12) yields

$$1 - \frac{k_1}{k_2} z = e^{-k_1 t}. \quad (E-13)$$

Substituting the expression from Equation (E-4) for z into Equation (E-13) and rearranging yields

$$\frac{k_1}{k_2} (k_2 t - k_1 C) = 1 - e^{-k_1 t}. \quad (E-14)$$

By solving for C , the resulting expression is

$$C = \frac{-1}{k_1} \left[\frac{k_2}{k_1} (1 - e^{-k_1 t}) - k_2 t \right] \quad (E-15)$$

which, upon rearranging, is

$$C = \frac{-k_2}{k_1} \left[\frac{1}{k_1} (1 - e^{-k_1 t}) - t \right]. \quad (E-16)$$

Substituting G_{NAR}/V for k_2 yields

$$C = \frac{G_{NAR}}{k_1 V} \left[t - \frac{1}{k_1} + \frac{e^{-k_1 t}}{k_1} \right]. \quad (E-17)$$

The Equation to calculate the average concentration for any interval of time where the time at the end of exposure is less than or equal to t_1 is obtained by integrating Equation (E-17) with respect to time and dividing the resulting equation by the length of the exposure interval. The resulting expression is

$$C_{ave} = \frac{G_{NAR}}{k_1 V (t_b - t_e)} \left[\frac{t^2}{2} - \frac{t}{k_1} - \frac{e^{-k_1 t}}{k_1^2} \right]_{t = t_e}^{t = t_b}. \quad (E-18)$$

where

t_b = time at the beginning of the desired time interval

t_e = time at the end of the desired time interval.

(2) For $t_1 < t < t_2$

The mass balance equation and the physical interpretation of each group of terms is

$$V \frac{dC}{dt} = G_N A R t_1 - m Q C. \quad (E-19)$$

$$\left\{ \begin{array}{l} \text{The net mass of} \\ \text{chemical substance} \\ \text{in air in the room} \end{array} \right\} = \left\{ \begin{array}{l} \text{The mass of chemical} \\ \text{substance released} \\ \text{to air in the room} \end{array} \right\} - \left\{ \begin{array}{l} \text{The mass of chemical} \\ \text{substance removed by} \\ \text{air leaving the room} \end{array} \right\}.$$

If Equation (E-19) is divided by V, Equation (E-19) becomes

$$\frac{dC}{dt} = \frac{G_N A R t_1}{V} - \frac{m Q C}{V}. \quad (E-20)$$

By letting

$$k_1 = \frac{m Q}{V} \text{ and } k_2 = \frac{G_N A R t_1}{V}$$

and substituting k_1 and k_2 , as appropriate into Equation (E-20), one obtains the resulting expression of

$$\frac{dC}{dt} = k_2 - k_1 C. \quad (E-21)$$

Rearranging Equation (E-21) yields the resulting expression

$$\frac{dC}{k_2 - k_1 C} = dt \quad (E-22)$$

which, when multiplied by k_2 , becomes

$$\frac{dC}{1 - (k_1/k_2)C} = k_2 dt. \quad (E-23)$$

Integrating Equation (E-23) yields the following expression

$$\frac{-k_2}{k_1} \ln \left(1 - \frac{k_1}{k_2} C \right) = k_2 t + C^*. \quad (E-24)$$

Solving for C by dividing by $-k_2/k_1$ yields

$$\ln\left(1 - \frac{k_1}{k_2} C\right) = -k_1 t + C^* \quad (\text{E-25})$$

Taking the antilog of Equation (E-25) yields

$$1 - \frac{k_1}{k_2} C = C^* e^{-k_1 t} \quad (\text{E-26})$$

To determine C^* , substitute the expression for C in Equation (E-17) for the parameter, C, in Equation (E-26). Substitute t_1 for the parameter, t, in Equation (E-17). The resulting expression after these substitutions are made is

$$1 - \frac{k_1}{k_2} \left[\frac{G_{NAR}}{k_1 V} \left(t_1 - \frac{1}{k_1} + \frac{e^{-k_1 t_1}}{k_1} \right) \right] = C^* e^{-k_1 t_1} \quad (\text{E-27})$$

$G_{NAR}/k_1 V$ in Equation (E-27) can be simplified if one multiplies by t_1/t_1 . The parameter k_2 can be substituted for $G_{NAR}t_1/V$, after which Equation (E-28) is obtained:

$$1 - \frac{k_1}{k_2} \left[\frac{k_2}{k_1 t_1} \left(t_1 - \frac{1}{k_1} + \frac{e^{-k_1 t_1}}{k_1} \right) \right] = C^* e^{-k_1 t_1} \quad (\text{E-28})$$

Equation (E-28) can be simplified to Equation (E-29) by cancelling like terms:

$$1 - \frac{1}{t_1} \left(t_1 - \frac{1}{k_1} + \frac{e^{-k_1 t_1}}{k_1} \right) = C^* e^{-k_1 t_1} \quad (\text{E-29})$$

Multiplying Equation (E-29) by $e^{k_1 t_1}$ and cancelling like terms yields

$$e^{k_1 t_1} \left(1 - 1 + \frac{1}{k_1 t_1} - \frac{e^{-k_1 t_1}}{k_1 t_1} \right) = C^* \quad (\text{E-30})$$

Equation (E-30) can be further simplified to Equation (E-31).

$$C^* = \frac{e^{k_1 t_1}}{k_1 t_1} \left(1 - e^{-k_1 t_1} \right) \quad (\text{E-31})$$

or

$$C^* = \frac{1}{k_1 t_1} (e^{k_1 t_1} - 1). \quad (\text{E-32})$$

Substituting the expression for C^* in Equation (E-32) for C^* in Equation (E-26) yields

$$C = \frac{-k_2}{k_1} \left[\frac{1}{k_1 t_1} (e^{k_1 t_1} - 1) e^{-k_1 t} - 1 \right]. \quad (\text{E-33})$$

Multiplying Equation (E-33) by -1 and rearranging yields

$$C = \frac{k_2}{k_1} \left[1 - \frac{1}{k_1 t_1} (e^{k_1(t_1-t)} - e^{-k_1 t}) \right]. \quad (\text{E-34})$$

Substituting $G_{NAR} t_1 / V$ for k_2 in Equation (E-34) yields

$$C = \frac{G_{NAR} t_1}{k_1 V} \left[1 - \frac{1}{k_1 t_1} (e^{k_1(t_1-t)} - e^{-k_1 t}) \right]. \quad (\text{E-35})$$

or

$$C = \frac{G_{NAR}}{k_1 V} \left[t_1 - \frac{1}{k_1} (e^{k_1(t_1-t)} - e^{-k_1 t}) \right]. \quad (\text{E-36})$$

Simplifying Equation (E-36) yields

$$C = \frac{G_{NAR}}{k_1 V} \left[t_1 - \frac{e^{k_1(t_1-t)}}{k_1} + \frac{e^{-k_1 t}}{k_1} \right]. \quad (\text{E-37})$$

Rearranging Equation (E-37) yields

$$C = \frac{G_{NAR}}{k_1 V} \left[t_1 - \frac{e^{-k_1(t-t_1)}}{k_1} + \frac{e^{-k_1 t}}{k_1} \right]. \quad (\text{E-38})$$

The equation to calculate the average concentration for any interval of time less where t_e is less than or equal to t_2 and t_b is greater than or equal to t_1 is obtained by integrating Equation (E-38) with respect to time and dividing the resulting equation by the length of the exposure interval. The resulting expression is

$$C_{ave} = \frac{G_{NAR}}{k_1 V (t_e - t_b)} \left\{ t_1 t + \frac{e^{-k_1(t-t_1)}}{k_1^2} - \frac{e^{-k_1 t}}{k_1^2} \right\}_{t=t_b}^{t=t_e} \quad (E-39)$$

(3) For $t_2 < t < t_r$

The mass balance equation and the physical interpretation of each group of terms is

$$V \frac{dC}{dt} = G_{NAR} (t_r - t) - mQ C. \quad (E-40)$$

$$\left\{ \begin{array}{l} \text{The net mass of} \\ \text{chemical substance} \\ \text{in air in the room} \end{array} \right\} = \left\{ \begin{array}{l} \text{The mass of chemical} \\ \text{substance released} \\ \text{to air in the room} \end{array} \right\} - \left\{ \begin{array}{l} \text{The mass of chemical} \\ \text{substance removed by} \\ \text{air leaving the room} \end{array} \right\}.$$

Dividing Equation (E-40) by V yields

$$\frac{dC}{dt} = \frac{G_{NAR}}{V} (t_r - t) - \frac{mQ}{V} C. \quad (E-41)$$

By letting

$$k_1 = \frac{mQ}{V} \text{ and } k_2 = \frac{G_{NAR}}{V}$$

and by substituting k_1 and k_2 , as appropriate, into Equation (E-41), one obtains

$$\frac{dC}{dt} = k_2(t_r - t) - k_1 C. \quad (E-42)$$

If we let

$$z = k_2(t_r - t) - k_1 C \quad (E-43)$$

and differentiate with respect to time, the resulting expression is

$$\frac{dz}{dt} = -k_2 - k_1 \frac{dC}{dt}. \quad (E-44)$$

Upon being rearranged, Equation (E-44) becomes

$$\frac{-1}{k_1} \left(\frac{dz}{dt} + k_2 \right) = \frac{dC}{dt}. \quad (E-45)$$

If Equations (E-43) and (E-45) are substituted into Equation (E-42), the resulting expression is

$$\frac{-1}{k_1} \left(\frac{dz}{dt} + k_2 \right) = z. \quad (E-46)$$

Multiplying Equation (E-46) by $-k_1$ yields

$$\frac{dz}{dt} + k_2 = -k_1 z. \quad (E-47)$$

Rearranging Equation (E-47) yields

$$\frac{dz}{dt} = -(k_2 + k_1 z). \quad (E-48)$$

Rearranging Equation (E-48) yields

$$\frac{dz}{k_2 + k_1 z} = -dt. \quad (E-49)$$

Integrating Equation (E-49) with respect to

$$\frac{1}{k_1} \ln (k_2 + k_1 z) = -t + \beta''. \quad (E-50)$$

Multiplying Equation (E-50) by k_1 yields

$$\ln (k_2 + k_1 z) = -k_1 t + \beta'. \quad (E-51)$$

If one takes the antilog of Equation (E-51), the resulting expression is

$$k_2 + k_1 z = \beta e^{-k_1 t}. \quad (E-52)$$

To determine β in Equation (E-52), substitute the expression for z from Equation (E-43) in Equation (E-52). When t equals t_2 , C is equal to Ct_2 . Therefore, substitute t_2 for t and Ct_2 for C to determine β . Ct_2 is calculated by substituting t_2 for t in Equation (E-37). The resulting expression is

$$k_2 + k_1 \left[k_2 (t_r - t_2) - k_1 Ct_2 \right] = \beta e^{-k_1 t_2}. \quad (E-53)$$

Rearranging Equation (E-53) yields

$$\beta = e^{k_1 t_2} [k_2 + k_1 k_2 (t_r - t_2) - k_1^2 C t_2]. \quad (\text{E-54})$$

Substituting the expression for z from Equation (E-43) into Equation (E-52) yields

$$k_2 + k_1 [k_2 (t_r - t) - k_1 C] = \beta e^{-k_1 t}. \quad (\text{E-55})$$

Multiplying the expression in brackets in Equation (E-55) by k_1 yields

$$k_2 + k_1 k_2 (t_r - t) - k_1^2 C = \beta e^{-k_1 t}. \quad (\text{E-56})$$

Rearranging Equation (E-56) yields

$$-k_1^2 C = \beta e^{-k_1 t} - k_2 - k_1 k_2 (t_r - t). \quad (\text{E-57})$$

Substituting the expression for β from Equation (E-54) into Equation (E-57) yields

$$-k_1^2 C = e^{-k_1 t} \left\{ e^{k_1 t_2} [k_2 + k_1 k_2 (t_r - t_2) - k_1^2 C t_2] \right\} - [k_2 + k_1 k_2 (t_r - t)]. \quad (\text{E-58})$$

Simplifying Equation (E-58) results in

$$-k_1^2 C = e^{(-k_1 t + k_1 t_2)} [k_2 + k_1 k_2 (t_r - t_2) - k_1^2 C t_2] - [k_2 + k_1 k_2 (t_r - t)]. \quad (\text{E-59})$$

Simplifying Equation (E-59) results in

$$-k_1^2 C = e^{-k_1(t-t_2)} [k_2 + k_1 k_2 (t_r - t_2) - k_1^2 C t_2] - [k_2 + k_1 k_2 (t_r - t)]. \quad (\text{E-60})$$

Dividing Equation (E-60) by $-k_1^2$ yields

$$C = e^{-k_1(t-t_2)} \left[-\frac{k_2}{k_1^2} - \frac{k_2}{k_1} (t_r - t_2) + C t_2 \right] + \left[\frac{k_2}{k_1^2} + \frac{k_2}{k_1} (t_r - t) \right]. \quad (\text{E-61})$$

Substituting G_{NAR}/V for k_2 in Equation (E-61) and rearranging yields

$$C = -e^{-k_1(t-t_2)} \left[\frac{G_{NAR}}{k_1^2 V} + \frac{G_{NAR}}{k_1 V} (t_r - t_2) - Ct_2 \right] + \left[\frac{G_{NAR}}{k_1^2 V} + \frac{G_{NAR}}{k_1 V} (t_r - t) \right]. \quad (E-62)$$

Ct_2 is calculated using Equation (E-38) by setting t equal to t_2 . The equation to calculate the average concentration for any interval of time where t_e is less than or equal to t_r and t_b is greater than or equal to t_2 is derived by integrating Equation (E-62) with respect to time and dividing the resulting equation by the length of the exposure interval. The resulting expression is

$$C_{ave} = \frac{1}{(t_e - t_b)} \left\{ \frac{e^{-k_1(t-t_2)}}{k_1} \left[\frac{G_{NAR}}{k_1^2 V} + \frac{G_{NAR}}{k_1 V} (t_r - t_2) - Ct_2 \right] \right\}_{t=t_b}^{t=t_e} + \left[\frac{G_{NAR}}{k_1^2 V} + \frac{G_{NAR}}{k_1 V} (t_r - \frac{t}{2}) \right]_{t=t_b}^{t=t_e}. \quad (E-63)$$

(4) For $t > t_r$

Equation (3-7) with Ct_r substituted for C_0 and with $(t-t_r)$ substituted for t is used to calculate the concentration at any time after t_r . Ct_r is calculated by substituting t_r for t in Equation (E-62). As the time during this interval increases, the concentration decreases exponentially as air containing the chemical flows out of the room.

$$C = Ct_r \left[e^{-m(Q/V)(t-t_r)} \right] \quad (E-64)$$

The equation to calculate the average concentration for any interval of time where t_e and t_b are greater than or equal to t_r is derived by integrating Equation (E-64) with respect to time. The resulting expression is

$$C_{ave} = Ct_r \left[\frac{-e^{-k(t-t_r)}}{k^2} \right]_{t=t_b}^{t=t_e}. \quad (E-65)$$