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EMISSION SCENARIO DOCUMENT ON THE BLENDING OF FRAGRANCE OILS INTO COMMERCIAL AND CONSUMER PRODUCTS

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EMISSION SCENARIO DOCUMENT ON THE BLENDING OF FRAGRANCE OILS INTO COMMERCIAL AND CONSUMER PRODUCTS

IOMC

INTER-ORGANISATION PROGRAMME FOR THE SOUND MANAGEMENT OF CHEMICALS

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EXPLANATORY NOTES

Purpose and background

This OECD Emission Scenario Document (ESD) is intended to provide information on the sources, use patterns and release pathways of chemicals used in the electronics industry, to assist in the estimation of releases of chemicals into the environment.

This ESD should be seen as a 'living' document, which provides the most updated information available. As such, an ESD can be updated to take account of changes and new information, and extended to cover the industry area in countries other than the lead (the United States). Users of the document are encouraged to submit comments, corrections, updates and new information to the OECD Environment, Health and Safety Division (env.riskassessment@oecd.org). The comments received will be forwarded to the OECD Task Force on Exposure Assessment, which will review the comments every two years so that the lead country can update the document. The comments will also be made available to users within the OECD web-site (www.oecd.org/env/riskassessment).

How to use this document

The user of this ESD needs to consider how the information contained in the document covers the situation for which they wish to estimate releases of chemicals. The document could be used as a framework to identify the information needed, or the approaches in the document could be used together with the suggested default values to provide estimates. Where specific information is available it should be used in preference to the defaults. At all times, the values inputted and the results should be critically reviewed to assure their validity and appropriateness.

How this document was developed

This ESD was developed under the leadership of the United States. The proposal to develop this ESD was approved by the OECD Task Force on Environmental Exposure Assessment (TFEEA) in September 2004. Since then the first, second and the third drafts were circulated to the Task Force for their comments in 2005, 2006 and 2008 respectively.

With regard to these drafts, relevant data and information were provided by Canada in 2006 and the Research Institute for Fragrance Materials (RIFM) in 2009, which were incorporated as Appendices of this document. Finally the draft ESD was approved by the Task Force on Exposure Assessment which replaced TFEEA in early 2009, at its first meeting in November-December 2009.

This document is published on the responsibility of the Joint Meeting of the Chemicals Committee and the Working Party on Chemicals, Pesticides and Biotechnology of the OECD.

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1. INDUSTRY SUMMARY AND BACKGROUND

The scope of this ESD includes the blending of fine and functional fragrance oils into consumer and commercial products. The manufacture of aroma chemicals and the formulation of fragrance oil are outside the scope of this scenario. However, these industrial operations are discussed in this section as an introduction to the fragrance industry as a whole. The following life-cycle diagram demonstrates the applicability of this scenario.

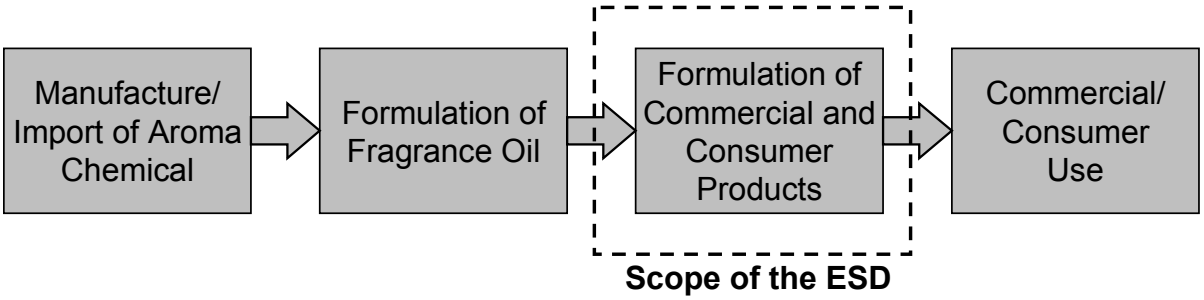


Figure 1-1. Life-Cycle Diagram – Aroma Chemical

It should be noted that certain operations covered in the 1994 Generic Scenario for Manufacture and Use of Fragrances (e.g., the use of fragrances in mixing and packaging detergents, cosmetics, etc.) fall within the scope of this scenario. Where the two scenarios overlap, this ESD is an update of the 1994 Generic Scenario.

1.1 Aroma Chemical Manufacturing

The manufacture of fragrance oils consists of blending an array of aroma chemicals with other additives to produce a desired smell. Aroma chemicals can either be extracted from nature or synthetically manufactured through a chemical process. Natural aroma chemicals are extracted from fragrant blossoms, leaves, roots, fruits and woods by steam distillation, crushing, or solvent extraction (Kirk-Othmer, 2005). Synthetic aroma chemicals were first created in the mid-nineteenth century to recreate natural fragrances and later to create new scents. Synthetics have a greater market share due to their abundance, lower cost, and simple purification. They are also independent of supply interruptions caused by inclement growing conditions. Synthetics are generally manufactured in a batch process and then distilled to remove impurities having a negative affect on the aroma. The ability to control the purity of a synthetic chemical eliminates the uncertainty of exposure to other unknown components found in natural chemicals (FMA, 2006). Environmental releases and worker exposures during natural chemical extraction and synthetic aroma chemical manufacturing are outside the scope of this ESD.

The majority of aroma chemicals are manufactured in small quantities. Below is a breakdown of the approximately 3,000 aroma chemicals used in blending or compounding fragrances, based on a market profile from 1985 (Grant, 1985):

- 88% were used in quantities less than 1,000 kg/yr, with many less than 100 kg/yr;[1]
- 8.3% were used in quantities from 1,000 to 10,000 kg/yr;
- 2% were used in quantities from 10,000 to 100,000 kg/yr;
- 1.3% were used in quantities from 100,000 to 1,000,000 kg/yr; and,
- 0.7% were used in quantities greater than 1,000,000 kg/yr.

A search of the 2005 Premanufacture Notice (PMN) Initial Review Engineering Reports (IRERs) shows that of the 20 reports concerning aroma chemicals all had production volumes of 10,000 kg or less. The median production volume of the reports was 900 kg, which substantiates the market profile (EPA, 2006a). It should be noted that these production volumes are the maximum amount potentially produced, not the actual production volumes.

1.2 Fragrance Oil Formulation

Individual aroma chemicals can be blended with hundreds of other aroma chemicals to create fragrance oil. Stabilizers (to reduce the rate of volatilization) and solvents (to help dissolve solids) may also be added to enhance the function of the oil. Concentrations of an aroma chemical in a fragrance oil can range from parts per million to 20 weight percent (Kirk-Othmer, 2005). The concentration of the aroma chemical depends upon the intended use of the final product. Some aroma chemicals are added to provide a strong initial scent, while others provide a pleasant, lingering odor. Fragrance oil formulators typically have thousands of aroma chemicals available as they develop the fragrance oil.

Fragrance oil formulators are classified under the North American Industry Classification System (NAICS) code 32562, Toilet Preparations Manufacturing, and specifically under the Perfume Oil Mixtures and Blends Manufacturing subcategory. According to the 2002 Economic Census, 33 companies were listed under the Perfume Oil Mixtures and Blends Manufacturing subcategory (USCB, 2002).

Fragrance oils are designed and formulated for a specific end use. For the purpose of this scenario, fragrance oils are classified by two categories, fine and functional fragrances. Fine fragrance oils are those used in the formulation of perfumes, colognes, and aftershaves. Functional fragrance oils are those used in personal and household products such as cosmetics, shampoos, detergents, soaps, and other cleaning formulations. There are no major differences in the processes used to formulate the two types of fragrance oil. The only significant difference between the oils themselves is the relative strength (i.e., concentration) and variety of aroma.

[1]Note: original data converted from Mton/yr by multiplying by 1,000 kg/Mton.

1.3 Formulation of Commercial and Consumer Products

The aromatic strength of fragrance oils results from the concentration of the specific aroma chemicals. Table 1-1 lists the concentration of functional fragrance oils in several types of consumer products. While functional fragrance oils may be incorporated at higher concentrations for products specifically designed for their aromatic purposes (e.g., scented candles, air fresheners), they are typically incorporated into commercial and consumer products at concentrations of 2% or less (e.g., most cleaning products) (Kirk-Othmer, 2005; EPA, 2006b)[1].

Table 1-1. Concentration of Fragrances in Various Consumer Products

Product Type	Concentration of Fragrance Oil(s) (Percent)
Scented candle	3 to 7
Scented gel air freshener, plug-in	60 to 100
Scented gel air freshener, non-plug-in	1 to 3
Carpet & room deodorizer	0.5 to 5
Toilet bowl cleaner/deodorizer	<10
Laundry detergent	0.5
Pet care products	<1 to 6
Liquid auto products	0 to 10
Paste auto products	<1
Aerosol auto products	<1 to 5

Source: Household Products Database (NLM, 2006).

Fine fragrance oils are present in the final products at much higher concentrations, because the aromatic effect imparted by the fragrance oil is the primary function of the product. These oils are present at concentrations of 20-35% in women's perfumes and 2-12% in men's colognes and aftershaves (Kirk-Othmer, 2005).

Commercial and consumer product formulators are classified under NAICS code 3256, Soap, Cleaning Compound, and Toilet Preparations Manufacturing. According to the 2002 Economic Census, 2,356 U.S. sites employed 113,041 workers in 2002 (USCB, 2002). This scenario assumes that all facilities classified under NAICS codes 32561 and 32562 manufacture commercial and consumer

[1] Under EPA's Design for the Environment (DfE) Branch's Formulator Partnership, companies may submit the chemical constituents and concentrations of their formulations to DfE for review. DfE reviews the formulation and may suggest safer chemical substitutes. EPA reviewed the concentration of fragrance oils in the approximately 150 recognized formulations (as of August 2006). Most formulations reviewed to date are cleaning products (e.g., laundry detergent, dishwashing detergent, surface cleaners, carpet cleaners/deodorizers). With one exception, fragrance oils were blended into cleaning products at 2% concentration or less (typically less than 1%). The one exception identified is a holding tank cleaner/deodorizer (e.g., toilet bowl deodorizers), which is specifically designed to keep a tank smelling fresh. Fragrance oils may be expected in these products at <10% concentration.

products containing functional fragrance oils. One exception is facilities in subcode 3256204 under NAICS code 32562 which are assumed to be the perfume and cologne formulators using fine fragrance oils. Table 1-2 lists the number of establishments and workers for NAICS code 3256.

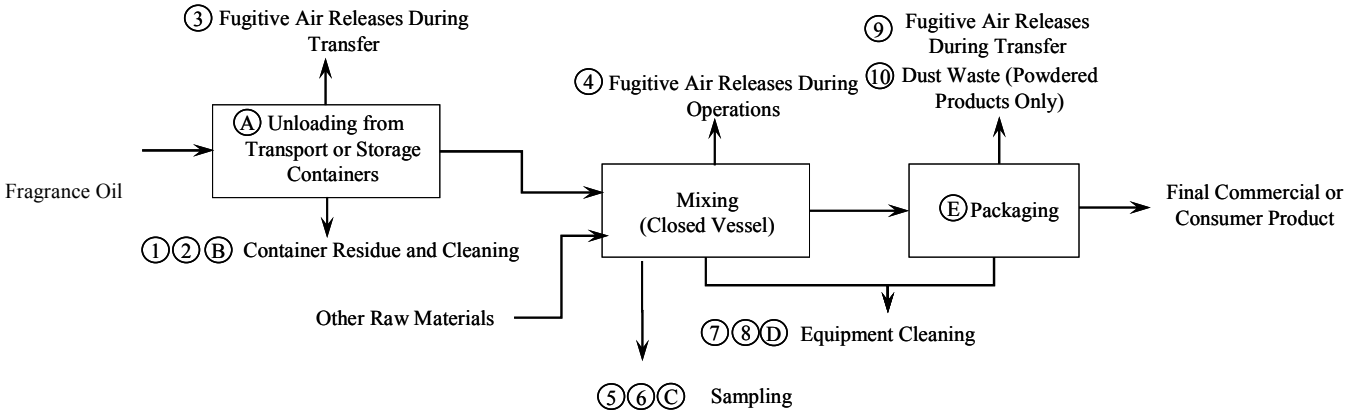
Table 1-2. Number of Sites and Number of Workers in NAICS code 3256

NAICS Code	NAICS Code Title	Product	Number of Sites[a]	Total Number of Employees[a]	Average Number of Workers per Site	Average Number of Production Workers per Site	Percentage of Production Workers[a]
3256-	Soap, cleaners, and toilet preparation mfg	All products in codes 32561 and 32562	2,356	113,041	48	29	60
-1	Soap and cleaning compound mfg	All products in codes 325611, 325612, and 325613	1,534	48,327	32	18	56
-11	Soap and other detergent mfg	Laundry detergents, dishwashing detergents, toothpaste gels and powders, natural glycerin	761	23,296	31	20	64
-12	Polish and sanitation goods mfg	Bleach, air fresheners, fabric softeners, laundry dryer sheets; glass, toilet bowl, and upholstery cleaners; auto, floor, and furniture cleaners and polishes	604	17,679	29	17	58
-13	Surface active agent mfg	Wetting agents, emulsifiers, and penetrants for manufacturing textiles and leather finishing agents	169	7,352	44	20	47
-2	Toilet preparation mfg	Shampoos, shaving cream, denture cleaners, deodorants, sunscreen, cosmetics, perfumes, colognes, and other lotions	822	64,714	79	50	63
-204	Perfumes, toilet waters, and colognes	Perfumes, colognes, and fragrance oils	35	4,185	120	60	50

a - Source: U.S. Census Bureau, 2002 Economic Census (USCB, 2002).

2. PROCESS DESCRIPTION

The processes used to formulate commercial and consumer products containing fine and functional fragrance oil into may vary widely; however, the major processes used are essentially the same. This section presents generic process descriptions for both fragrance oil types and identifies potential environmental release and occupational exposure points for each process. Figure 2-1 summarizes the release and exposure points in a generic process flow diagram.



Environmental Releases:

1. Release to water, incineration, or land from container residue.
2. Fugitive losses to air during container cleaning.
3. Transfer operation losses to air from unloading the chemical.
4. Fugitive losses to air during operations.
5. Release to water, incineration, or land from sampling residue.
6. Fugitive losses to air during sampling.
7. Release to water, incineration, or land from equipment cleaning.
8. Fugitive losses to air during equipment cleaning.
9. Transfer operation losses to air from loading final product.
10. Dust waste generated from conveying, mixing, and packaging powdered detergents released to water, incineration, land, or air.

Occupational Exposures:

A. Dermal and inhalation exposure to liquids during unloading from transport containers and charging the aroma chemical.
B. Dermal and inhalation exposure to liquids and vapors during container cleaning.
C. Dermal and inhalation exposure to liquids and vapors during sampling.
D. Dermal and inhalation exposure to liquids and vapors during equipment cleaning.
E. Dermal and inhalation exposure to liquids, vapors or solids during the packaging of commercial and consumer products.

Figure 2-1. Process Flow Diagram – Fine and Functional Fragrance Oil

When the specific end-use of an aroma chemical is unknown, this scenario assumes that the chemical is used in functional fragrance oil, which is in turn formulated into powdered commercial and consumer products. For volatile chemicals, both vapor and dust inhalation exposures are assessed. These assumptions (discussed in greater detail in Section 3) results in the most comprehensive assessment of the possible end use of the aroma chemical.

2.1 Production of Commercial and Consumer Products Using Functional Fragrance Oils

The particular manufacturing process used to incorporate functional fragrance oils into commercial and consumer products varies greatly. Heated processes are used in the manufacturing of many cleaning products; however, because they are heat-sensitive, fragrance oils are generally added after the product

has been cooled down to room temperature. If fragrance oils are mixed into a warm consumer product, the aroma chemicals could potentially evaporate or degrade (Aroma, 2004). In unheated processes, the fragrance oil may be blended with other materials during the manufacturing process. Once the process is complete, the final commercial and consumer product is packaged for shipment and sale. Some specific process descriptions are listed below:

- Powdered detergents may be formed in a spray drying, agglomeration, or dry mixing process. In spray drying, ingredients are combined in a slurry or viscous liquid. The liquid is heated and sprayed under high pressure through nozzles at the top of a tower then falls in small droplets through a current of hot air, drying into solid granules (SDA, 2006). Fragrances and other heat-sensitive materials are blended with the solid granules, which are then packaged in either a small container for consumers (approximately 1 gallon) or larger containers (drums) for industrial or commercial use, such as industrial or institutional laundries. Conveying, mixing, and packaging powdered detergents may also generate dust, resulting in exposure and emission (EPA, 1993).

- Liquid detergents or cleaning products may be produced in batch or continuous processes (SDA, 2006). Surfactants and other cleaning ingredients are blended with the fragrance. Stabilizers may be added to ensure the final product is stable and uniform. After blending, the product is packaged for sale in containers ranging from an 8-ounce bottle of special purpose cleaner to totes of industrial or institutional laundry detergent.

- Solid bar soaps are typically made in a continuous or semi-continuous process (Aroma, 2004). Fats and oils are saponified with inorganic water-soluble bases, and by-products such as glycerin are removed, producing soap in a liquid form. The soap is then vacuum-spray dried to convert the neat soap into dry pellets. Pellets are blended together with fragrance oils, colorants, and other heat-sensitive ingredients in a large enclosed mixer called an amalgamator. The mixture is further refined and homogenized through rolling mills and refining plodders to achieve uniformity (SDA, 2006). The mixture is finally extruded, cut into individual bars, and stamped into its final shape.

- Gel air fresheners consist of fragrance oils blended with organic or inorganic gelling materials, such as silica, and coloring. Scented gels with high solids concentrations and low fragrance concentrations (1-3 percent) may be formed into sticks or cones for use in air fresheners with adjustable plastic housings. Gels with high fragrance concentrations (greater than 60 percent) may be dispensed into cartridges in a form-fill-seal process for use in plug-in air fresheners. In these products, a permeable membrane allows aroma chemicals to evaporate from the cartridge when the gel is warmed by electric current. (Thomson-Gale, 2006)

- Aerosol air fresheners and cleaners are made by first blending the fragrance oil with a solvent, surfactants, and other additives. The concentration of the fragrance oil in an aerosol air freshener is typically 1 percent (Thomson-Gale, 2006). The mixture is added to the unsealed aerosol can through the valve stem, which is then crimped closed while a vacuum is drawn in the container. The propellant filler forms a seal around the head of the can, and under pressure, forces the propellant through the valve stem into the can (Kirk-Othmer, 2005). Cans are generally placed in a warm water bath (approximately 130°F) (NIOSH, 1992) to check for leaks. Because the containers are sealed before they are heated, an air release or vapor exposure is possible but not expected.

Generic Process Description for Functional Fragrance Oils – Default

This subsection describes the general process for incorporating functional fragrance oil into commercial and consumer products, which is a compilation of the specific process descriptions presented above. Because functional fragrance oils may be used in a variety of commercial and consumer products, EPA uses this general process description to develop estimates of environmental releases and occupational exposures. If the physical state of the final product is unknown, the fragrance oil is assumed to be formulated into powdered products, resulting in additional estimates of dust waste during packaging.

The fragrance oil is received in transport containers (drums or smaller) and poured or pumped into a mixing tank (Exposure A). Due to the volatility of the aroma chemicals, fugitive air releases may occur during transfers (Release 3). No industry-specific information on container handling was found (see Section 8.0 for a list of specific sources investigated); however, empty containers are likely to be rinsed with water or an organic solvent, as residual fragrance oil may affect the scent of future fragrance oil stored in the container (Exposure B). The containers may not be cleaned on site but sent directly to a landfill (Release 1). Volatile aroma chemicals may also evaporate during the container cleaning, resulting in fugitive air releases (Release 2).

The fragrance oil and other heat-sensitive materials are blended into the product formulation after the formulation has been cooled to room temperature. Even at room temperature, fugitive air releases are may occur during the blending process due to the volatility of the aroma chemicals (Release 4). The mixture may be homogenized and refined through a mesh screen, rolling mill, or plodder.

Although no industry-specific data were found regarding product sampling practices at product formulators, it is generally assumed that some amount of product quality analysis/quality control (QA/QC) sampling is performed as part of the formulation process (engineering judgment). Releases and associated exposures may occur as a result of sampling activities (Release 5, Release 6, and Exposure C).

Because many of the manufacturing processes are continuous or semi-continuous, tanks and process equipment may only be cleaned intermittently (Exposure D). During the cleaning, fugitive releases to air may occur due to the volatility of the aroma chemicals (Release 8). Industry-specific information on equipment cleaning practices was unavailable; therefore, the release of equipment cleaning residue is assessed to the default media of water, incineration or landfill (Release 7). Automated packaging machines typically load consumer products into small containers. Workers may load large volume commercial products, such as industrial and institutional laundry detergents, into drums or totes and may be exposed while connecting transfer lines (Exposure E). Fugitive air releases may occur during the transfer (Release 9). Packaging a powder product may generate dust (Release 10), which results in an additional inhalation exposure to particulate during the loading of transport containers (Exposure E).

2.2 Production of Consumer Products Using Fine Fragrance Oils

Fine fragrances are formulated into consumer products such as perfumes and colognes. Commercial use of products containing fine fragrance oils is possible but not expected. The formulations containing fine fragrance oil are designed to be pleasant, diffusive, and long lasting, as well as compatible with the skin and body.

Generic Process Description for Fine Fragrance Oils

The process for manufacturing consumer products containing fine fragrance oils is generally consistent for all products. The fragrance oils are generally blended with denatured alcohol (Flick, 1989), bottled, and shipped to consumers. This subsection describes the general process for incorporating fine fragrance oil into consumer products.

The fragrance oil is unloaded from storage containers or pumped directly from the fragrance oil formulation vessel into a mixing tank (Exposure A). Because most aroma chemicals are volatile, fugitive air releases may occur during transfers (Release 3). No industry-specific information on container handling was found (see Section 8.0 for a list of specific sources investigated); however, containers are likely to be rinsed with water or an organic solvent, as residual fragrance oil may affect the scent of future fragrance oil stored in the container (Exposure B). The containers may not be cleaned on site but sent directly to a landfill (Release 1). Volatile aroma chemicals may also evaporate during the container cleaning (Release 2).

Denatured alcohol and the fine fragrance oil are blended together in a batch process. This process does not usually involve heating because of degradation and volatilization concerns; however, fugitive air releases may occur due to the volatility of the aroma chemicals (Release 4).

Although no industry-specific data were found regarding product sampling practices at product formulators, it is generally assumed that some amount of product quality analysis/quality control (QA/QC) sampling is performed as part of the formulation process (engineering judgment). Releases and associated exposures may occur as a result of sampling activities (Release 5, Release 6, and Exposure C).

The process equipment will likely be used to formulate multiple types of consumer products; therefore, the process equipment will be cleaned after every batch because the residual fragrance oil will affect the aroma of subsequent batches (Exposure D). During the cleaning, fugitive releases to air may occur due to the volatility of the aroma chemicals (Release 8). Industry-specific information on equipment cleaning practices was unavailable; therefore, the release of equipment cleaning residue is assessed to the default media of water, incineration or landfill (Release 7). Workers load the formulated product into automated bottling machines for packaging (Exposure E). The automated bottling machines typically load the perfume or cologne into small containers (<20 fluid ounces) for sale to consumers. Fugitive air releases may occur during the transfer (Release 9).

2.3 Physical Properties of Aroma Chemicals

This ESD focuses on aroma chemicals used in the manufacturing of commercial and consumer fragrance products. Aroma chemicals are generally volatile, oily liquids. Their molecular weight typically ranges from 100 to 300, with most chemicals containing between 10 and 18 carbon atoms. A majority of aroma chemicals contain one oxygenated functional group, but some may contain more. Nitrogen- and sulfur-containing compounds are also common (Kirk-Othmer, 2005). Table 2-1 presents the physical properties of chemical compounds representing different aroma chemical categories presented in Kirk-Othmer. The chemicals were chosen to be representative of the category; however, physical properties may vary across the category. The physical property data are intended only to provide the reader with a general understanding of the physical properties of each category.

Table 2-1. Chemical Property Data of Representative Aroma Chemicals

Component Category	Chemical (CAS)	Neat Physical State	Molecular Weight	Vapor Pressure (torr at 25°C)	Boiling Point (°C)	Melting Point (°C)	Water Solubility (mg/L at 25°C)	Other (Density, Octanol-Water Partition Coefficient)
Ester	Benzyl acetate (140-11-4)	Liquid[a]	150.2[b]	0.177[c]	213[a,c]	-51.3[b]	3,100[c]	$\rho = 1.06$[d] $\log K_{OW} = 1.96$[c]
Alcohol	Citronellol (106-22-9)	Liquid[a]	156.3[b]	0.0441[c]	224.5[a,c]	<25[c]	212[c]	$\rho = 0.86$[d] $\log K_{OW} = 3.91$[c]
Aldehyde	Citral (5392-40-5)	Liquid[a]	152.2[b]	0.0913[c]	227[c]	<-10[c]	1,340 (at 34°C)[c]	$\rho = 0.89$[d] $\log K_{OW} = 3.45$[c]
Hydrocarbon	Limonene (138-86-3)	Liquid[a]	136.2[b]	1.55[c]	176[c]	-95[c]	7.57[c]	$\rho = 0.84$[d] $\log K_{OW} = 4.57$[c]
Ketone	Carvone (99-49-0)	Liquid[a]	150.2[b]	0.16[c]	230-231[a]	9.8[a]	1,300[c]	$\rho = 0.96$[d] $\log K_{OW} = 3.07$[c]
Lactones	Coumarin (91-64-5)	Solid[a]	146.1[b]	0.00098[c]	301.7[c]	71[c]	1,900 (at 20°C)[c]	$\rho = 0.94$[d] $\log K_{OW} = 1.39$[c]
Ether	Galaxolide (1222-05-5)	Liquid[d]	258.4[b]	0.000545[c]	325[c]	-5[c]	1.75[c]	$\rho = 1.00$[d] $\log K_{OW} = 5.90$[c]
Nitrile	Cinnamonitrile (4360-47-8)	Solid or Liquid[d]	129.2[b]	0.0129[c]	253-254[d]	-4 (*cis*)[d] 22 (*trans*)[d]	1,070[c]	$\rho = 1.03$[b] $\log K_{OW} = 1.84$[c]
Polyfunctional	Isoeugenol (97-54-1)	Liquid[a]	164.2[b]	0.012[c]	266[a]	-10[a]	356[c]	$\rho = 1.09$[d] $\log K_{OW} = 3.04$[c]

a – Source: Merck, 1996.
b – Source: ChemFinder, 2006.
c – Source: SRC, 2006.
d – Source: Wavelength, 2005.

3. GENERAL FACILITY ESTIMATES

This ESD presents EPA's standard approach for estimating environmental releases of and worker exposures to aroma chemicals during the formulation of commercial and consumer products. This section covers the blending of fragrance oils into commercial and consumer products.

The estimation methods described in this document utilize available industry-specific information and data to the greatest extent possible; however, EPA acknowledges several areas in which additional fragrance industry data are needed. These data needs are summarized in Section 7 of this ESD. It should be noted that the default values cited throughout this ESD are intended to be used only when appropriate site-specific or industry-specific information is not available.

Because this ESD presents several alternative default assumptions or values for some estimation parameters, one must consider carefully how the selection of these defaults will affect the final assessment results.

This section of the ESD presents general facility calculations for formulators, which estimate daily use rates of fragrance oil and aroma chemical, the number of formulation sites using the chemical of interest, and the number of days the chemical is expected to be used in the formulation process.

Section 4 of the ESD presents the environmental release assessments for the formulation of commercial and consumer products containing fragrance oils, which use the general facility estimates to estimate the quantity of chemical released from various points in the formulation process and the most likely media of release for each release source.

Section 5 of the ESD presents the occupational exposure assessments for the formulation of commercial and consumer products containing fragrance oils, which use both the general facility estimates and release estimates to estimate the number of workers potentially exposed while performing various process activities and the corresponding potential level (quantity) and routes of those exposures.

3.1 Introduction to the General Facility Estimates

When a new fragrance chemical is identified, the specific type of end-use commercial or consumer product (containing fine or functional fragrance oil) is generally unknown. Aroma chemicals are blended into fragrance oil that may be sold either directly to consumers or to additional sites for further formulation into commercial and consumer products. When the end-use of the aroma chemical is unknown, a conservative estimate is that the entire volume of an aroma chemical would be formulated into functional fragrance oils and shipped off site for formulation into commercial and consumer products. It is assumed, at the general facility, that the chemical is incorporated into powdered commercial and consumer products. This assumption provides the most comprehensive assessment of the possible end use of the chemical. Table 3-1 summarizes the general facility parameters calculated in this section. Table A-4 in Appendix A summarizes EPA's default values that could be used for general facility estimates, accompanied by their references.

Table 3-1. Summary of General Facility Parameters

Parameter	Description	ESD Section
$TIME_{working_days}$	Number of operating days the fragrance oil is formulated into commercial and consumer products (days/yr).	3.2
F_{chem_final}	Weight fraction of aroma chemical in final commercial and consumer product (kg aroma chemical/kg product).	3.3
$Q_{chem_site_day}$	Daily use rate of aroma chemical (kg aroma chemical/site-day).	3.4
N_{sites}	Number of sites using the fragrance oil containing the aroma chemical (sites).	3.5
$N_{container_unload_site_yr}$	Number of transport containers unloaded at each site per year (containers/site-yr).	3.6
$N_{container_load_site_yr}$	Number of transport containers loaded at each site per year (container/site-yr).	3.7

The method described in the remaining sections incorporates certain assumptions in cases where industry-specific data were not found. These key assumptions are presented throughout this section and are accompanied by a discussion of their uncertainties and potential effects on the estimates.

3.2 Days of Operation ($TIME_{working_days}$)

In the absence of industry-specific information, the total number of operating days ($TIME_{operating_days}$) for the commercial and consumer product formulator may be assumed to be 250 days/yr (CEB, 1991). This is based on a five-day workweek and a two-week operation shut down for maintenance and holidays.

While the fragrance oil containing the aroma chemical of interest may only be formulated into a portion of the commercial and consumer products produced by the formulator, data on the number of fragrance oils used by each site was unavailable at the time of publication. Therefore, EPA assumes that all products formulated at each site contain the fragrance oil containing the aroma chemical of interest (i.e., $F_{products}$ is equal to 1 kg of product formulated containing the chemical of interest per kg of total products formulated). If chemical-specific or site-specific information is available, these data should be used in lieu of this assumption. The impact of this assumption is discussed in greater detail in Section 3.4.

$$TIME_{working_days} = TIME_{operating_days} \times F_{products} \quad (3\text{-}1)$$

Where:

$TIME_{working_days}$ = Number of operating days fragrance oil is formulated into commercial and consumer products (days/yr)

$TIME_{operating_days}$ = Total facility operating days (Default: 250 days/yr)

$F_{products}$ = Fraction of products formulated at each site containing the chemical of interest (Default: 1 kg of product formulated containing chemical of interest/ kg of all products formulated)

3.3 Concentration of the Aroma Chemical (F_{chem_final})

The concentration of an aroma chemical in fragrance oil can range from parts per million to 20 weight percent (Kirk-Othmer, 2005). If chemical-specific information is unavailable, a conservative estimate of 20% aroma chemical in the fragrance oil (F_{chem_oil}) may be assumed. To calculate the concentration of the aroma chemical in the final product, the following guidelines should be considered:

- Functional fragrance oils (default scenario) are typically used at concentrations of 2% or less in consumer products (Kirk-Othmer, 2005; EPA, 2006b). If the end use product is unknown and the concentration of the fragrance oil in the final commercial and consumer product is unknown, a default of 2% is assumed. However, if the final commercial and consumer product is known, alternative defaults may be selected from Table 1-1.

- Fine fragrance oils are used in a much larger range of concentrations. Table 3-2 provides guidance if the specific end-use of the fragrance oil is known. If the end-use of the fragrance oil is unknown, the upper end of the concentration range of 35% is assumed.

Table 3-2. Concentration of Fine Fragrance Oils in Consumer Products

Product Type	Concentration of Fragrance Oil
Women's Perfumes	20% to 35%
Women's Colognes	12% to 22%
Men's Colognes and Aftershaves	2% to 12%

Source: Kirk-Othmer, 2005.

If the type of fragrance oil in which the aroma chemical will be blended is unknown, it may be assumed that the aroma chemical will be incorporated into functional fragrance oil. This estimate is based on the U.S Census data presented in Table 1-2, which demonstrates that, of the 2,356 sites identified as potentially incorporating fragrance oil into final products, only 35 manufacture products, such as perfume and cologne, with fine fragrance oil.

The concentration of an aroma chemical in the final product can be calculated using the following equation:

$$F_{chem_final} = F_{chem_oil} \times F_{oil_final} \quad (3\text{-}2)$$

Where:

F_{chem_final} = Weight fraction of aroma chemical in final product (kg aroma chemical/ kg product)

F_{chem_oil} = Weight fraction of aroma chemical in fragrance oil (Default: 0.2 kg aroma chemical/ kg fragrance oil)

F_{oil_final} = Weight fraction of fragrance oil in final product (Default: 0.02 kg fragrance oil/ kg product; see Tables 1-1 and 3-2 for alternative defaults)

3.4 Daily Use Rate of Aroma Chemical ($Q_{chem_site_day}$)

Due to the wide range of company and facility sizes, estimates for the daily use rate of an aroma chemical presented in this ESD are based on census data and engineering judgment. Table 3-3 presents the 2002 Economic Census data indicating the quantity of fragrance oil used for two of the four NAICS codes of interest. No data were available for NAICS code 325613 Surface Active Agent Manufacturing or 325620 Toilet Preparations Manufacturing. The average use rate of the two NAICS codes presented in

Table 3-3 may be appropriate to use for estimating purposes if the specific end use of the commercial and consumer product is unknown or if the end use falls under another NAICS code.

Table 3-3. Consumption of Fragrance Oils in Consumer Cleaning Products

NAICS Code	Fragrance Oils Consumed in 2002 (million kg)[a]	Sites	Average Annual Use Rate (kg/site-yr)[b]
325611 Soap and Other Detergent Manufacturing	21.7	761	28,500
325612 Polish and Other Sanitation Goods Manufacturing	6.4[c]	604	10,600
Totals and Average Use Rate	**28.1**	**1,368**	**20,500**

a - Source: USCB, 2002. Original data converted from pounds to kilograms.
b - Calculated by dividing the 2002 consumption of fragrance oils by the number of sites.
c - 2002 value was not reported. Value is estimated by applying the growth rate of fragrance oil reported for NAICS code 325611 from the Economic Census for years 1997-2002 to the 1997 Economic Census value of fragrance oil reported for NAICS code 325612.

The average daily use of fragrance oil containing the chemical of interest can be estimated using the following equation:

$$Q_{oil_site_day} = \frac{Q_{oil_site_yr} \times F_{products}}{TIME_{working_days}} \quad (3\text{-}3)$$

Where:

$Q_{oil_site_day}$ = Daily use of fragrance oil (kg fragrance oil/site-day)
$Q_{oil_site_yr}$ = Average annual facility use of fragrance oil (Default: 20,500 kg fragrance oil/site-yr; see Table 3-3 for alternative defaults)
$TIME_{working_days}$ = Number of operating days fragrance oil is formulated into commercial and consumer products (days/yr) (see Section 3.2)
$F_{products}$ = Fraction of products formulated at each site containing the chemical of interest (Default: 1 kg of product formulated containing chemical of interest/ kg of all products formulated)

The daily use rate of fragrance oil ($Q_{oil_site_day}$) can then be used to determine the daily use rate of the aroma chemical ($Q_{chem_site_day}$), by multiplying the weight fraction of the aroma chemical in the fragrance oil (F_{chem_oil}) by the daily use rate of the fragrance oil, as shown below.

$$Q_{chem_site_day} = Q_{oil_site_day} \times F_{chem_oil} \quad (3\text{-}4)$$

Where:

$Q_{chem_site_day}$ = Daily use rate of aroma chemical (kg aroma chemical/site-day)
$Q_{oil_site_day}$ = Daily use rate of fragrance oil (kg fragrance oil/site-day) (see Equation 3-3)
F_{chem_oil} = Weight fraction of the aroma chemical in the fragrance oil (Default: 0.2 kg aroma chemical/kg fragrance oil; see Section 3.3)

The following key assumptions and limitations in this method of determining the use rate of the aroma chemical should be noted:

- All sites listed in the Economic Census under NAICS codes 325611 and 325612 are assumed to use fragrance oil. EPA recognizes that not all sites listed under these NAICS codes formulate products with fragrance oil (e.g., unscented industrial laundry detergents). Using this assumption underestimates the daily use rate of the aroma chemical and result in more conservative exposure assessments (i.e., greater number of workers) but less conservative release assessment (i.e., smaller daily release amount).

- All sites are assumed to use only one fragrance oil. EPA recognizes that facilities will likely formulate multiple products containing different fragrance oils; however, industry-specific information was not available (see Section 8.0 for a list of the specific sources investigated). Using this assumption may overestimate the daily use rate of the aroma chemical and result in less conservative exposure assessments but more conservative release assessments.

EPA typically presents methodology to estimate both a "typical" and "high-end" use rates to provide ranges for these assumptions. However, at the time of publication, no industry-specific information was identified to develop methodology to characterize facilities by size. If such information becomes available, EPA will revise its methodology to provide both "typical" and "high-end" use rates for the fragrance oil containing the aroma chemical of interest.

3.5 Number of Sites (N_{sites})

Using the daily use rate estimated above and the annual production volume of the aroma chemical, the number of sites using the aroma chemical can be estimated using the following equation:

$$N_{sites} = \frac{Q_{chem_yr}}{Q_{chem_site_day} \times TIME_{working_days}} \quad (3\text{-}5)$$

Where:

N_{sites}[1] = Number of sites using the fragrance oil containing the aroma chemical (sites)

Q_{chem_yr} = Annual production volume of aroma chemical (kg aroma chemical/yr)

$Q_{chem_site_day}$ = Daily use rate of aroma chemical (kg aroma chemical/site-day) (see Equation 3-4)

[1]The value for N_{sites}, calculated using Equation 3-5 should be rounded up to the nearest integer value. $Q_{chem_site_day}$ should then be adjusted for the N_{sites} integer value (to avoid errors due to rounding):

$$Q_{chem_site_day} = \frac{Q_{chem_yr}}{N_{sites} \times TIME_{working_days}}$$

Note: If the number of formulation sites is known, the previous equation may also be used to estimate the resulting average annual production rate for use in subsequent calculations.

$TIME_{working_days}$ = Number of operating days fragrance oil is formulated into commercial and consumer products (days/yr) (see Equation 3-1)

Based on 2002 Economic Census data, there are 2,321 sites using functional fragrance oil and 35 sites using fine fragrance oil (see Table 1-2). Therefore, if the estimated number of sites exceeds the corresponding Census value, default values may be adjusted accordingly (i.e., increasing the weight fraction of the aroma chemical, which will decrease the number of sites using the fragrance oil).

Summary of the Relationship of General Facility Parameters

The values for days of operation, daily use rate of the chemical of interest (Q_{chem_day}), and number of sites (N_{sites}) are related. This ESD presents one method for estimating Q_{chem_day} using estimated default values for: 1) the total U.S. production volume of fragrance oil; 2) the fraction of the aroma chemical in the fragrance oil; and 3) number of operating days ($TIME_{working_days}$).

If N_{sites} and $TIME_{working_days}$ are known, $Q_{chem_site_day}$ can be calculated directly, without using Equation 3-4. This alternative calculation is:

$$Q_{chem_site_day} = \frac{Q_{chem_yr}}{N_{sites} \times TIME_{working_days}}$$

Alternatively, if only N_{sites} is known, $Q_{chem_site_day}$ could be calculated utilizing the following alternate equations:

$$Q_{chem_site_yr} = \frac{Q_{chem_yr}}{N_{sites}}$$

$$TIME_{working_days} = \frac{TIME_{operating_days} \times Q_{chem_site_yr}}{Q_{oil_site_yr} \times F_{chem_oil}}$$

$$Q_{chem_site_day} = \frac{Q_{chem_yr}}{TIME_{working_days}}$$

However, it is recommended to calculate the chemical of interest throughput based on the methodology presented in Section 3.4, and compare it to the throughput based on number of sites and operating days, as calculated above.

3.6 Number of Transport Containers Unloaded per Site ($N_{container_unload_site_yr}$)

The number of fragrance oil containers unloaded annually per site can be estimated based on the daily use rate, container size, and weight fraction of the aroma chemical in the component. Industry-specific information on the types of containers used by the fragrance industry was not found in the references reviewed for this ESD (see Section 8.0 for a list of the specific sources investigated). EPA suggests that a default transportation container size of a 55-gallon drum can be used in the absence of site-specific information. Engineering judgment may be used to determine if another container type or size is

more appropriate (e.g., a 5-gallon pail may be more appropriate for highly concentrated fragrance oils). If the density of the fragrance oil is not known, the density of water can be used as a default (1 kg/L).

$$N_{container_unload_site_yr} = \frac{Q_{chem_site_day} \times TIME_{working_days}}{F_{chem_oil} \times V_{container_oil} \times RHO_{oil}} \quad (3\text{-}6)$$

Where:

$N_{container_unload_site_yr}$ = Number of transport containers unloaded at each site per year (containers/site-yr)

$Q_{chem_site_day}$ = Daily use rate of aroma chemical (kg aroma chemical/site-day) (see Equation 3-4)

F_{chem_oil} = Weight fraction of the aroma chemical in the fragrance oil (Default: 0.2 kg aroma chemical/kg fragrance oil; see Section 3.3)

$TIME_{working_days}$ = Number of operating days fragrance oil is formulated into commercial and consumer products (days/yr) (see Equation 3-1)

$V_{container_oil}$ = Volume of fragrance oil container (Default: 208 L fragrance oil/container (for 55-gallon drum))

RHO_{oil} = Density of fragrance oil (Default: 1 kg fragrance oil/L fragrance oil; assumed to be similar to water)

3.7 Number of Transport Containers Filled per Site ($N_{container_load_site_yr}$)

The number of containers filled annually with the final product per site can be estimated similarly to estimating the number of fragrance oil containers that are emptied (see Section 3.6). The calculation is based on the daily use rate of fragrance oil, container size, and weight fraction of the aroma chemical in the final product. The following guidelines should be considered when evaluating the container size parameter for the calculation:

- For products containing fine fragrance oils: 20-ounce bottle;
- For products containing functional fragrance oil designed for industrial or institutional use: 55-gallon drums;
- For products containing functional fragrance oil designed for commercial and/or consumer use: 1-gallon containers; and,
- If the end use of the product is unknown: 1-gallon containers (default).

$$N_{container_load_site_yr} = \frac{Q_{chem_site_day} \times TIME_{working_days}}{F_{chem_final} \times V_{container_final} \times RHO_{final}} \quad (3\text{-}7)$$

Where:

$N_{container_load_site_yr}$	=	Number of transport containers unloaded at each site per year (container/site-yr)
$Q_{chem_site_day}$	=	Daily use rate of aroma chemical (kg aroma chemical/site-day) (see Equation 3-4)
F_{chem_final}	=	Weight fraction of aroma chemical in final product (kg aroma chemical/ kg product) (see Equation 3-2)
$TIME_{working_days}$	=	Number of operating days fragrance oil is formulated into commercial and consumer products (days/yr) (see Equation 3-1)
$V_{container_final}$	=	Volume of final product container (Default: 3.78 L product/container (for 1-gallon container))
RHO_{final}	=	Density of final product formulation (Default: 1 kg product/L product; assumed to be similar to water)

4. ENVIRONMENTAL RELEASE ASSESSMENTS

This section presents an approach for calculating the amount of aroma chemical released for each identified release source. The release sources are discussed in the order that they occur in the process (see Figure 2-1). The most likely media of release (i.e., air, water, landfill, or incineration) are also identified. Table 4-1 presents the release sources, the likely media of release, and the models used to estimate the release. Table A-4 in Appendix A provides default values used for release and exposure estimates, accompanied by their respective references.

Table 4-1. Summary of Environmental Releases and Likely Media of Release

Release	Description	Model(s)	Standard EPA Model (✓)
1	Container cleaning residue released to water, incineration, or land.	*EPA/OPPT Bulk Transport Residual Model, Drum Residual Model, or Small Container Residual Model*	✓
2	Fugitive releases of volatile chemical to air during container cleaning.	*EPA/OPPT Penetration Model*	✓
3	Fugitive releases of volatile chemical to air during unloading.	*EPA/OAQPS AP-42 Loading Model*	✓
4	Fugitive releases of volatile chemical to air during mixing operation.	*EPA/OPPT Penetration Model*	✓
5	Product sampling wastes disposed to non-air media.	No methodology for quantifying the release from this source has been developed	
6	Fugitive releases of volatile chemical to air during product sampling.	*EPA/OPPT Penetration Model*	✓
7	Equipment cleaning residue released to water, incineration, or land.	*EPA/OPPT Multiple Vessel Residual Model or Solid Residuals in Transport Containers Model*	✓
8	Fugitive releases of volatile chemical to air during equipment cleaning.	*EPA/OPPT Mass Transfer Coefficient Model*	✓
9	Fugitive releases of volatile chemical to air during product loading.	*EPA/OAQPS AP-42 Loading Model*	✓
10	Dust emissions to water, incineration, land, or air from conveying powder products.	*AP-42 Emission Factor*	

OPPT – Office of Pollution Prevention and Toxics.
OAQPS – Office of Air Quality Planning and Standards.

It is generally assumed that during commercial and consumer product formulation, the losses of the aroma chemical are minimized in actual practice; however, it is likely that some pre-process or other upstream releases occur. Because losses are assumed to be minimized, the methodology presented in this section for estimating the releases of the chemical of interest from the formulation process does not include adjustments to account for pre-process or other upstream releases of the chemical (e.g., while some material may remain in the transport container, the entire volume received in the container is assumed when estimating equipment cleaning releases). These omissions of mass balance adjustments

should not result in a negative throughput of the chemical of interest in these calculations (i.e., the total amount of chemical released from the process should not exceed the amount that enters the process).

All release equations below estimate daily rates for a given site. To estimate annual releases for all sites for a given source, the daily release rates must be multiplied by the number of days of release and by the total number of product formulation sites using the aroma chemical (N_{sites}, see Equation 3-5).

Some of the process releases may occur to the same receiving medium on the same days. Therefore, daily and annual releases to a given medium may be summed to yield total amounts released per site-day and per year, respectively.

No industry-specific release data were available for this industry except for an emission factor for powdered detergent and soap manufacturing (see Section 4.12). Therefore, most of the environmental release estimates presented in this document are based on standard EPA release models. Note that the model default values cited are current as of the date of this ESD; however, EPA may update these models as additional data become available. It is recommended that the most current version of the models be used in these calculations.

EPA has developed a software package (ChemSTEER) containing these models as well as all current EPA defaults. Because of the complexity of the air release models, ChemSTEER is recommended for estimating air releases. Appendix B provides additional information on ChemSTEER, including instructions for obtaining the program, as well as background information, model equations, and default values for several parameters for all standard EPA models.

4.1 Control Technologies

No specific data were found on typical pollution control technologies for water releases used by the fragrance industry, although it is likely that some sites may pretreat their process wastewaters. EPA suggests that as a default, it should be assumed that all aqueous wastes are discharged to surface waters (potentially to a publicly owned treatment works (POTW) in the United States). This assumption allows a conservative estimate on the releases to the environment. If site-specific information about control technologies is available, the assessments may be revised. See Section 4.12 for a discussion of pollution control technologies for air releases.

4.2 Adjusted Vapor Pressure

Many of the releases presented in Section 4 estimate vapor emissions of the aroma chemical. The quantity released is dependent on the vapor pressure or volatility of the aroma chemical of interest. For example, for chemicals with vapor pressures less than 0.001 torr, EPA typically assumes environmental releases of vapors are negligible.

However, the vapor pressure of a chemical within a mixture is different than the vapor pressure of a pure component. ChemSTEER utilizes a vapor pressure correction factor, $F_{correction_factor}$, and the following equation to adjust the vapor pressure for diluted chemicals.

$$VP_{chem_adjusted} = F_{correction_factor} \times VP_{chem_pure} \quad (4\text{-}1)$$

Where:

$VP_{chem_adjusted}$ = Adjusted vapor pressure of the aroma chemical within the formulation (torr)

$F_{correction_factor}$ = Vapor pressure correction factor (dimensionless)

VP_{chem_pure} = Vapor pressure of the pure aroma chemical (torr)

For many screening level estimates, EPA assumes that the chemical-containing material in the evaporating pool exhibits the vapor pressure of the chemical of interest (i.e., $F_{correction_factor} = 1$), and this assumption may be conservative. However, since aroma chemicals may be present in fragrance oils at low concentrations, this assumption may not be reasonable.

Alternatively, Raoult's Law may be utilized to estimate a vapor pressure correction factor (i.e., $F_{correction_factor}$ may be set equivalent to the chemical's mole fraction in the mixture). However, to estimate the true mole fraction of the chemical of interest within the fragrance oil, the weight fractions and molecular weights of all other components of the oil must be known. Due to the proprietary nature of most fragrance oil formulations, this information is likely not available. However, since many other chemicals in the fragrance oil (e.g., solvents, stabilizers, other aroma chemicals) may have a similar molecular weight as the aroma chemical of interest, the weight fraction may be assumed to be a realistic estimate of the mole fraction for the fragrance oil as it is received (i.e., $F_{correction_factor} = F_{chem_oil}$ for Releases 2 and 3) (CEB, 1998).

However, the molecular weights of the chemicals the fragrance oil is blended with to manufacture commercial and consumer products are unknown and are likely higher than the molecular weight of the aroma chemical (e.g., surfactants). Therefore, the weight fraction of the aroma chemical in the final commercial and consumer product would not be an appropriate approximation of the mole fraction of the aroma chemical. In this case (and as a general default, the vapor pressure correction factor for the aroma chemical of interest in the final product may be assumed to be equal to the weight fraction of the aroma chemical as it is received in the fragrance oil (i.e., $F_{correction_factor} = F_{chem_oil}$ for Releases 4, 6, 8, and 9).

When determining how to estimate the vapor releases presented in this ESD, the adjusted vapor pressure may be generally more appropriate than the vapor pressure of the pure component.

4.3 Release to Water, Incineration, or Land from Container Residue (Release 1)

The amount of fragrance oil remaining in the transportation containers depends on the size of the transport container. In the absence of industry-specific data, the following standard EPA models, which are included in ChemSTEER, may be used to estimate container residue releases:

- *EPA/OPPT Bulk Transport Residual Model* can be used for large containers (e.g., totes, tank trucks, rail cars) containing greater than or equal to 100 gallons of liquid;
- *EPA/OPPT Drum Residual Model* can be used for drums containing between 20 and 100 gallons of liquid (Default); and,
- *EPA/OPPT Small Container Residual Model* can be used for liquid containers containing less than 20 gallons.

The rationale, defaults, and limitations of these models are further explained in Appendix B. The release estimates are based on the most current version of each model (as of the date of this ESD). Because standard EPA/OPPT models are subject to change, EPA recommends using the current version.

EPA suggests that a 55-gallon drum be used as a default transport container in the absence of site-specific information. Therefore, the default model for estimating releases of container residue is the

EPA/OPPT Drum Residual Model, which estimates 3 percent of the fragrance oil remains in the drum as container residue. FMA provided industry-specific data on the quantity of residue that may remain in empty containers. Based on FMA data, 0.31 percent of the fragrance oil may remain as container residue if the drum is emptied by pumping. For pouring, 0.18 percent may remain as residue. EPA is currently revising the *EPA/OPPT Drum Residual Model* based on these and other available data on container residual. For conservative screening-level estimates, EPA recommends assuming 3 percent residual until the revised model is completed.

No industry-specific information was found on transport container cleaning. Typical industrial container handling may include rinsing the container with water or solvent. The residual wash is then released to water or incinerated. If the containers are not washed, they may be sent directly to a landfill or a drum recycler/reconditioner.

If the number of containers used per site per year ($N_{container_unload_site_yr}$, Equation 3-6) is fewer than the days of operation ($TIME_{working_days}$), the days of release equals the number of containers and the daily release is calculated based on the following equation:

$$Elocal_{container_residue_disp} = V_{container_oil} \times RHO_{oil} \times F_{chem_oil} \times F_{container_residue} \times 1\frac{container}{site-day} \qquad (4\text{-}2a)$$

This release will occur over [$N_{container_unload_site_yr}$] days/year from [$N_{sites}$] sites.

Where:

$Elocal_{container_residue_disp}$	=	Daily release of aroma chemical from container residue (kg aroma chemical/site-day)
$V_{container_oil}$	=	Volume of fragrance oil container (Default: 208 L fragrance oil/container (for 55-gallon drum))
RHO_{oil}	=	Density of fragrance oil (Default: 1 kg fragrance oil/L fragrance oil; assumed to be similar to water)
F_{chem_oil}	=	Weight fraction of the aroma chemical in the fragrance oil (Default: 0.2 kg aroma chemical/kg fragrance oil; see Section 3.3)
$F_{container_residue}$	=	Fraction of chemical remaining in the container as residue (Default for larger liquid containers: 0.03 kg container residue/kg fragrance oil supplied in drums; see Appendix B for defaults for other container types)

If the number of containers used per site per year ($N_{container_unload_site_yr}$) is greater than the days of operation, the days of release equal the days of operation, and the average daily release is calculated based on the following equation. Note that it is assumed most sites use less than one container per day. Also, Equation 4-2b may be used if a container size is not assumed in Equation 4-2a and the number of containers used per site per year is unknown.

$$Elocal_{container_residue_disp} = Q_{chem_site_day} \times F_{container_residue} \qquad (4\text{-}2b)$$

This release will occur over [$TIME_{working_days}$] days/year from [N_{sites}] sites.

Where:

$Elocal_{container_residue_disp}$	=	Daily release of aroma chemical from container residue (kg aroma chemical/site-day)
$Q_{chem_site_day}$	=	Daily use rate of aroma chemical (kg aroma chemical/site-day)
$F_{container_residue}$	=	Fraction of chemical remaining in the container as residue (Default for larger liquid containers: 0.03 kg container residue/kg fragrance oil supplied in drums; see Appendix B for defaults for other container types)

4.4 Fugitive Air Releases During Transport Container Cleaning (Release 2)

For those aroma chemicals with a low adjusted vapor pressure within the fragrance oil, (e.g., those with an adjusted vapor pressure < 0.001 torr), releases to air are expected to be negligible. However, the majority of aroma chemicals are expected to volatilize (see Section 4.2). .If the chemical is volatile, it may vaporize while empty containers are being rinsed and cleaned; therefore, a release to air from container cleaning may occur ($Elocal_{air_cleaning}$). The EPA standard model for estimating releases to air from container cleaning may be used (*EPA/OPPT Penetration Model*).

Table 4-2 lists the model inputs and default values. The models and all current EPA defaults have been programmed into ChemSTEER, and EPA recommends using this software to calculate fugitive losses to air during container cleaning. Appendix B provides background information, model equations, and default values for several parameters the model uses to estimate daily releases to air.

Table 4-2. Transport Container Cleaning Default Values for *EPA/OPPT Penetration Model*

Input Parameter	Default Values
Diameter of Opening	EPA default: 2 in. (5.08 cm) for all containers less than 5,000 gallons (CEB, 1991) (see Appendix B for alternative default diameters)
Frequency of Use	Equal to $TIME_{working_days}$ (see Equation 3-1) or the number of containers ($N_{container_unload_site_yr}$) (see Equation 3-6), whichever is fewer (see Section 4.3)
Molecular Weight	Specific chemical parameter
Number of Sites	Calculated in Section 3.5, Equation 3-5
Operating Hours for the Activity	Number of containers per site, per day[1] divided by the unload/fill rate (CEB, 2002) (Default: 20 containers/hr for volumes between 20 and 1,000 gallons (CEB, 1991); alternative default unload/fill rates are found in Appendix B)

[1]The daily number of containers unloaded per site may be estimated as (consistent with Section 4.3):

$$N_{container_unload_site_day} = \frac{N_{container_unload_site_yr}}{TIME_{working_days}}$$

($N_{container_site_day}$ should be rounded up to the nearest integer)

Where:

Vapor Pressure	Specific chemical parameter
Air Speed	Standard EPA default: 100 ft/min (CEB, 1991)
Vapor Pressure Correction Factor	$F_{chem\ oil}$ (see Section 4.2)

Note: The model also assumes standard temperature and pressure along with ideal gas interactions.

4.5 Fugitive Air Releases from Unloading Transport Containers (Release 3)

For those aroma chemicals with a low adjusted vapor pressure within the fragrance oil, (e.g., those with an adjusted vapor pressure < 0.001 torr), releases to air are expected to be negligible. However, the majority of aroma chemicals are expected to volatilize (see Section 4.2). If the chemical is volatile, it may vaporize while containers are being unloaded; therefore, a release to air from container unloading may occur ($Elocal_{air_unload}$). The standard EPA estimation model for transfer operations (*EPA/OAQPS AP-42 Loading Model*) may be used to estimate the release to air. This model provides typical and worst-case estimates for releases during transfer operations.

Table 4-3 lists the model inputs and default values. The models and all current EPA defaults have been programmed into ChemSTEER, and EPA recommends using this software to calculate air releases and exposures from transfer operations. Appendix B provides background information, model equations, and default values for several parameters the model uses to estimate daily releases to air.

Table 4-3. Transport Container Unloading Default Values for *EPA/OAQPS AP-42 Loading Model*

Input Parameter	Default Values
Saturation Factor	EPA defaults 0.5 (typical) and 1 (worst case) for all containers less than 5,000 gallons (CEB, 2002) (see Appendix B for alternative default saturation factors)
Frequency of Use	Equal to $TIME_{working_days}$ (see Equation 3-1) or the number of containers ($N_{container_unload_site_yr}$) (see Equation 3-6), whichever is fewer (see Section 4.3)
Molecular Weight	Specific chemical parameter
Number of Sites	Calculated in Section 3.5, Equation 3-5
Operating Hours for the Activity	Number of containers unloaded per site, per day divided by the unload/fill rate (CEB, 2002) (Default: 20 containers/hr for volumes between 20 and 1,000 gallons (CEB, 1991); alternative default unload/fill rates are found in Appendix B)
Unloading Rate	EPA default: 20 containers/hr for volumes between 20 and 1,000 gallons (CEB, 1991) (alternative default unload/fill rates are found in Appendix B)

$N_{container_unload_site_day}$ = Number of containers emptied containing chemical of interest per site per day (containers/site-day)

$N_{container_unload_site_yr}$ = Annual number of containers emptied containing chemical of interest per site (containers/site-yr) (see Equation 3-6)

$TIME_{working_days}$ = Operating days (see Equation 3-1)

Container Volume	EPA Default: 55-gallon drum (208 L) (for other container sizes, see Appendix B)
Vapor Pressure	Specific chemical parameter
Vapor Pressure Correction Factor	$F_{chem\ oil}$ (see Section 4.2)

Note: The model also assumes standard temperature and pressure along with ideal gas interactions.

4.6 Fugitive Air Releases During Mixing Operations (Release 4)

For those aroma chemicals with a low adjusted vapor pressure within the fragrance oil, (e.g., those with an adjusted vapor pressure < 0.001 torr), releases to air are expected to be negligible. However, the majority of aroma chemicals are expected to volatilize (see Section 4.2). Although heated mixing is generally avoided, volatile chemicals can potentially to be released to the air during mixing even at room temperature. EPA uses the *EPA/OPPT Penetration Model* as the default model to calculate this release.

Two parameters required for using the model are release time and diameter of the opening. While the typical process time for bar soaps is six hours (Aroma, 2004), many commercial and consumer cleaning products are formulated in a semi-continuous process. Therefore, it can be conservatively assumed that this release occurs over a 24-hour period for functional fragrance oil (default). For fine fragrance oil, a batch time of 8 hours may be assumed. If a mixing vessel is closed (default), it may be assumed that the vent has an opening diameter of 4 inches (engineering judgment[1]). These defaults should only be used in the absence of site-specific data for the *EPA/OPPT Penetration Model*. Table 4-4 lists model inputs and default values.

If the fragrance oil is mixed in an open vessel (not the default scenario), assume the diameter of the vessel can be substituted as the diameter of the opening. The vessel may be assumed to be cylindrical with the capacity comparable to the batch size. If the batch size is unknown, a default batch size of 500 kg may be assumed (Sigma, 2002). The diameter of the opening can be calculated using the following equation:

$$D_{opening} = \left[\frac{4 \times Q_{final_batch} \times 1000\left(cm^3 / L\right)}{\pi \times RHO_{final}} \right]^{1/3} \quad (4\text{-}3)$$

Where:

$D_{opening}$ = Diameter of the mixing vessel opening (cm)

Q_{final_batch} = Mass of final product formulated per batch (kg product/batch) (Sigma, 2002) (Default: 500 kg/batch)

[1] Note: The 4-inch vent diameter default is based on professional experience in the radiation-curable adhesives formulation, fermentation, and petroleum processing industries. Based on these industries, a 4-inch vent is assumed to provide conservative estimates for potential air releases during operations. Similar vent sizes are anticipated in the fragrances industry; however, the applicability of this default to the fragrance industry is uncertain. Additionally, the vessel may be vented through control technologies (e.g., scrubber, condenser, thermal oxidizer); however, industry-specific information on vent sizes or control technologies for volatile components was not identified.

RHO_{final} = Density of final product (Default: 1 kg product/L product; assumed to be similar to water)

Note that this equation assumes an aspect ratio (height/diameter) of one, which was found in McCabe, Smith, and Harriott, Unit Operations of Chemical Engineering, 5th Edition to relate mixing time for various types of impellers and Reynolds Number.

Table 4-4. Mixing Operations Default Values for *EPA/OPPT Penetration Model*

Input Parameter	Default Values
Diameter of Opening	Closed Vessel: 10 cm (4 in) (default) Open Vessel: see Equation 4-3
Frequency of Use	Equal to $TIME_{working\ days}$ (see Equation 3-1)
Molecular Weight	Specific chemical parameter
Number of Sites	Calculated in Section 3.5, Equation 3-5
Operating Hours for the Activity	Functional fragrances (default) = 24 hr/day, fine fragrances = 8 hr/batch
Vapor Pressure	Specific chemical parameter
Air Speed	Standard EPA default: 100 ft/min (CEB, 1991)
Vapor Pressure Correction Factor	$F_{chem\ oil}$ (see Section 4.2)

Note: The model also assumes standard temperature and pressure along with ideal gas interactions.

4.7 Product Sampling Wastes Disposed to Water, Incineration, or Landfill (Release 5)

EPA generally assumes that formulation processes incorporate product sampling activities for quality assurance/quality control (QA/QC) and that this sampling will generate some amount of waste that will be disposed of to either water, incineration, or landfill (engineering judgment). EPA found no industry-specific data in the references reviewed for this ESD, nor does EPA currently have data on QA/QC sampling waste amounts that can be used to generally quantify the release of these process wastes to non-air media.

It should be noted that EPA expects releases of the aroma chemical from product sampling activities to be relatively low in comparison to the other sources of release in the product formulation process.

4.8 Open Surface Losses to Air During Product Sampling (Release 6)

For those aroma chemicals with a low adjusted vapor pressure within the fragrance oil, (e.g., those with an adjusted vapor pressure < 0.001 torr), releases to air are expected to be negligible (see Section 4.2). However, if the chemical is volatile, it may volatilize and be emitted from the process during product QA/QC sampling activities ($Elocal_{air_sample}$). The EPA standard model for estimating releases to air from sampling activities performed indoors (*EPA/OPPT Penetration Model*) may be used. It should be noted that EPA expects releases of the aroma chemical from product sampling activities to be relatively low in comparison to the other sources of release in the product formulation process; however, the model is included to provide a vapor generation rate to estimate the corresponding occupational exposure during this activity (see Section 5.5).

Table 4-5 lists the model inputs and default values. The models and all current EPA defaults have been programmed into ChemSTEER, and EPA recommends this software for calculating open surface losses to air during sampling. Appendix B provides background information, model equations, and default values for several parameters the model uses to estimate daily releases to air.

Table 4-5. Product Sampling Default Values for *EPA/OPPT Penetration Model*

Input Parameter	Default Values
Diameter of Opening	EPA defaults for sampling: 1 in. (2.5 cm) typical and 4 in. (10 cm) worst case (CEB, 2002)
Frequency of Release	Equal to $TIME_{working\ days}$ (see Equation 3-1)
Molecular Weight	Specific chemical parameter
Number of Sites	Calculated in Section 3.5, Equation 3-5
Operating Hours for the Activity	EPA default for sampling: 1 hour/day (CEB, 1991)
Vapor Pressure	Specific chemical parameter
Air Speed	Standard EPA default: 100 ft/min (CEB, 1991)
Vapor Pressure Correction Factor	$F_{chem\ oil}$ (see Section 4.2)

Note: The model also assumes standard temperature and pressure along with ideal gas interactions.

4.9 Release to Water, Incineration, or Landfill from Equipment Cleaning (Release 7)

The amount of residual fragrance oil remaining in the process equipment may be estimated using the *EPA/OPPT Multiple Vessel Residual Model* for fragrance oil formulated into liquid products and *EPA/OPPT Solid Residuals in Transport Containers Model* for fragrance oil formulated into solid products (default). The *EPA/OPPT Multiple Vessel Residual Model* assumes that no more than 2% of the batch size or capacity of the process remains in the equipment as residue and released as equipment cleaning waste. The *Multiple Vessel Residual Model* is suggested as opposed to the *Single Vessel Residual Model* because automated loading equipment and transfer lines will also have to be cleaned. The *EPA/OPPT Solid Residuals in Transport Containers Model* assumes that no more than 1% of the batch size or capacity of the process remains in the equipment as residue and released as equipment cleaning waste.

Semi-continuous manufacturing equipment is not likely to be cleaned daily; however, the batch equipment used for to formulate perfumes and colognes may be cleaned after each batch. If the fragrance oil is used in commercial and consumer products containing functional fragrance oil, it may be assumed that cleaning occurs weekly (50 times/year) between product changes (CEB, 1991). Daily cleaning may be assumed for equipment used to produce of products containing fine fragrance oil.

No industry-specific information was found on the likely media of release for equipment cleaning. Equipment may be rinsed with water or organic solvent; therefore, container residue may be released to water, incineration, or landfill. The release from equipment cleaning can be estimated using the following equation:

$$Elocal_{equipment_residue_disp} = Q_{chem_site_day} \times F_{equipment_residue} \quad (4\text{-}4)$$

This release will occur over [$TIME_{working_days}$] days/year for fine fragrance oils and [50] days/year for functional fragrance oils from [N_{sites}] sites.

Where:

$Elocal_{equipment_residue_disp}$ = Daily release of aroma chemical from equipment residue (kg aroma chemical/site-day)

$Q_{chem_site_day}$ = Daily use rate of aroma chemical (kg aroma chemical/site-day) (see Section 3.4)

$F_{equipment_residue}$ = Fraction of aroma chemical remaining in the equipment as residue (Default: 0.02 kg equipment residue/kg in equipment for liquids and 0.01 kg equipment residue/kg in equipment for solids) (CEB, 1992)

4.10 Fugitive Air Releases During Equipment Cleaning (Release 8)

For those aroma chemicals with a low adjusted vapor pressure within the fragrance oil, (e.g., those with an adjusted vapor pressure < 0.001 torr), releases to air are expected to be negligible (see Section 4.2). However, for volatile chemicals, fugitive releases may occur during equipment cleaning operations. The standard EPA estimation model for open surface releases during cleaning operations (*EPA/OPPT Mass Transfer Coefficient Model*) may be used to estimate the release to air. The EPA standard diameter of the opening of a vessel for cleaning operations is 92 cm (3-foot manhole).

Table 4-6 lists the model inputs and default values. The model and all current EPA defaults have been programmed into ChemSTEER, and the software is recommended to calculate open surface losses to air during container cleaning. Appendix B provides background information, model equations, and default values for several parameters the model uses to estimate daily releases to air.

Table 4-6. Equipment Cleaning Default Values for *EPA/OPPT Mass Transfer Coefficient Model*

Input Parameter	Default Values
Diameter of Opening	EPA default for cleaning operations: 92 cm (3-foot manhole)
Frequency of Use	Equal to $TIME_{working\ days}$ (see Equation 3-1)
Molecular Weight	Specific chemical parameter
Number of Sites	Calculated in Section 3.5, Equation 3-5
Operating Hours for the Activity	EPA default for multiple vessel cleaning operations: 4 hrs (CEB, 1991)
Vapor Pressure	Specific chemical parameter
Air Speed	Standard EPA default: 100 ft/min (CEB, 1991)
Vapor Pressure Correction Factor	$F_{chem\ oil}$ (see Section 4.2)

Note: The model also assumes standard temperature and pressure along with ideal gas interactions.

4.11 Fugitive Air Releases During Product Packaging (Release 9)

For those aroma chemicals with a low adjusted vapor pressure within the fragrance oil, (e.g., those with an adjusted vapor pressure < 0.001 torr), releases to air are expected to be negligible. However, the majority of aroma chemicals are expected to volatilize (see Section 4.2). If the chemical is volatile, it may vaporize while containers are being loaded; therefore, a release to air from container loading may occur ($Elocal_{air_load}$). If the final product is a solid, an estimate for this release is made, as it is foreseeable that the aroma chemical could still vaporize.

To estimate the release of volatile aroma chemicals during the transfer of the final product to transport containers, the *EPA/OAQPS AP-42 Loading Model* may be used. Parameters may be based on size of the containers. Table 4-7 lists model inputs and default values. The models and all current EPA defaults have been programmed into ChemSTEER, and EPA recommends using this software to calculate fugitive losses to air during product packaging. Appendix B provides background information, model equations, and default values for several parameters the model uses to estimate daily releases to air.

Table 4-7. Product Packaging Default Values for *EPA/OAQPS AP-42 Loading Model*

Input Parameter	Default Values
Saturation Factor	EPA defaults 0.5 (typical) and 1 (worst case) for all containers less than 5,000 gallons (CEB, 2002) (see Appendix B for alternative default saturation factors)
Frequency of Use	Equal to $TIME_{working\ days}$ (see Equation 3-1)
Molecular Weight	Specific chemical parameter
Number of Sites	Calculated in Section 3.5, Equation 3-5
Operating Hours for the Activity	Number of containers loaded per site, per day[1] divided by the unload/fill rate (CEB, 2002) (Default: 20 containers/hr for volumes between 20 and 1,000 gallons (CEB, 1991); alternative default unload/fill rates are found in Appendix B)
Vapor Pressure	Specific chemical parameter
Container Volume	EPA default: 1-gallon container (see Section 3.7)
Vapor Pressure Correction Factor	$F_{chem\ oil}$ (see Section 4.2)

Note: The model also assumes standard temperature and pressure along with ideal gas interactions.

[1]The daily number of containers unloaded per site may be estimated as (consistent with Section 4.3):

$$N_{container_unload_site_day} = \frac{N_{container_unload_site_yr}}{TIME_{working_days}}$$

($N_{container_site_day}$ should be rounded up to the nearest integer)

Where:

$N_{container_unload_site_day}$ = Number of containers emptied containing chemical of interest per site per day (containers/site-day)

$N_{container_unload_site_yr}$ = Annual number of containers emptied containing chemical of interest per site (containers/site-yr) (see Equation 3-6)

$TIME_{working_days}$ = Operating days (see Equation 3-1)

Note: The default scenario assumes the fragrance oil is blended into powder products. The *EPA/OAQPS AP-42 Loading Model* may not properly assess air releases from loading powdered products into transport containers because volatile components do not evaporate from solid powders at the same rate as from liquid solutions. While the rate of evaporation of volatile chemicals from solid powders is unknown, the model can be used as a conservative estimate. In addition, the model provides the vapor generation rate necessary to assess inhalation exposures to vapors as well as particulate.

4.12 Release to Water, Incineration, Land, or Air from Dust Waste Generated from Conveying, Mixing, and Packaging Powdered Commercial and Consumer Products (Release 10)

If the end-use product is unknown, a conservative estimate assumes that fragrance oil is used in powder products because conveying, mixing, and packaging powder products produce all forms of emissions, including dust emissions. Release of the final product during pneumatic transfer is expected; however, air pollution control devices, such as those designed for spray dryers, recycle most of the recovered particulate back into the process (EPA, 1993). Table 4-8 presents the efficiencies of common control devices. No information was available on the media of release for dust waste; however, in some cases, the particulate may be small enough to travel several miles from the facility, resulting in environmental and human exposures beyond the boundaries of the site. Therefore, the release is assessed to the default media of water, incineration, land, or air.

It is estimated that the uncontrolled releases from a spray-drying unit are 4.5% of the product produced (45 kg particulates emitted per Mg product) (EPA, 1993). Therefore, a product loss fraction ($F_{dust_generation}$) of 4.5 percent may be used to estimate particulate emissions from the conveying, mixing, and packaging operations. Note that this estimate is more conservative than the 0.5 percent loss fraction utilized by the *EPA/OPPT Dust Emissions from Solid Transfers Model* (CEB, 2007a) (see Appendix B).

Dust is typically passed through a cyclone to remove most particulate, followed by a scrubber or ESP to remove smaller particulate and vapors. Table 4-8 presents efficiencies for common air pollution control devices used at powdered detergent manufacturing facilities. While particulate captured by a cyclone filter or fabric filter is typically recycled back into the process and not released into the environment (EPA, 1993), wet scrubber wastes may be harder to recycle. Wet scrubber wastes may be passed through a wiped film evaporator to concentrate the material for recycle; however, wastes from this operation may also be incinerated (CEB, 2007b). If site-specific information about the control device used is not available, it can conservatively be assumed that a device with 85% removal efficiency is used. A higher removal efficiency is not recommended, unless information is known on how wastes from secondary control technologies are handled.

Table 4-8. Efficiencies of Air Pollution Control Devices

Control Device	F_{APCD}
Cyclone	0.85
Cyclone with Spray Chamber	0.92
Cyclone with Packed Scrubber	0.95
Cyclone with Venturi Scrubber	0.97
Cyclone with Wet Scrubber	0.99
Cyclone with Wet Scrubber/ESP	0.999
Cyclone with Packed Bed/ESP	0.99
Fabric Filter	0.99

Source: EPA, 1993.

The following equation can be used to estimate the dust waste generated from conveying, mixing, and packaging powdered detergents:

$$Elocal_{dust_generation} = Q_{chem_site_day} \times F_{dust_generation} \times (1 - F_{APCD}) \quad (4\text{-}5)$$

This release will occur over [$TIME_{working_days}$] days/year from [N_{sites}] sites.

Where:

$Elocal_{dust_generation}$ = Daily release of aroma chemical from dust generation (kg aroma chemical/site-day)

$Q_{chem_site_day}$ = Daily use rate of aroma chemical (kg aroma chemical/site-day)

$F_{dust_generation}$ = Fraction of product released as dust (Default: 0.045 kg released/kg product transferred)

F_{APCD} = Air pollution control device efficiency (Default: 0.85; see Table 4-8 for alternative defaults)

Note that dust captured by control technologies is typically recycled back into the process and is not released into the environment (EPA, 1993). Therefore, this quantity is not estimated.

5. OCCUPATIONAL EXPOSURE ASSESSMENTS

As seen in Figure 2-1, worker activities at facilities incorporating fine and functional fragrances into commercial and consumer products include transferring fragrance oil to the mixing vessel, container cleaning, product sampling, equipment cleaning, and loading final products into transport containers. This section presents methodologies for estimating occupational exposures during these activities. Table 5-1 summarizes the source, physical state encountered, route, and model used to assess each exposure.

Table 5-1. Summary of Occupational Exposures

Exposure[a]	Description	Route of Exposure/Physical Form	Model	Standard EPA Model (✓)
A	Unloading Transport Containers	Inhalation of volatile liquid vapors.	*EPA/OPPT Mass Balance Model*	✓
		Dermal exposure to liquid chemical.	*EPA/OPPT 2-Hand Dermal Contact with Liquid Model*	✓
B	Transport Container Cleaning	Inhalation of volatile liquid vapors.	*EPA/OPPT Mass Balance Model*	✓
		Dermal exposure to liquid chemical.	*EPA/OPPT 2-Hand Dermal Contact with Liquid Model*	✓
C	Product Sampling	Inhalation of volatile liquid vapors.	*EPA/OPPT Mass Balance Model*	✓
		Dermal exposure to liquid product.	*EPA/OPPT 2-Hand Dermal Contact with Liquid Model*	✓
D	Equipment Cleaning	Inhalation of volatile liquid vapors.	*EPA/OPPT Mass Balance Model*	✓
		Dermal exposure to liquid product.	*EPA/OPPT 2-Hand Dermal Contact with Liquid Model*	✓
		Dermal exposure to solid product.	*EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model*	✓
E	Product Loading	Inhalation of volatile liquid vapors.	*EPA/OPPT Mass Balance Model*	✓
		Inhalation of particulate.	*OSHA Total Particulates Not Otherwise Regulated (PNOR) PEL-Limiting Model or EPA/OPPT Small Volume Solids Handling Inhalation Model*	✓
		Dermal exposure to liquid product.	*EPA/OPPT 2-Hand Dermal Contact with Liquid Model*	✓
		Dermal exposure to solid product.	*EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model*	✓

a - See Figure 2-1 for a list of occupational exposures.

Note that the model default values cited are current as of the date of this ESD; however, EPA may update these models as additional data become available. It is recommended that the most current version of the models be used for these calculations.

Industry-specific occupational exposure information was not found in the references reviewed for this ESD (see Section 8.0 for a list of specific sources investigated). All of the occupational exposure estimates presented in this document are based on standard EPA exposure models. Because of the complexity of the inhalation exposure to vapor models, ChemSTEER is recommended for estimating these exposures. Appendix B provides additional information on ChemSTEER, including information on obtaining the program, as well as background information, model equations, and default values for several parameters for all standard EPA models.

5.1 Personal Protective Equipment (PPE)

No specific information was identified about the typical PPE used during the formulation of commercial and consumer products containing fragrance oil. According to a study by the European Commission on worker exposures to benzene C_{10-13} alkyl derivatives, a common component of soap in liquid and powdered detergents, workers are "likely" to wear PPE[1]; however, the specific type of PPE was not mentioned (ECB, 1999). Typical Material Safety Data Sheets (MSDS) for fragrance oil suggest wearing gloves, goggles, and impervious clothing when handling the fragrance oil. A respirator with an organic vapor cartridge is also frequently recommended (for instance, in poorly ventilated spaces). To provide a conservative estimate, EPA standard exposure models assume that no PPE is used.

5.2 Number of Workers Exposed Per Site

U.S. Census Bureau information associated with NAICS codes can be used to estimate the total number of workers at each facility. If the NAICS code is unknown, it can be assumed that fine fragrance oils are classified under NAICS code 3256204 and functional fragrance oils (default) under NAICS code 3256. Once the NAICS code has been identified, the total number of production workers per site can be obtained from Table 1-2.

Industry-specific data on the numbers of workers potentially exposed while performing each of the commercial and consumer product formulation activities were not found in the references reviewed for this ESD (see Section 8.0 for a list of specific sources investigated). According to the 2002 Economic Census for the industry (NAICS code 3256), an average of 48 workers are employed at each facility (USCB, 2002); however, not all of these are expected to work in the production areas. The 2002 Economic Census estimates approximately 60% of these workers are *production* workers (USCB, 2002), which are defined by the U.S. Census Bureau to include:

> *"… workers (up through the line-supervisor level) engaged in fabricating, processing, assembling, inspecting, receiving, storing, handling, packing, warehousing, shipping (but not delivering), maintenance, repair, janitorial and guard services, product development, auxiliary production for plant's own use (e.g., power plant), record keeping, and other services closely associated with these production operations at the establishment." (USCB, 2002)*

[1] Note that, while PPE was likely to be worn, as a conservative estimate, exposure estimation in the study assumed PPE was not worn.

All other "non-production" employees include:

> *"… those engaged in supervision above the line-supervisor level, sales (including driver-salespersons), sales delivery (highway truck drivers and their helpers), advertising, credit, collection, installation and servicing of own products, clerical and routine office functions, executive, purchasing, financing, legal, personnel (including cafeteria, medical, etc.), professional, technical employees, and employees on the payroll of the manufacturing establishment engaged in the construction of major additions or alterations utilized as a separate work force." (USCB, 2002)*

It is therefore assumed that 60% of the 48 workers per site, or ***up to 29 workers per site***, are potentially exposed to the aroma chemical while performing formulation process activities. No information was found that would provide bases for estimating the specific numbers of these 29 workers that perform each of the exposure activities discussed in this section. Therefore, it can be conservatively estimated that all 29 workers per site are exposed during each activity.

No information was found on the typical hours of operation per day or the number of shifts supporting operations at product formulation facilities; however, this section presents an estimate for the exposure duration for each worker activity (based on standard EPA defaults and methodology).

5.3 Exposure from Unloading Transport Containers into Mixing Vessel (Exposure A)

Workers may connect transfer lines or manually unload the fragrance oil from transport containers into the mixing tanks. Exposure to solids is possible but not expected, since almost all fragrance oils are received in liquid form. Up to 29 workers per site may be exposed during this activity.

Inhalation Exposure:

Inhalation exposure is assumed to be negligible for chemicals with low adjusted vapor pressures within the fragrance oil (e.g., adjusted vapor pressure < 0.001 torr; see Section 4.2). If the aroma chemical is volatile, the vapor generation rate calculated in Release 3 and the EPA standard model for estimating inhalation exposure due to volatile chemicals evaporation (*EPA/OPPT Mass Balance Model*) during transfer operations may be used to estimate the exposure. The model and all current EPA defaults have been programmed into ChemSTEER, and the software is recommended to calculate inhalation exposures from transfer operations. Appendix B explains the background and derivation of the model, and provides EPA default values for several model parameters.

The ventilation rate of a perfume and air freshener formulation facility evaluated in a NIOSH Health Hazard Evaluation (HHE) was found to be 3,500-4,000 ft^3/min (NIOSH, 1992). This is comparable to the EPA default of 3,000 ft^3/min for typical exposure; therefore, the EPA default can be used when site-specific information is not available.

Table 5-2 lists the model inputs and default values. Note that the exposure hours per day is equivalent to the operating hours per day for this activity (consistent with Section 4.5 calculations), but EPA assumes a maximum exposure duration of eight hours per day. Similarly, the exposure days per site, per year should be consistent with the release days, but EPA assumes a maximum of 250 days per year.

These exposure duration maximum defaults are based on full-time employment and considers an individual worker's vacation, sick, and weekend time (i.e., a 40-hour work week over 50 weeks per year).

Table 5-2. Transport Container Unloading Default Values for *EPA/OPPT Mass Balance Model*

Input Parameter	Default Values
Inhalation Rate	Standard EPA default: 1.25 m^3/hr (CEB, 1991)
Exposure Days	Frequency of release determined in Section 4.5, up to 250 days per year
Vapor Generation Rate	Calculated by the *EPA/OAQPS AP-42 Loading Model* (Section 4.5)
Exposure Duration	Operating hours determined in Section 4.5
Mixing Factor	EPA defaults: 0.5 (typical) and 0.1 (worst case) (CEB, 1991)
Molecular Weight	Specific chemical parameter
Number of Sites	Calculated in Section 3.5, Equation 3-5
Ventilation Rate	EPA defaults: 3,000 ft^3/min (typical) and 500 ft^3/min (worst case) for indoor conditions (default for containers less than 1,000 gallons (CEB, 1991) (see Appendix B for alternative default ventilation rates)
Vapor Pressure	Specific chemical parameter
Vapor Pressure Correction Factor	$F_{chem\ oil}$ (see Section 4.2)

Note: The model also assumes standard temperature and pressure along with ideal gas interactions.

Dermal Exposure:

There is potential for dermal exposure during both metered and manual loading. Metered loading systems (e.g., pumps) limit worker exposure, but workers may still be exposed when connecting transfer lines. If metered loading systems are not used, workers manually pour the fragrance oil into the mixing vessel. No dermal monitoring data on the transfer of aroma chemicals were available at the time of publication. In the absence of data, the *EPA/OPPT 2-Hand Dermal Contact with Liquid Model* can be used to estimate dermal exposure to the aroma chemical in a liquid formulation during these activities (CEB, 1991). Appendix B discusses the rationale, defaults, and limitations of this model.

To estimate the potential worker exposure to the aroma chemical for this activity, the following equation may be used:

$$EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_oil} \quad (5\text{-}1)$$

This exposure will occur over the lesser of $N_{container_unload_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.5), up to [250] days per year.

Where:

EXP_{dermal} = Potential dermal exposure to the aroma chemical per day (mg aroma chemical/day)

Q_{liquid_skin}	=	Quantity of liquid fragrance oil remaining on skin (Defaults: 2.1 mg fragrance oil/cm^2-incident (high-end) and 0.7 mg fragrance oil/cm^2-incident (low-end) for routine or incidental contact (CEB, 2000))
$AREA_{surface}$	=	Surface area of contact (Default: 840 cm^2 for 2 hands (CEB, 2000))
$N_{exp_incident}$[1]	=	Number of exposure incidents per day (Default: 1 incident/day)
F_{chem_oil}	=	Weight fraction of the aroma chemical in the fragrance oil (Default: 0.2 kg aroma chemical/kg fragrance oil; see Section 3.3)

5.4 Exposure During Transport Container Cleaning (Exposure B)

Exposure to the aroma chemical may occur during container cleaning. If the weight fraction of the aroma chemical in the fragrance oil (F_{chem_oil}) is unknown, the default value of 20% weight fraction is used as a conservative estimate (see Section 3.3). Up to 29 workers per site may be exposed during this activity (see Section 5.2). The exposure route and rate presented for this activity are similar to those presented for Exposure A

Inhalation Exposure:

Inhalation exposure is assumed to be negligible for chemicals with low adjusted vapor pressures within the fragrance oil (e.g., adjusted vapor pressure < 0.001 torr; see Section 4.2). For volatile liquids, the *EPA/OPPT Mass Balance Model* can be used to calculate worker inhalation exposure due to volatilization during cleaning operations based on the vapor generation rate calculated in Release 2. The default ventilation rates and mixing factors provide worst-case and typical estimates of exposure.

The model and all current EPA defaults have been programmed into ChemSTEER, and use of the software is recommended to calculate inhalation exposure to volatile chemicals during container cleaning. Appendix B explains the background and derivation of the model and provides EPA default values for several model parameters.

Table 5-3 lists the model inputs and default values. Note that the exposure hours per day is equivalent to the operating hours per day for this activity (consistent with Section 4.4 calculations), but EPA assumes a maximum exposure duration of eight hours per day. Similarly, the exposure days per site, per year should be consistent with the release days, but EPA assumes a maximum of 250 days per year, as previously discussed in Section 5.2.

Table 5-3. Container Cleaning Default Values for *EPA/OPPT Mass Balance Model*

Input Parameter	Default Values

[1]Only one contact per day ($N_{exp_incident}$ = 1 event/worker-day) is assumed because Q_{liquid_skin}, with few exceptions, is not expected to be significantly affected either by wiping excess chemical material from skin or by repeated contacts with additional chemical material (i.e., wiping excess from the skin does not remove a significant fraction of the small layer of chemical material adhering to the skin and additional contacts with the chemical material do not add a significant fraction to the layer). Exceptions to this assumption may be considered for chemicals with high volatility and/or with very high rates of absorption into the skin.

Inhalation Rate	Standard EPA default: 1.25 m^3/hr (CEB, 1991)
Exposure Days	Frequency of release determined in Section 4.4, up to 250 days per year
Vapor Generation Rate	Calculated by the *EPA/OPPT Penetration Model* (Section 4.4)
Exposure Duration	Operating hours determined in Section 4.4, up to 8 hours per day
Mixing Factor	EPA defaults: 0.5 (typical) and 0.1 (worst case) (CEB, 1991)
Molecular Weight	Specific chemical parameter
Number of Sites	Calculated in Section 3.5, Equation 3-5
Ventilation Rate	EPA defaults are 3,000 ft^3/min (typical) and 500 ft^3/min (worst case) for indoor conditions (default for containers less than 1,000 gallons (CEB, 1991) (see Appendix B for alternative default ventilation rates)
Vapor Pressure	Specific chemical parameter
Vapor Pressure Correction Factor	$F_{chem\ oil}$ (see Section 4.2)

Note: The model also assumes standard temperature and pressure along with ideal gas interactions.

Dermal Exposure:

There is potential for dermal exposure during transport containers cleaning. No industry-specific dermal monitoring data on transport containers cleaning were found. In the absence of data, the *EPA/OPPT 2-Hand Dermal Contact with Liquid Model* can be used to estimate dermal exposure to the aroma chemical in a liquid formulation during these activities. Appendix B discusses the rationale, defaults, and limitations of these models.

To estimate the potential worker exposure to the aroma chemical in the fragrance oil for this activity, the following equation may be used:

$$EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_oil} \quad (5\text{-}2)$$

This exposure will occur over the lesser of $N_{container_unload_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.4), up to [250] days per year.

Where:

EXP_{dermal} = Potential dermal exposure to the aroma chemical per day (mg aroma chemical/day)

Q_{liquid_skin} = Quantity of liquid fragrance oil remaining on skin (Defaults: 2.1 mg fragrance oil/cm^2-incident (high-end) and 0.7 mg fragrance oil/cm^2-incident (low-end) for routine or incidental contact (CEB, 2000))

$AREA_{surface}$ = Surface area of contact (Default: 840 cm^2 for 2 hands (CEB, 2000))

$N_{exp_incident}$ = Number of exposure incidents per day (Default: 1 incident/day; see footnote to Equation 5-1)

F_{chem_oil} = Weight fraction of the aroma chemical in the fragrance oil (Default: 0.2 kg aroma chemical/kg fragrance oil; see Section 3.3)

5.5 Exposure from Sampling Product Formulation (Exposure C)

Workers may collect samples of the product formulation for quality analysis/quality control (QA/QC). Up to 29 workers per site may be exposed during this activity.

Inhalation Exposure:

Inhalation exposure is assumed to be negligible for chemicals with low adjusted vapor pressures within the fragrance oil (e.g., adjusted vapor pressure < 0.001 torr; see Section 4.2).

Using the vapor generation rate calculated in Release 6, the *EPA/OPPT Mass Balance Model* can be used to calculate worker inhalation exposure to volatile chemicals during sampling activities. The default ventilation rates and mixing factors provide a typical and worst-case estimate of exposure. Table 5-4 lists the model inputs and default values. Note that the exposure hours per day is equivalent to the operating hours per day for this activity (consistent with Section 4.8 calculations), but EPA assumes a maximum exposure duration of eight hours per day. Similarly, the exposure days per site, per year should be consistent with the release days, but EPA assumes a maximum of 250 days per year, as previously discussed in Section 5.2.

The model and all current EPA defaults have been programmed into ChemSTEER, and EPA recommends this software to calculate inhalation exposure to volatile chemicals during packaging/loading activities. Appendix B explains the background and derivation of the model and provides EPA default values for several model parameters.

Table 5-4. Sampling Parameter Default Values for *EPA/OPPT Mass Balance Model*

Input Parameter	Default Values
Inhalation Rate	Standard EPA default: 1.25 m^3/hr (CEB, 1991)
Exposure Days	Frequency of release determined in Section 4.8, up to 250 days per year
Vapor Generation Rate	Calculated by the *EPA/OPPT Penetration Model* (Section 4.8)
Exposure Duration	Operating hours determined in Section 4.8 (default: 1 hour/day (CEB, 1991))
Mixing Factor	EPA defaults: 0.5 (typical) and 0.1 (worst case) (CEB, 1991)
Molecular Weight	Specific chemical parameter
Number of Sites	Calculated in Section 3.5, Equation 3-5
Ventilation Rate	EPA defaults: 3,000 ft^3/min (typical) and 500 ft^3/min (worst case) for indoor conditions (default for containers less than 1,000 gallons (CEB, 1991) (see Appendix B for alternative default ventilation rates)
Vapor Pressure	Specific chemical parameter
Vapor Pressure Correction Factor	F_{chem_oil} (see Section 4.2)

Note: The model also assumes standard temperature and pressure along with ideal gas interactions.

Dermal Exposure:

Dermal exposure to liquid product may occur during sampling activities. The *EPA/OPPT 1-Hand Dermal Contact with Liquid Model* may be used to estimate dermal exposure to the chemical of interest in a liquid formulation during these activities. Appendix B discusses the rationale, defaults, and limitations of this model.

To estimate the potential worker exposure to the chemical of interest in a liquid product formulation, the following equation is used:

$$EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_final} \quad (5\text{-}3)$$

This exposure will occur over the lesser of $N_{container_load_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.8), up to 250 days per year.

Where:

EXP_{dermal}	=	Potential dermal exposure to the aroma chemical per day (mg aroma chemical/day)
Q_{liquid_skin}	=	Quantity of liquid final product remaining on skin (Defaults: 2.1 mg product/cm^2-incident (high-end) and 0.7 mg product/cm^2-incident (low-end) for routine or incidental contact (CEB, 2000))
$AREA_{surface}$	=	Surface area of contact (Default: 420 cm^2 for 1 hand (CEB, 2000))
$N_{exp_incident}$	=	Number of exposure incidents per day (Default: 1 incident/day)
F_{chem_final}	=	Weight fraction of aroma chemical in final product (kg aroma chemical/ kg product) (see Equation 3-2)

5.6 Exposure During Equipment Cleaning (Exposure D)

Workers may be exposed to the aroma chemical when they manually wipe down the equipment. Up to 29 workers per site may be exposed during this activity. The days of activity should be consistent with the frequency of equipment cleaning associated with each formulation, as discussed for Release 7 in Section 4.9. The concentration of the aroma chemical in the product formulation is calculated in Section 3.3.

Inhalation Exposure:

Inhalation exposure is assumed to be negligible for chemicals with low adjusted vapor pressures within the fragrance oil (e.g., adjusted vapor pressure < 0.001 torr; see Section 4.2).

For volatile liquids, the *EPA/OPPT Mass Balance Model* can be used to calculate worker inhalation exposure due to volatilization during equipment cleaning operations based on the vapor generation rate calculated in Release 8. The default ventilation rates and mixing factors provide a typical and worst case estimate of exposure. Table 5-5 lists the model inputs and default values. Note that the exposure hours per day is equivalent to the operating hours per day for this activity (consistent with Section 4.10 calculations), but EPA assumes a maximum exposure duration of eight hours per day. Similarly, the exposure days per site, per year should be consistent with the release days, but EPA assumes a maximum of 250 days per year, as previously discussed in Section 5.2.

The model and all current EPA defaults have been programmed into ChemSTEER, and use of the software is recommended to calculate inhalation exposure to volatile chemicals during equipment cleaning. Appendix B explains the background and derivation of the model and provides EPA default values for several model parameters.

Table 5-5. Equipment Cleaning Default Values for *EPA/OPPT Mass Balance Model*

Input Parameter	Default Values
Inhalation Rate	Standard EPA default: 1.25 m^3/hr (CEB, 1991)
Exposure Days	Frequency of release determined in Section 4.10, up to 250 days per year
Vapor Generation Rate	Calculated by the *EPA/OPPT Penetration Model* (Section 4.10)
Exposure Duration	Operating hours determined in Section 4.10, up to 8 hours per day
Mixing Factor	EPA defaults: 0.5 (typical) and 0.1 (worst case) (CEB, 1991)
Molecular Weight	Specific chemical parameter
Number of Sites	Calculated in Section 3.5, Equation 3-5
Ventilation Rate	EPA defaults: 3,000 ft^3/min (typical) and 500 ft^3/min (worst case) for indoor conditions (CEB, 1991) (see Appendix B for alternative default ventilation rates)
Vapor Pressure	Specific chemical parameter
Vapor Pressure Correction Factor	$F_{chem\ oil}$ (see Section 4.2)

Note: The model also assumes standard temperature and pressure along with ideal gas interactions.

Dermal Exposure:

There is potential for dermal exposure during process equipment cleaning. No dermal monitoring data for this operation were found. In the absence of data, the EPA/OPPT standard models for estimating dermal exposures from industrial activities can be used.

Liquids

The *EPA/OPPT 2-Hand Dermal Contact with Liquid Model* may be used to estimate dermal exposure to the aroma chemical in a liquid formulation during these activities. Appendix B discusses the rationale, defaults, and limitations of these models.

To estimate the potential worker exposure to the aroma chemical in the fragrance oil for this activity, the following equation may be used:

$$EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_final} \quad (5\text{-}4)$$

This exposure will occur over the lesser of $N_{container_unload_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.10), up to [250] days per year.

Where:

EXP_{dermal} = Potential dermal exposure to the aroma chemical per day (mg aroma chemical/day)

Q_{liquid_skin} = Quantity of liquid final product remaining on skin (Defaults: 2.1 mg product/cm^2-incident (high-end) and 0.7 mg product/cm^2-incident (low-end) for routine or incidental contact (CEB, 2000))

$AREA_{surface}$ = Surface area of contact (Default: 840 cm^2 for 2 hands (CEB, 2000))

$N_{exp_incident}$ = Number of exposure incidents per day (Default: 1 incident/day)

F_{chem_final} = Weight fraction of the aroma chemical in the final product formulation (kg aroma chemical/kg product; see Section 3.3)

Solids

To estimate the potential worker exposure to the aroma chemical in a solid commercial or consumer product for this activity, the *EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model* may be used.

$$EXP_{dermal} = \text{up to } 3{,}100 \frac{\text{mg product}}{\text{day}} \times F_{chem_final} \quad (5\text{-}5)$$

This exposure will occur over the lesser of $N_{container_unload_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.10), up to [250] days per year.

Where:

EXP_{dermal} = Potential dermal exposure to the aroma chemical per day (mg aroma chemical/day)

F_{chem_final} = Weight fraction of the aroma chemical in the final product formulation (kg aroma chemical/kg product; see Section 3.3)

5.7 Exposure from Packaging of Commercial and Consumer Products (Exposure E)

Loading processes for consumer and commercial products may be automated to minimize exposure; however, workers may connect transfer lines to load chemicals into transport containers. The final product may be a liquid or solid powder. As discussed in Section 4.11, if the physical state of the product is unknown, it may be assumed that the aroma chemical is a component of a solid powder product. This assumption yields a more conservative inhalation estimate, as it includes an exposure estimate for both vapor and dust inhalation. Up to 29 workers per site may be exposed during this activity. The concentration of the aroma chemical in the product formulation is calculated in Section 3.3.

Inhalation Exposure:

For the default scenario, it is assumed that the fragrance oil is blended into powdered commercial and consumer products. While the rate of evaporation of volatile chemicals from solid powders is unknown, both vapor and dust inhalation may be assessed for this activity if the aroma chemical is volatile.

Liquids:

Inhalation exposure is assumed to be negligible for chemicals with low adjusted vapor pressures within the fragrance oil (e.g., adjusted vapor pressure < 0.001 torr; see Section 4.2).

For volatile chemicals, the *EPA/OPPT Mass Balance Model* may be used to estimate vapor exposures due to volatilization during loading operations based on the vapor generation rate from Release 9. The default ventilation rates and mixing factors provide a typical and worst case estimate of exposure. Table 5-6 lists model inputs and default values. Note that the exposure hours per day is equivalent to the

operating hours per day for this activity (consistent with Section 4.11 calculations), but EPA assumes a maximum exposure duration of eight hours per day. Similarly, the exposure days per site, per year should be consistent with the release days, but EPA assumes a maximum of 250 days per year, as previously discussed in Section 5.2.

The model and all current EPA defaults have been programmed into ChemSTEER, and use of the software is recommended to calculate inhalation exposure to volatile chemicals during equipment cleaning. Appendix B explains the background and derivation of the model and provides EPA default values for several model parameters.

Table 5-6. Product Packaging Default Values for *EPA/OPPT Mass Balance Model*

Input Parameter	Default Values
Inhalation Rate	Standard EPA default: 1.25 m^3/hr (CEB, 1991)
Exposure Days	Frequency of release determined in Section 4.11, up to 250 days per year
Vapor Generation Rate	Calculated by the *EPA/OPPT Penetration Model* (Section 4.11)
Exposure Duration	Operating hours determined in Section 4.11, up to 8 hours per day
Mixing Factor	EPA defaults: 0.5 (typical) and 0.1 (worst case) (CEB, 1991)
Molecular Weight	Specific chemical parameter
Number of Sites	Calculated in Section 3.5, Equation 3-5
Ventilation Rate	EPA defaults: 3,000 ft^3/min (typical) and 500 ft^3/min (worst case) for indoor conditions (CEB, 1991) (see Appendix B for alternative default ventilation rates)
Vapor Pressure	Specific chemical parameter
Vapor Pressure Correction Factor	$F_{chem\ oil}$ (see Section 4.2)

Note: The model also assumes standard temperature and pressure along with ideal gas interactions.

Solids:

Transferring powdered commercial and consumer products from mixing vessels to transport containers is expected to generate particulates. The degree of inhalation exposure to particulates depends on the potential concentration of the product in the worker's breathing zone ($C_{particulate}$) and the weight fraction of the aroma chemical in the final product (F_{chem_final}). Appendix B provides additional explanation, including the background and model defaults, of the two standard EPA models used to estimate inhalation exposure to solid powder.

Two NIOSH HHEs for Purex Corporation and The Clorox Company were used to estimate inhalation exposures to solids in the 1994 generic scenario for this industry. Based on the monitoring data from these facilities, the scenario presents a concentration range of respirable particles of 0.14 to 2.82 mg/m^3 and of total dust particulate of 0.19 to 18.9 mg/m^3. These data support the use of the OSHA PEL for particulate not otherwise regulated (15 mg/m^3), as a conservative estimate, to assess inhalation exposure to solid particulate.

The quantity of final product handled per day is first calculated to determine which model is more appropriate for estimating inhalation exposures to solids.

$$Q_{final_site_day} = \frac{Q_{chem_site_day}}{F_{chem_final}} \quad (5\text{-}6)$$

Where:

$Q_{final_site_day}$ = Daily amount of final product that is transferred into transport containers (kg product/site-day)

$Q_{chem_site_day}$ = Daily use rate of the aroma chemical used to formulate the product (kg aroma chemical/site-day) (see Equation 3-4)

F_{chem_final} = Weight fraction of the aroma chemical in the final product formulation (kg aroma chemical/kg product; see Section 3.3)

If the transfer rate of the solid powder containing the aroma chemical ($Q_{final_site_day}$) is **greater than** 54 kg/site-day, the *OSHA Total Particulates Not Otherwise Regulated (PNOR) PEL-Limiting Model* is used. See Appendix B for more information on this model.

$$EXP_{inhalation} = C_{particulate} \times RATE_{breathing} \times TIME_{exposure} \times F_{chem_final} \quad (5\text{-}7)$$

This exposure will occur over the lesser of $N_{container_load_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.11), up to [250] days/year.

Where:

$EXP_{inhalation}$ = Inhalation exposure to the aroma chemical per day (mg aroma chemical/day)

$C_{particulate}$ = Concentration of particulate in the workers' breathing zone (Default: 15 mg product/m^3; based on OSHA Total PNOR PEL (8-hr TWA*) (29 CFR 1910.1000))

$RATE_{breathing}$ = Typical worker breathing rate (Default: 1.25 m^3/hr (CEB, 1991))

$TIME_{exposure}$ = Duration of exposure (Default: 8 hrs/day (NOTE: the default value for $C_{particulate}$ is an 8-hr TWA*; therefore, the 8 hrs/day value must be used))

F_{chem_final} = Weight fraction of the aroma chemical in the final product formulation (kg aroma chemical/kg product; see Section 3.3)

*TWA = Time-weighted average.

The accuracy of solid component inhalation estimates is controlled by the estimated airborne concentration of the aroma chemical and the assumed breathing rate.

If the transfer rate of the solid powder containing the aroma chemical ($Q_{final_site_day)}$ is **less than or equal to** 54 kg/site-day, the *EPA/OPPT Small Volume Solids Handling Inhalation Model* is used. See Appendix B for more information on this model.

$$EXP_{inhalation} = Q_{final_site_day} \times F_{chem_final} \times F_{exposure} \quad (5\text{-}8)$$

This exposure will occur over the lesser of $N_{container_load_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.11), up to [250] days/year.

Where:

$EXP_{inhalation}$	=	Inhalation exposure to the aroma chemical per day (mg aroma chemical/day)
$Q_{final_site_day}$	=	Daily amount of final product that is transferred to the transport containers (kg product/site-day) (see Equation 5-2)
F_{chem_final}	=	Weight fraction of the aroma chemical in the final product formulation (kg aroma chemical/kg product; see Section 3.3)
$F_{exposure}$	=	Weight fraction of the total particulate in the workers breathing zone (Default: 0.0477 (typical) to 0.161 (worst) mg product exposure/kg of product handled (CEB, 1992))

Note: The use of Equation 5-7 versus 5-8 is based on the amount of product the worker transfers per day ($Q_{final_site_day}$), not the amount of aroma chemical the worker is exposed to ($Q_{chem_site_day}$).

Dermal Exposure:

There is potential for dermal exposure during the packaging of the final product. In the absence of industry-specific data, the EPA/OPPT standard models for estimating dermal exposures from industrial activities can be used. The *EPA/OPPT 2-Hand Dermal Contact with Liquid Model* can be used to estimate dermal exposure to the aroma chemical in a liquid formulation during these activities. The *EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model* can be used to estimate dermal exposure to the aroma chemical in a solid powder formulation. Appendix B discusses the rationale, defaults, and limitations of these models.

Liquids:

To estimate the potential worker exposure to the aroma chemical in a liquid commercial or consumer product for this activity, the following equation can be used:

$$EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_final} \quad (5\text{-}9)$$

This exposure will occur over the lesser of $N_{container_load_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.11), up to [250] days per year.

Where:

EXP_{dermal}	=	Potential dermal exposure to the aroma chemical per day (mg aroma chemical/day)
Q_{liquid_skin}	=	Quantity of liquid final product remaining on skin (Defaults: 2.1 mg product/cm^2-incident (high-end) and 0.7 mg product/cm^2-incident (low-end) for routine or incidental contact (CEB, 2000))
$AREA_{surface}$	=	Surface area of contact (Default: 840 cm^2 for 2 hands (CEB, 2000))
$N_{exp_incident}$	=	Number of exposure incidents per day (Default: 1 incident/day)
F_{chem_final}	=	Weight fraction of the aroma chemical in the final product formulation (kg aroma chemical/kg product; see Section 3.3)

Solids:

To estimate the potential worker exposure to the aroma chemical in a solid commercial or consumer product for this activity, the following equation can be used:

$$EXP_{dermal} = \text{up to } 3{,}100 \frac{\text{mg product}}{\text{day}} \times F_{chem_final} \quad (5\text{-}10)$$

This exposure will occur over the lesser of $N_{container_load_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.11), up to [250] days per year.

Where:

EXP_{dermal}	=	Potential dermal exposure to the aroma chemical per day (mg aroma chemical/day)
F_{chem_final}	=	Weight fraction of the aroma chemical in the final product formulation (kg aroma chemical/kg product; see Section 3.3)

6. SAMPLE CALCULATIONS

This section presents an example using all of the equations introduced in Sections 3, 4, and 5 of this ESD. Table A-4 in Appendix A summarizes the parameters, default values if applicable, and the sources used throughout the scenario. The hypothetical operating scenario presented in this section demonstrates how the equations in Sections 3, 4, and 5 might be used to estimate releases of and exposures to an aroma chemical used in functional fragrance oil, which is then formulated into a powdered consumer product. The default values used in these calculations are presented in Sections 3, 4, and 5 and are appropriate only in the absence of site-specific information.

The following values are chemical-specific and should be provided by the manufacturer of the aroma chemical. The following values were chosen to demonstrate the use of conservative estimates in the methodologies presented in this document:

1. Production volume of aroma chemical: $Q_{chem_site_yr}$ = 10,000 kg chemical/yr;
2. Vapor pressure of aroma chemical: VP = 0.1 torr @ 25°C; and,
3. Molecular weight of the chemical = 100.

6.1 General Facility Estimates

6.1.1 Days of Operation ($TIME_{working_days}$)

Using the default values presented in Section 3.2, the number of days the fragrance oil is formulated into commercial and consumer products is calculated as:

$$TIME_{working_days} = TIME_{operation_days} \times F_{products} \quad \text{[Eqn. 3-1]}$$

$$TIME_{working_days} = 250\ \frac{days}{yr} \times 1\ \frac{kg\ product\ containing\ chemical}{kg\ all\ products\ formulated}$$

$$TIME_{working_days} = 250\ \frac{days}{yr}$$

6.1.2 Weight Fraction of Aroma Chemical in Commercial or Consumer Product (F_{chem_final})

Using the logic presented in Section 3.3, the weight fraction of the aroma chemical in the final product for the default scenario is calculated as:

$$F_{chem_final} = F_{chem_oil} \times F_{oil_final} \quad \text{[Eqn. 3-2]}$$

$$F_{chem_final} = 0.2 \frac{\text{kg aroma chemical}}{\text{kg fragrance oil}} \times 0.02 \frac{\text{kg fragrance oil}}{\text{kg product}}$$

$$F_{chem_final} = 0.004 \frac{\text{kg aroma chemical}}{\text{kg product}}$$

6.1.3 Daily Use Rate of Aroma Chemical ($Q_{chem_site_day}$)

The daily use rate of the chemical interest is calculated using the following equations:

$$Q_{oil_site_day} = \frac{Q_{oil_site_yr} \times F_{products}}{TIME_{working_days}} \quad \text{[Eqn. 3-3]}$$

$$Q_{chem_site_day} = Q_{oil_site_day} \times F_{chem_oil} \quad \text{[Eqn. 3-4]}$$

Using the default value of 20,500 kg fragrance oil per year from Table 3-2, the default daily use rate of the aroma chemical is calculated below.

$$Q_{oil_site_day} = \frac{20{,}500 \frac{\text{kg fragrance oil}}{\text{site - yr}}}{250 \frac{\text{days}}{\text{yr}}} \times 1 \frac{\text{kg product containing chemical}}{\text{kg all products}}$$

$$Q_{oil_site_day} = 82 \ \frac{\text{kg fragrance oil}}{\text{site - day}}$$

$$Q_{chem_site_day} = 82 \frac{\text{kg fragrance oil}}{\text{site - day}} \times 0.2 \frac{\text{kg aroma chemical}}{\text{kg fragrance oil}}$$

$$Q_{chem_site_day} = 16.4 \frac{\text{kg aroma chemical}}{\text{site - day}}$$

6.1.4 Number of Sites (N_{sites})

The number of sites using the aroma chemical is calculated using the following equation:

$$N_{sites} = \frac{Q_{chem_yr}}{Q_{chem_site_day} \times TIME_{working_days}} \quad \text{[Eqn. 3-5]}$$

Using the annual production volume ($Q_{chem_site_yr}$) of 10,000 kg/yr as specified in Section 6.0, and the daily use rate calculated above ($Q_{chem_site_day}$), the number of sites using the aroma chemical is:

$$N_{sites} = \frac{10{,}000\ \frac{\text{kg aroma chemical}}{\text{yr}}}{16.4\ \frac{\text{kg aroma chemical}}{\text{site - day}} \times 250\ \frac{\text{days}}{\text{yr}}}$$

$$N_{sites} = 2.44 \text{ sites or } N_{sites} = 3 \text{ sites}$$

Since the number of sites is rounded, the daily use rate of the aroma chemical must be recalculated using the following equation:

$$Q_{chem_site_day} = \frac{Q_{chem_yr}}{N_{sites} \times TIME_{working_days}}$$

$$Q_{chem_site_day} = \frac{10{,}000\ \frac{\text{kg aroma chemical}}{\text{year}}}{3 \text{ sites} \times 250\ \frac{\text{days}}{\text{yr}}}$$

$$Q_{chem_site_day} = 13.3\ \frac{\text{kg aroma chemical}}{\text{site - day}}$$

6.1.5 Number of Fragrance Oil Transport Containers ($N_{container_unload_site_yr}$)

The number of containers containing fragrance unloaded at each site on a yearly basis is calculated using the following equation. See Table A-4 in Appendix A for default values.

$$N_{container_unload_site_yr} = \frac{Q_{chem_site_day} \times TIME_{working_days}}{F_{chem_oil} \times V_{container_oil} \times RHO_{oil}} \qquad \text{[Eqn. 3-6]}$$

$$N_{container_unload_site_yr} = \frac{13.3\ \frac{\text{kg aroma chemical}}{\text{site - day}} \times 250\ \frac{\text{days}}{\text{yr}}}{0.2\ \frac{\text{kg aroma chemical}}{\text{kg fragrance oil}} \times 208\ \frac{\text{L fragrance oil}}{\text{container}} \times 1\ \frac{\text{kg fragrance oil}}{\text{L fragrance oil}}}$$

$$N_{container_unload_site_yr} = 80\ \frac{\text{containers}}{\text{site - yr}}$$

6.1.6 Number of Final Product Transport Containers ($N_{container_load_site_yr}$)

The number of containers used to load the final product at each site on a yearly basis is calculated using the following equation. See Table A-4 in Appendix A for default values.

$$N_{container_load_site_yr} = \frac{Q_{chem_site_day} \times TIME_{working_days}}{F_{chem_final} \times V_{container_final} \times RHO_{final}} \quad \text{[Eqn. 3-7]}$$

$$N_{container_load_site_yr} = \frac{13.3 \ \frac{\text{kg aroma chemical}}{\text{site - day}} \times 250 \ \frac{\text{days}}{\text{yr}}}{0.004 \ \frac{\text{kg aroma chemical}}{\text{kg final product}} \times 3.78 \ \frac{\text{L final product}}{\text{container}} \times 1 \ \frac{\text{kg final product}}{\text{L final product}}}$$

$$N_{container_load_site_yr} = 220{,}000 \ \frac{\text{container}}{\text{site - yr}}$$

6.2 Release Assessments

6.2.1 Release from Container Residue (Release 1)

Since $N_{container_unload_site_yr}$ is not greater than $TIME_{working_days}$, it is assumed that no more than one container is emptied on each operating day. Therefore, the following equation is used to estimate the daily release:

$$Elocal_{container_residue_disp} = V_{container_oil} \times RHO_{oil} \times F_{chem_oil} \times F_{container_residue} \times 1 \frac{\text{container}}{\text{site} - \text{day}} \quad \text{[Eqn. 4-2a]}$$

$$Elocal_{container_residue_disp} = 208 \ \frac{\text{L fragrance oil}}{\text{container}} \times 1 \ \frac{\text{kg fragrance oil}}{\text{L fragrance oil}} \times 0.2 \ \frac{\text{kg aroma chemical}}{\text{kg fragrance oil}} \times 0.03 \ \frac{\text{kg residual}}{\text{kg supplied}} \times 1 \ \frac{\text{container}}{\text{site} - \text{day}}$$

$$Elocal_{container_residue_disp} = 1.25 \ \frac{\text{kg aroma chemical}}{\text{site - day}}$$

…over 80 days/year from 3 sites.

Media of release: water, land, or incineration

6.2.2 Fugitive Air Releases During Transport Container Cleaning (Release 2)

The following equation is used by ChemSTEER to calculate the vapor generation rate ($Q_{vapor_generation}$) for the *EPA/OPPT Penetration Model*, which estimates releases to air from evaporation of a chemical from an open, exposed liquid surface.

[Eqn. B-1]

$$Q_{vapor_generation} = \frac{(8.24 \times 10^{-8}) \times MW_{chem}^{0.835} \times F_{correction_factor} \times VP_{chem} \times \left(1/29 + 1/MW_{chem} \right)^{0.25} \times RATE_{air_speed}^{0.5} \times AREA_{opening}}{TEMP_{ambient}^{0.05} \times D_{opening}^{0.5} \times P_{ambient}^{0.5}}$$

Table 6-1. Summary of ChemSTEER Inputs for Release 2

Parameter	Units	ChemSTEER Input
MW_{chem}	g/mol	100
$F_{correction\ factor}$	dimensionless	0.2
VP_{chem}	torr	0.1
$RATE_{air\ speed}$	Ft/min	100
$AREA_{opening}$	cm^2	20.3
$TEMP_{ambient}$	K	298
$D_{opening}$	cm	5.08
$P_{ambient}$	atm	1

Therefore:

$$Q_{vapor_generation} = 2.4 \times 10^{-6}\ g/s$$

Using $Q_{vapor_generation}$ calculated in Equation B-1 and the other standard default values presented in Table 4-2 for container cleaning, the model then estimates the daily release to air using the following equation:

$$Elocal_{air} = Q_{vapor_generation} \times TIME_{activity_hours} \times \frac{3600\ sec/hr}{1000\ g/kg} \qquad [Eqn.\ B\text{-}2]$$

$$Elocal_{air} = 2.4 \times 10^{-6}\ g/sec \times \frac{1\ containers/site\text{ - }day}{20\ containers/hr} \times \frac{3600\ sec/hr}{1000\ g/kg}$$

$$Elocal_{air} = 1.4 \times 10^{-7}\ \frac{kg\ aroma\ chemical}{site\text{ - }day}$$

…over 80 days/year from 3 sites.

Media of release: air

6.2.3 Fugitive Air Releases from Unloading Transport Containers (Release 3)

ChemSTEER uses the following equation to calculate the vapor generation rate ($Q_{vapor_generation}$) for the *EPA/OAQPS AP-42 Loading Model*, which estimates releases to air from the displacement of air containing chemical vapor as a container/vessel is filled with a liquid. The *EPA/OAQPS AP-42 Loading Model* calculates a **typical** and **worst-case** estimate.

[Eqn. B-5]

$$Q_{vapor_generation} = \frac{F_{saturation_factor} \times MW_{chem} \times \left(V_{container} \times \frac{3785.4\ cm^3}{gal} \right) \times \left(\frac{RATE_{fill}}{3600\ sec/hr} \right) \times F_{correction_factor} \times \left(\frac{VP_{chem}}{760\ torr/atm} \right)}{R \times TEMP_{ambient}}$$

Table 6-2. Summary of ChemSTEER Inputs for Release 3

Parameter	Units	ChemSTEER Input
MW_{chem}	g/mol	100
$F_{saturation_factor}$	dimensionless	Typical = 0.5 Worst Case = 1
VP_{chem}	torr	0.1
$V_{container}$	gal	55
$RATE_{fill}$	containers/hour	20
$TEMP_{ambient}$	K	298
$F_{correction\ factor}$	dimensionless	0.2
R	atm	82.05

Therefore:

$Q_{vapor_generation} = 6.2 \times 10^{-5}$ g/s for typical and $Q_{vapor_generation} = 1.2 \times 10^{-4}$ g/s for worst case

Using $Q_{vapor_generation}$ calculated in Equation B-1 and the other standard default values presented in Table 4-3 for unloading, the model then estimates the daily release to air using the following equation:

$$Elocal_{air} = Q_{vapor_generation} \times TIME_{activity_hours} \times \frac{3600\ sec/hr}{1000\ g/kg} \qquad \text{[Eqn. B-6]}$$

$$Elocal_{air} = (6.2 \times 10^{-5} \text{ or } 1.2 \times 10^{-4})\ g/s \times 1.6 \times 10^{-2} \frac{hrs}{site\text{-}day} \times \frac{3600\ sec/hr}{1000\ g/kg}$$

$$Elocal_{air} = (3.6 \times 10^{-6} \text{ or } 7.2 \times 10^{-6}) \frac{kg\ aroma\ chemical}{site\text{-}day}$$

…over 80 days/year from 3 sites.

Media of release: air

6.2.4 Fugitive Air Releases During Mixing Operations (Release 4)

The following equation is used by ChemSTEER to calculate the vapor generation rate ($Q_{vapor_generation}$) for the *EPA/OPPT Penetration Model*, which estimates releases to air from evaporation of a chemical from an open, exposed liquid surface.

[Eqn. B-1]

$$Q_{vapor_generation} = \frac{(8.24\times10^{-8}) \times MW_{chem}^{0.835} \times F_{correction_factor} \times VP_{chem} \times \left(1/29 + 1/MW_{chem}\right)^{0.25} \times RATE_{air_speed}^{0.5} \times AREA_{opening}}{TEMP_{ambient}^{0.05} \times D_{opening}^{0.5} \times P_{ambient}^{0.5}}$$

Table 6-3. Summary of ChemSTEER Inputs for Release 4

Parameter	Units	ChemSTEER Input
MW_{chem}	g/mol	100
$F_{correction\ factor}$	dimensionless	0.2
VP_{chem}	torr	0.1
$RATE_{air\ speed}$	ft/min	100
$AREA_{opening}$	cm^2	5,808
$TEMP_{ambient}$	K	298
$D_{opening}$	cm	86
$P_{ambient}$	atm	1

To demonstrate the use of Equation 4-3, for this example it is assumed that mixing the fragrance oil into the final product formulation occurs in an open vessel; note, however, that closed mixing is the scenario default. The following equation is used to calculate the diameter of the vessel ($D_{opening}$).

$$D_{opening} = \left[\frac{4\times Q_{final_batch}\times 1000\left(cm^3/L\right)}{\pi \times RHO_{final}}\right]^{1/3} \qquad \text{[Eqn. 4-3]}$$

$$D_{opening} = \left[\frac{4\times 500\ kg/batch\times 1000\left(cm^3/L\right)}{\pi \times 1\dfrac{kg\ product}{L\ product}}\right]^{1/3}$$

$$D_{opening} = 86\ cm$$

Therefore:

$$Q_{vapor_gene\ ration} = 1.7\times10^{-4}\ g/s$$

Using $Q_{vapor_generation}$ calculated in Equation B-1 and the other standard default values presented in Table 4-4 for mixing, the model then estimates the daily release to air using the following equation:

$$\text{Elocal}_{\text{air}} = \text{Q}_{\text{vapor_generation}} \times \text{TIME}_{\text{activity_hours}} \times \frac{3600 \text{ sec/hr}}{1000 \text{ g/kg}} \qquad \text{[Eqn. B-2]}$$

$$\text{Elocal}_{\text{air}} = 1.7 \times 10^{-4} \text{ g/s} \times 24 \frac{\text{hrs}}{\text{site - day}} \times \frac{3600 \text{ sec/hr}}{1000 \text{ g/kg}}$$

$$\text{Elocal}_{\text{air}} = 0.014 \frac{\text{kg aroma chemical}}{\text{site - day}}$$

…over 250 days/year from 3 sites.

Media of release: air

6.2.5 Fugitive Air Releases from Product Sampling (Release 6)

The following equation is used by ChemSTEER to calculate the vapor generation rate ($Q_{vapor_generation}$) for the *EPA/OPPT Penetration Model*, which estimates releases to air from evaporation of a chemical from an open, exposed liquid surface.

[Eqn. B-1]

$$\text{Q}_{\text{vapor_generation}} = \frac{(8.24 \times 10^{-8}) \times \text{MW}_{\text{chem}}^{\ 0.835} \times \text{F}_{\text{correction_factor}} \times \text{VP}_{\text{chem}} \times \left(1/29 + 1/\text{MW}_{\text{chem}} \right)^{0.25} \times \text{RATE}_{\text{air_speed}}^{\ 0.5} \times \text{AREA}_{\text{opening}}}{\text{TEMP}_{\text{ambient}}^{\ 0.05} \times \text{D}_{\text{opening}}^{\ 0.5} \times \text{P}_{\text{ambient}}^{\ 0.5}}$$

Table 6-4. Summary of ChemSTEER Inputs for Release 6

Parameter	Units	ChemSTEER Input
MW_{chem}	g/mol	100
$F_{correction\ factor}$	dimensionless	0.2
VP_{chem}	torr	0.1
$RATE_{air\ speed}$	ft/min	100
$AREA_{opening}$	cm^2	4.9-78.5
$TEMP_{ambient}$	K	298
$D_{opening}$	cm	2.5-10
$P_{ambient}$	atm	1

Therefore:

$\text{Q}_{\text{vapor_generation}} = 8.3 \times 10^{-7}$ g/s for typical and $\text{Q}_{\text{vapor_generation}} = 6.6 \times 10^{-6}$ g/s for worst case

Using $Q_{vapor_generation}$ calculated in Equation B-1 and the other standard default values presented in Table 4-5 for sampling, the model then estimates the daily release to air using the following equation:

$$\text{Elocal}_{air} = Q_{vapor_generation} \times \text{TIME}_{activity_hours} \times \frac{3600 \text{ sec/hr}}{1000 \text{ g/kg}} \qquad \text{[Eqn. B-2]}$$

$$\text{Elocal}_{air} = (8.3 \times 10^{-7} \text{ or } 6.6 \times 10^{-6}) \text{ g/s} \times 1 \frac{\text{hr}}{\text{site - day}} \times \frac{3600 \text{ sec/hr}}{1000 \text{ g/kg}}$$

$$\text{Elocal}_{air} = (3.0 \times 10^{-6} \text{ or } 2.4 \times 10^{-5}) \frac{\text{kg aroma chemical}}{\text{site - day}}$$

…over 250 days/year from 3 sites.

Media of release: air

6.2.6 Release from Equipment Cleaning (Release 7)

$$\text{Elocal}_{equipment_residue_disp} = Q_{chem_site_day} \times F_{equipment_residue} \qquad \text{[Eqn. 4-4]}$$

$$\text{Elocal}_{equipment_residue_disp} = 13.3 \frac{\text{kg aroma chemical}}{\text{site - day}} \times 0.02 \frac{\text{kg residue}}{\text{kg processed in equipment}}$$

$$\text{Elocal}_{equipment_residue_disp} = 0.27 \frac{\text{kg aroma chemical}}{\text{site - day}}$$

…over 50 days/year from 3 sites.

Media of Release: water, land, or incineration

6.2.7 Fugitive Air Releases During Equipment Cleaning (Release 8)

ChemSTEER uses the following equation to calculate the vapor generation rate ($Q_{vapor_generation}$) for the *EPA/OPPT Mass Transfer Coefficient Model*, which estimates releases to air from the evaporation of a chemical from an open, exposed liquid surface.

[Eqn. B-3]

$$Q_{vapor_generation} = \frac{(1.93 \times 10^{-7}) \times MW_{chem}^{0.78} \times F_{correction_factor} \times VP_{chem} \times \left(\frac{1}{29} + \frac{1}{MW_{chem}}\right)^{0.33} \times RATE_{air_speed}^{0.78} \times AREA_{opening}}{TEMP_{ambient}^{0.4} \times D_{opening}^{0.11} \times \left(TEMP_{ambient}^{0.5} - 5.87\right)^{2/3}}$$

Table 6-5. Summary of ChemSTEER Inputs for Release 8

Parameter	Units	ChemSTEER Input
MW_{chem}	g/mol	100
$F_{correction\ factor}$	dimensionless	0.2
VP_{chem}	torr	0.1
$RATE_{air\ speed}$	ft/min	440
$AREA_{opening}$	cm^2	6,647
$TEMP_{ambient}$	K	298
$D_{opening}$	cm	92

Therefore,

$$Q_{vapor_generation} = 4.7 \times 10^{-4}\ g/s$$

Using $Q_{vapor_generation}$ calculated in Equation B-3 and the other standard default values presented in Table 4-6 for equipment cleaning, the model then estimates the daily release to air using the following equation:

$$Elocal_{air} = Q_{vapor_generation} \times TIME_{activity_hours} \times \frac{3600\ sec/hr}{1000\ g/kg} \qquad [Eqn.\ B\text{-}4]$$

$$Elocal_{air} = 4.7 \times 10^{-4}\ g/s \times 4 \frac{hrs}{site\text{-}day} \times \frac{3600\ sec/hr}{1000\ g/kg}$$

$$Elocal_{air} = 6.8 \times 10^{-3} \frac{kg\ aroma\ chemcial}{site\text{-}day}$$

…over 50 days/year from 3 sites.

Media of Release: air

6.2.8 Fugitive Air Releases During Product Packaging (Release 9)

ChemSTEER uses the following equation to calculate the vapor generation rate ($Q_{vapor_generation}$) for the *EPA/OAQPS AP-42 Loading Model*, which estimates releases to air from the displacement of air containing chemical vapor as a container/vessel is filled with a liquid.

[Eqn. B-5]

$$Q_{vapor_generation} = \frac{F_{saturation_factor} \times MW_{chem} \times \left(V_{container} \times \frac{3785.4\ cm^3}{gal} \right) \times \left(\frac{RATE_{fill}}{3600\ sec/hr} \right) \times F_{correction_factor} \times \left(\frac{VP_{chem}}{760\ torr/atm} \right)}{R \times TEMP_{ambient}}$$

Table 6-6. Summary of ChemSTEER Inputs for Release 9

Parameter	Units	ChemSTEER Input
MW_{chem}	g/mol	100
$F_{saturation_factor}$	dimensionless	Typical = 0.5 Worst Case = 1
VP_{chem}	torr	0.1
$V_{container}$	gal	1
$RATE_{fill}$	containers/hour	60
$TEMP_{ambient}$	K	298
$F_{correction\ factor}$	dimensionless	0.2
R	atm	82.05

Therefore,

$Q_{vapor_generation}$ =3.4 × 10^{-6} g/s for typical and $Q_{vapor_generation}$ = 6.8 × 10^{-6} g/s for worst case

Using $Q_{vapor_generation}$ calculated in Equation B-1 and the other standard default values presented in Table 4-7 for product loading, the model then estimates the daily release to air using the following equation:

$$Elocal_{air} = Q_{vapor_generation} \times TIME_{activity_hours} \times \frac{3600\ sec/hr}{1000\ g/kg} \qquad \text{[Eqn. B-6]}$$

$$Elocal_{air} = (3.4 \times 10^{-6} \text{ or } 6.8 \times 10^{-6})\ g/s \times 14.6 \frac{hrs}{site\text{-}day} \times \frac{3600\ sec/hr}{1000\ g/kg}$$

$$Elocal_{air} = (1.8 \times 10^{-4} \text{ or } 3.6 \times 10^{-4}) \frac{kg\ aroma\ chemical}{site\text{-}day}$$

…over 250 days/year from 3 sites.

Media of release: air

6.2.9 Dust Waste Generated from Conveying, Mixing, and Packaging Powdered Commercial and Consumer Products (Release 10)

The amount of dust released as a result of conveying, mixing, and packaging a solid final product is calculated using the following equation:

$$Elocal_{dust_generation} = Q_{chem_site_day} \times F_{dust_generation} \times (1 - F_{APCD}) \qquad \text{[Eqn. 4-5]}$$

$$Elocal_{dust_generation} = 13.3 \frac{kg\ aroma\ chemical}{site\text{-}day} \times 0.045 \frac{kg\ released}{kg\ transferred} \times (1 - 0.85)$$

$$\text{Elocal}_{\text{dust_generation}} = 0.09 \frac{\text{kg aroma chemical}}{\text{site - day}}$$

…over 250 days/year from 3 sites.

Media of Release: water, incineration, land, or air

6.3 Occupational Exposure Assessments

6.3.1 Total Number of Workers Potentially Exposed to the Chemical

It is assumed that 29 workers are potentially exposed to the aroma chemical at each site; therefore, the total number of workers is calculated as:

$$29 \frac{\text{workers}}{\text{site}} \times N_{\text{sites}} = 29 \frac{\text{workers}}{\text{site}} \times 3 \text{ sites} = 87 \text{ total workers}$$

Note that all 87 workers are assumed to be exposed during each of the exposure activities performed at the three formulation sites.

6.3.2 Exposure from Unloading Transport Containers into Mixing Vessel (Exposure A)

Inhalation Exposure:

Using the vapor generation rate calculated in Release 3 and the EPA standard model for estimating inhalation exposure due to evaporation of volatile chemicals (*EPA/OPPT Mass Balance Model*), ChemSTEER calculates the worker exposure using the following equations:

Table 6-7. Summary of ChemSTEER Inputs for Exposure A

Parameter	Units	ChemSTEER Input
F_{mixing_factor}	dimensionless	Typical = 0.5 Worst Case = 0.1
$TEMP_{ambient}$	K	298
MW_{chem}	g/mol	100
$RATE_{ventilation}$	ft^3/min	Typical = 3000 Worst Case = 500
$Q_{vapor_generation}$	g/s	Typical = 6.2×10^{-5} Worst Case = 1.3×10^{-4}
$RATE_{breathing}$	m^3/hour	1.25
V_{molar}	L/mol	24.45
$TIME_{exposure}$	hours/day	0.016

$$C_{chem_volumetric} = \frac{(1.7 \times 10^5) \times TEMP_{ambient} \times Q_{vapor_generation}}{MW_{chem} \times RATE_{ventilation} \times F_{mixing_factor}} \quad \text{[Eqn. B-7]}$$

$C_{chem_volumetric} = 2.1 \times 10^{-2}$ ppm for typical and $C_{chem_volumetric} = 1.26$ ppm for worst case

Next, the volumetric concentration is converted to a mass concentration (C_{chem_mass}) by the following equation:

$$C_{chem_mass} = \frac{C_{chem_volumetric} \times MW_{chem}}{V_{molar}} \quad \text{[Eqn. B-9]}$$

$C_{chem_mass} = 8.6 \times 10^{-2}$ mg/m^3 for typical and $C_{chem_mass} = 5.2$ mg/m^3 for worst case

Finally, the mass concentration of the chemical and the standard default values presented in Table 5-2 for the container unloading activity are used to estimate the amount of inhalation exposure per worker using the following calculation:

$$EXP_{inhalation} = C_{chem_mass} \times RATE_{breathing} \times TIME_{exposure} \quad \text{[Eqn. B-10]}$$

$$EXP_{inhalation} = 1.7 \times 10^{-3} \frac{mg}{day} \text{ for typical and } EXP_{inhalation} = 0.10 \frac{mg}{day} \text{ for worst case}$$

…over 80 days/year.

Dermal Exposure:

The dermal exposure to the aroma chemical during transport container unloading is calculated using the following equation:

$$EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_oil} \quad \text{[Eqn. 5-1]}$$

$$EXP_{dermal} = 0.7 \text{ to } 2.1 \frac{mg \text{ fragrance oil}}{cm^2 \text{ - incident}} \times 840 \text{ cm}^2 \times 1 \frac{\text{incident}}{day} \times 0.2 \frac{\text{kg aroma chemical}}{\text{kg fragrance oil}}$$

$$EXP_{dermal} = 118 \text{ to } 353 \frac{mg \text{ aroma chemical}}{day}$$

…over 80 days/year.

6.3.3 Exposure During Transport Container Cleaning (Exposure B)

Inhalation Exposure:

Using the vapor generation rate calculated in Release 2 and the EPA standard model for estimating inhalation exposure due to evaporation of volatile chemicals (*EPA/OPPT Mass Balance Model*), ChemSTEER calculates the worker exposure using the following equations:

Table 6-8. Summary of ChemSTEER Inputs for Exposure B

Parameter	Units	ChemSTEER Input
F_{mixing_factor}	dimensionless	Typical = 0.5 Worst Case = 0.1
$TEMP_{ambient}$	K	298
MW_{chem}	g/mol	100
$RATE_{ventilation}$	ft^3/min	Typical = 3000 Worst Case = 500
$Q_{vapor\ generation}$	g/s	Typical =2.4 x 10^{-6}
$RATE_{breathing}$	m^3/hour	1.25
V_{molar}	L/mol	24.45
$TIME_{exposure}$	hours/day	0.016

$$C_{chem_volumetric} = \frac{(1.7\times10^{5})\times TEMP_{ambient}\times Q_{vapor_generation}}{MW_{chem}\times RATE_{ventilation}\times F_{mixing_factor}} \qquad \text{[Eqn. B-7]}$$

$C_{chem_volumetric} = 8.1 \times 10^{-4}$ ppm for typical and $C_{chem_volumetric} = 2.4 \times 10^{-2}$ ppm for worst case

Next, the volumetric concentration is converted to a mass concentration (C_{chem_mass}) by the following equation:

$$C_{chem_mass} = \frac{C_{chem_volumetric}\times MW_{chem}}{V_{molar}} \qquad \text{[Eqn. B-9]}$$

$C_{chem_mass} = 3.3\times10^{-3}$ mg/m^3 for typical and $C_{chem_mass} = 9.9\times10^{-2}$ mg/m^3 for worst case

Finally, the mass concentration of the chemical and the standard default values presented in Table 5-3 for the container cleaning activity are used to estimate the amount of inhalation exposure per worker using the following calculation:

$$EXP_{inhalation} = C_{chem_mass}\times RATE_{breathing}\times TIME_{exposure} \qquad \text{[Eqn. B-10]}$$

$EXP_{inhalation} = 6.6\times10^{-5}\ \frac{mg}{day}$ for typical and $EXP_{inhalation} = 2.0\times10^{-3}\ \frac{mg}{day}$ for worst case

…over 80 days/year.

Dermal Exposure:

The dermal exposure to the aroma chemical during transport container cleaning is calculated using the following equation:

$$EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_oil} \quad \text{[Eqn. 5-2]}$$

$$EXP_{dermal} = 0.7 \text{ to } 2.1 \frac{\text{mg fragrance oil}}{\text{cm}^2 \text{ - incident}} \times 840 \text{ cm}^2 \times 1 \frac{\text{incident}}{\text{day}} \times 0.2 \frac{\text{kg aroma chemical}}{\text{kg fragrance oil}}$$

$$EXP_{dermal} = 118 \text{ to } 353 \frac{\text{mg aroma chemical}}{\text{day}}$$

…over 80 days/year.

6.3.4 Exposure from Sampling Product Formulation (Exposure C)

Inhalation Exposure:

Using the vapor generation rate calculated in Release 6 and the EPA standard model for estimating inhalation exposure due to evaporation of volatile chemicals (*EPA/OPPT Mass Balance Model*), ChemSTEER calculates the worker exposure using the following equations:

Table 6-9. Summary of ChemSTEER Inputs for Exposure C

Parameter	Units	ChemSTEER Input
F_{mixing_factor}	dimensionless	Typical = 0.5 Worst Case = 0.1
$TEMP_{ambient}$	K	298
MW_{chem}	g/mol	100
$RATE_{ventilation}$	ft^3/min	Typical = 3000 Worst Case = 500
$Q_{vapor_generation}$	g/s	Typical = 8.3×10^{-7} Worst Case = 6.6×10^{-6}
$RATE_{breathing}$	m^3/hour	1.25
V_{molar}	L/mol	24.45
$TIME_{exposure}$	hours/day	0.016

$$C_{chem_volumetric} = \frac{(1.7 \times 10^5) \times TEMP_{ambient} \times Q_{vapor_generation}}{MW_{chem} \times RATE_{ventilation} \times F_{mixing_factor}} \quad \text{[Eqn. B-7]}$$

$C_{chem_volumetric} = 2.8 \times 10^{-4}$ ppm for typical and $C_{chem_volumetric} = 6.7 \times 10^{-2}$ ppm for worst case

Next, the volumetric concentration is converted to a mass concentration (C_{chem_mass}) by the following equation:

$$C_{chem_mass} = \frac{C_{chem_volumetric} \times MW_{chem}}{V_{molar}} \quad \text{[Eqn. B-9]}$$

$C_{chem_mass} = 1.1 \times 10^{-3}$ mg/m^3 for typical and $C_{chem_mass} = 0.3$ mg/m^3 for worst case

Finally, the mass concentration of the chemical and the standard default values presented in Table 5-4 for the product sampling activity are used to estimate the amount of inhalation exposure per worker using the following calculation:

$$EXP_{inhalation} = C_{chem_mass} \times RATE_{breathing} \times TIME_{exposure} \quad \text{[Eqn. B-10]}$$

$$EXP_{inhalation} = 1.4 \times 10^{-3} \frac{mg}{day} \text{ for typical and } EXP_{inhalation} = 0.3 \frac{mg}{day} \text{ for worst case}$$

…over 250 days/year.

Dermal Exposure:

The dermal exposure to the aroma chemical during equipment cleaning is calculated using the following equations:

Liquids:

$$EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_final} \quad \text{[Eqn. 5-3]}$$

$$EXP_{dermal} = 0.7 \text{ to } 2.1 \frac{\text{mg product}}{\text{cm}^2 \text{ - incident}} \times 420 \text{ cm}^2 \times 1 \frac{\text{incident}}{\text{day}} \times 0.004 \frac{\text{kg aroma chemical}}{\text{kg fragrance oil}}$$

$$EXP_{dermal} = 1.2 \text{ to } 3.5 \frac{\text{mg aroma chemical}}{\text{day}}$$

…over 250 days/year.

6.3.5 Exposure During Equipment Cleaning (Exposure D)

Inhalation Exposure:

Using the vapor generation rate calculated in Release 8 and the EPA standard model for estimating inhalation exposure due to evaporation of volatile chemicals (*EPA/OPPT Mass Balance Model*), ChemSTEER calculates the worker exposure using the following equations:

Table 6-10. Summary of ChemSTEER Inputs for Exposure D

Parameter	Units	ChemSTEER Input
F_{mixing_factor}	dimensionless	Typical = 0.5 Worst Case = 0.1
$TEMP_{ambient}$	K	298
MW_{chem}	g/mol	100
$RATE_{ventilation}$	ft^3/min	Typical = 3000 Worst Case = 500
$Q_{vapor\ generation}$	g/s	4.7×10^{-4}
$RATE_{breathing}$	m^3/hour	1.25
V_{molar}	L/mol	24.45
$TIME_{exposure}$	hours/day	4

$$C_{chem_volumetric} = \frac{(1.7 \times 10^5) \times TEMP_{ambient} \times Q_{vapor_generation}}{MW_{chem} \times RATE_{ventilation} \times F_{mixing_factor}} \quad \text{[Eqn. B-7]}$$

$C_{chem_volumetric} = 2.0 \times 10^{-3}$ ppm for typical and $C_{chem_volumetric} = 0.02$ ppm for worst case

Next, the volumetric concentration is converted to a mass concentration (C_{chem_mass}) by the following equation:

$$C_{chem_mass} = \frac{C_{chem_volumetric} \times MW_{chem}}{V_{molar}} \quad \text{[Eqn. B-9]}$$

$C_{chem_mass} = 8.3 \times 10^{-3}$ mg/m^3 for typical and $C_{chem_mass} = 7.4 \times 10^{-2}$ mg/m^3 for worst case

Finally, the mass concentration of the chemical and the standard default values presented in Table 5-5 for the process equipment cleaning activity are used to estimate the amount of inhalation exposure per worker using the following calculation:

$$EXP_{inhalation} = C_{chem_mass} \times RATE_{breathing} \times TIME_{exposure} \quad \text{[Eqn. B-10]}$$

$EXP_{inhalation} = 0.04 \frac{mg}{day}$ for typical and $EXP_{inhalation} = 0.4 \frac{mg}{day}$ for worst case

…over 50 days/year.

Dermal Exposure:

The dermal exposure to the aroma chemical during equipment cleaning is calculated using the following equations:

Liquids:

$$EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_final} \quad \text{[Eqn. 5-4]}$$

$$EXP_{dermal} = 0.7 \text{ to } 2.1 \frac{\text{mg product}}{\text{cm}^2 \text{ - incident}} \times 840 \text{ cm}^2 \times 1 \frac{\text{incident}}{\text{day}} \times 0.004 \frac{\text{kg aroma chemical}}{\text{kg fragrance oil}}$$

$$EXP_{dermal} = 2.3 \text{ to } 7.1 \frac{\text{mg aroma chemical}}{\text{day}}$$

…over 50 days/year.

Solids:

$$EXP_{dermal} = 3{,}100 \frac{\text{mg product}}{\text{day}} \times F_{chem_final} \quad \text{[Eqn. 5-5]}$$

$$EXP_{dermal} = 3{,}100 \frac{\text{mg product}}{\text{day}} \times 0.004 \frac{\text{kg aroma chemical}}{\text{kg product}}$$

$$EXP_{dermal} = 12.4 \frac{\text{mg aroma chemical}}{\text{day}}$$

…over 50 days/year.

6.3.6 Exposure from Packaging of Commercial and Consumer Products (Exposure E)

Inhalation Exposure:

Liquids:

Using the vapor generation rate calculated in Release 9 and the EPA standard model for estimating inhalation exposure due to evaporation of volatile chemicals (*EPA/OPPT Mass Balance Model*), ChemSTEER calculates the worker exposure using the following equations:

Table 6-11. Summary of ChemSTEER Inputs for Exposure E

Parameter	Units	ChemSTEER Input
F_{mixing_factor}	Dimensionless	Typical = 0.5 Worst Case = 0.1
$TEMP_{ambient}$	K	298
MW_{chem}	g/mol	100
$RATE_{ventilation}$	ft^3/min	Typical = 3000 Worst Case = 500
$Q_{vapor_generation}$	g/s	Typical = 6.2×10^{-6} Worst Case = 1.3×10^{-5}
$RATE_{breathing}$	m^3/hour	1.25
V_{molar}	L/mol	24.45
$TIME_{exposure}$	hours/day	8

$$C_{chem_volumetric} = \frac{(1.7 \times 10^5) \times TEMP_{ambient} \times Q_{vapor_generation}}{MW_{chem} \times RATE_{ventilation} \times F_{mixing_factor}} \quad \text{[Eqn. B-7]}$$

$C_{chem_volumetric} = 2.1 \times 10^{-3}$ ppm for typical and $C_{chem_volumetric} = 0.13$ ppm for worst case

Next, the volumetric concentration is converted to a mass concentration (C_{chem_mass}) by the following equation:

$$C_{chem_mass} = \frac{C_{chem_volumetric} \times MW_{chem}}{V_{molar}} \quad \text{[Eqn. B-9]}$$

$C_{chem_mass} = 8.6 \times 10^{-3}$ mg/m^3 for typical and $C_{chem_mass} = 0.5$ mg/m^3 for worst case

Finally, the mass concentration of the chemical and the standard default values presented in Table 5-6 for the product packaging activity are used to estimate the amount of inhalation exposure per worker using the following calculation:

$$EXP_{inhalation} = C_{chem_mass} \times RATE_{breathing} \times TIME_{exposure} \quad \text{[Eqn. B-10]}$$

$$EXP_{inhalation} = 0.09 \frac{mg}{day} \text{ for typical and } EXP_{inhalation} = 5.2 \frac{mg}{day} \text{ for worst case}$$

…over 250 days/year.

Solids:

The quantity of final product handled per day is first calculated to determine which model is more appropriate for calculating inhalation exposure to solids.

$$Q_{final_site_day} = \frac{Q_{chem_site_day}}{F_{chem_final}} \quad \text{[Eqn. 5-6]}$$

$$Q_{final_site_day} = \frac{13.3 \frac{kg\ aroma\ chemical}{site - day}}{0.004 \frac{kg\ aroma\ chemical}{kg\ product}}$$

$$Q_{final_site_day} = 3{,}325 \frac{kg\ product}{site - day}$$

Since $Q_{final_site_day}$ is greater than 54 kg/day, the *OSHA PNOR PEL-Limiting Model* is used to estimate the inhalation exposure to a solid powder:

$$EXP_{inhalation} = C_{particulate} \times RATE_{breathing} \times TIME_{exposure} \times F_{chem_final} \quad \text{[Eqn. 5-7]}$$

$$EXP_{inhalation} = 15 \frac{mg\ product}{m^3} \times 1.25 \frac{m^3}{hr} \times 8 \frac{hr}{day} \times 0.004 \frac{kg\ aroma\ chemical}{kg\ product}$$

$$EXP_{inhalation} = 0.60 \frac{mg\ aroma\ chemical}{day}$$

…over 250 days/year.

Dermal Exposure:

The dermal exposure to the aroma chemical during transport container loading is calculated using the following equations:

Liquids:

$$EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_final} \quad \text{[Eqn. 5-9]}$$

$$EXP_{dermal} = 0.7 \text{ to } 2.1 \frac{mg\ product}{cm^2 - incident} \times 840\ cm^2 \times 1 \frac{incident}{day} \times 0.004 \frac{kg\ aroma\ chemical}{kg\ fragrance\ oil}$$

$$EXP_{dermal} = 2.3 \text{ to } 7.1 \frac{mg\ aroma\ chemical}{day}$$

…over 50 days/year.

Solids:

$$EXP_{dermal} = 3{,}100 \frac{mg\ product}{day} \times F_{chem_final} \quad \text{[Eqn. 5-10]}$$

$$EXP_{dermal} = 3{,}100 \frac{mg\ product}{day} \times .004 \frac{kg\ aroma\ chemical}{kg\ fragrance\ oil}$$

$$EXP_{dermal} = 12.4 \frac{mg\ aroma\ chemical}{day}$$

…over 250 days/year.

7. DATA GAPS/UNCERTAINTIES AND FUTURE WORK

This ESD relies on anecdotal data and information gathered from various sources to generate general facility estimates, release estimates, and exposure estimates. EPA wishes to make this ESD as detailed and up-to-date as possible, such that the risk-screening assessments reflect current industrial practices. This ESD could be improved by collecting measured data and associated information to verify or supersede the anecdotal data and information.

EPA is most interested in obtaining information about the fragrance oil industry that is characterized as "typical" or "conservative" (i.e., worst case), and is applicable to a generic product formulation site. While EPA welcomes site-specific information as valuable to this ESD, additional qualifiers of how reflective it is to the industry are needed to ensure its transparency if used in the ESD. Reviewers should also feel free to recommend additional resources that may be useful to the development of this ESD.

The key data gaps are summarized below and are listed in order of importance (the first being most important):

1. The ESD incorporates average facility production rates that are estimated using U.S. Census Bureau data. The quality of these production rates could be improved with additional data on typical fragrance oil use rates or final product production rates (e.g., kg/batch, kg/site-day).

2. The ESD assumes that manufacturers use one specific fragrance oil (containing the aroma chemical) for all product formulations of the same type, and that each fragrance oil is incorporated into the final product during the entire year. Additional information on the validity of these assumptions, as well as typical formulation practices (e.g., typical campaign length, number of fragrance oils used at a time, etc.) would improve the quality of this ESD.

3. EPA found no specific information on the typical release control technologies used at product formulation sites (e.g., wastewater treatment). The releases calculated in this ESD reflect the amount of chemical released directly from the process. Information on control technologies and the prevalence of their use would further improve this ESD.

4. The default process description includes powdered products and volatile liquids, and the releases and exposures associated with these products. Additional information on the percentage of fragrance oils blended into solid powder products, and any specific monitoring data for these operations would improve the quality of this ESD.

5. EPA found no specific information on the typical personal protective equipment (PPE) used in product formulation processes (e.g., gloves, face shields, respirators). Specifically, EPA would be interested in monitoring data for all operations involving workers manually handling the formulated products would enhance the estimates. Further, the exposures calculated in this ESD reflect the potential amount of direct exposure with no mitigating PPE worn by the workers, as a worst case. Information on PPE and the prevalence of their use would further improve this ESD.

6. EPA found no information on the specific product shipping/packaging methods, container types, equipment residues, and waste handling practices. The ESD assumes that final products are packaged in 1-gallon containers. Additional information on specific mixing equipment (open versus closed mixing), and shipping/packaging methods would enhance the quality of the scenario.

EPA has previously contacted several trade associations to fill these data gaps; however, to date no additional information has been received. Should additional information be received, the ESD will be modified to reflect this new information.

8. REFERENCES

The specific information researched in the development of this document include process description, operating information, chemicals used, wastes generated, worker activities, and exposure information. Specific sources investigated in the development of this ESD include documents and data from the following sources:

- U.S. Environmental Protection Agency (EPA);
- U.S. Occupational Safety and Health Administration (OSHA);
- U.S. National Institute for Occupational Safety and Health (NIOSH);
- U.S. Census Bureau;
- Organisation for Economic Co-operation and Development (OECD);
- Environment Canada;
- North Carolina Division of Pollution Prevention and Environmental Assistance;
- Kirk-Othmer Encyclopedia of Technology;
- Various trade association websites (e.g., Fragrance Material Association (FMA) – www.fmafragrance.org, Cosmetic, Toiletry, and Fragrance Association (CTFA) – www.ctfa.org, Consumer Specialty Products Association (CSPA) – www.cspa.org, Soaps and Detergents Association (SDA) – www.cleaning101.com; and,
- Industry specific journals and technical literature (e.g., Aroma Creations, Inc. – www.aromacreations.com).

While each of these sources was reviewed for information, not all provided information specific to the blending of fragrance oils into commercial and consumer products. The references specifically cited in this ESD are provided below.

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APPENDIX A
ESTIMATION EQUATION SUMMARY AND DEFAULT VALUE DOCUMENTATION

Summary of Release and Exposure Estimation Equations

Table A-1 summarizes the equations introduced in Section 3, which are used to calculate the general facility parameters. Tables A-2 and A-3 summarize the equations used in evaluating releases of and exposures to aroma chemicals used in commercial and consumer products. Table A-4 summarizes the parameters for each equation, the default value if applicable and the source. The default values for the ChemSTEER models are presented in Appendix B.

Table A-1. General Facility Parameter Calculation Summary

General Facility Estimates	
Days of Operation (days/yr) ($TIME_{working_days}$): $$TIME_{working_days} = TIME_{operating_days} \times F_{products}$$	(Eqn. 3-1)
Weight fraction of the Aroma Chemical (F_{chem_final}): $$F_{chem_final} = F_{chem_oil} \times F_{oil_final}$$	(Eqn. 3-2)
Daily Use Rate of Fragrance Oil (kg/site-day), $Q_{oil_site_day}$: $$Q_{oil_site_day} = \frac{Q_{oil_site_yr} \times F_{products}}{TIME_{working_days}}$$	(Eqn. 3-3)
Daily Use Rate of Aroma Chemical (kg/site-day), $Q_{chem_site_day}$ (based on $Q_{facility_day}$): $$Q_{chem_site_day} = Q_{oil_site_day} \times F_{chem_oil}$$	(Eqn. 3-4)
Number of Sites (N_{sites}): $$N_{sites} = \frac{Q_{chem_yr}}{Q_{chem_site_day} \times TIME_{working_days}}$$	(Eqn. 3-5)
Number of Transport Containers Unloaded per Site, $N_{container_unload_site_yr}$: $$N_{container_unload_site_yr} = \frac{Q_{chem_site_day} \times TIME_{working_days}}{F_{chem_oil} \times V_{container_oil} \times RHO_{oil}}$$	(Eqn. 3-6)
Number of Transport Containers Loaded per Site, $N_{container_load_site_yr}$: $$N_{container_load_site_yr} = \frac{Q_{chem_site_day} \times TIME_{working_days}}{F_{chem_final} \times V_{container_final} \times RHO_{final}}$$	(Eqn. 3-7)

Table A-2. Environmental Release Calculation Summary

Source	Possible Medium	Daily Release Rates (kg/site-day), Elocal (for Given Sources)
Container Residue	Water Land Incineration	If $N_{container_unload_site_yr}$ is fewer than $TIME_{working_days}$: $Elocal_{container_residue_disp} = V_{container} \times RHO_{oil} \times F_{chem_oil} \times F_{container_residue} \times 1 \frac{container}{site - day}$ (Eqn. 4-2a) This release will occur over [$N_{container_unload_site_yr}$] days/year from [$N_{sites}$] sites. If $N_{container_unload_site_yr}$ is greater than $TIME_{working_days}$: $Elocal_{container_residue_disp} = Q_{chem_site_day} \times F_{container_residue}$ (Eqn. 4-2b) This release will occur over [$TIME_{working_days}$] days/year from [N_{sites}] sites.
Container Cleaning (Volatile Releases)	Air	*EPA/OPPT Penetration Model* (see Section 4.4)
Transfer Operations (Volatile Releases)	Air	*EPA/OAQPS AP-42 Loading Model* (see Section 4.5)
Operating Losses	Air	The following equation is used to determine the diameter of the opening, which is subsequently used in the *EPA/OPPT Penetration Model* (see Section 4.6). $D_{opening} = \left[\frac{4 \times Q_{final_batch} \times 1000 \left(cm^3 / L \right)}{\pi \times RHO_{final}} \right]^{1/3}$ (Eqn. 4-3)
Sampling	Water Land Incineration	No methodology has been developed at time of publication.
Sampling (Volatile Releases)	Air	*EPA/OPPT Penetration Model* (see Section 4.8)
Equipment Cleaning Residue	Water Land Incineration	$Elocal_{equipment_residue_disp} = Q_{chem_site_day} \times F_{equipment_residue}$ (Eqn. 4-4) This release will occur over [$TIME_{working_days}$] days/year for fine fragrance oils and [50] days/year for functional fragrance oils from [N_{sites}] sites.
Equipment Cleaning (Volatile Releases)	Air	*EPA/OPPT Mass Transfer Coefficient Model* (see Section 4.10)
Loading Product (Volatile Releases)	Air	*EPA/OAQPS AP-42 Loading Model* (see Section 4.11)
Dust Waste	Aire, Water, Incineration, Land	$Elocal_{dust_generation} = Q_{chem_site_day} \times F_{dust_generation} \times (1 - F_{APCD})$ (Eqn. 4-5)

Table A-3. Occupational Exposure Calculation Summary

Occupational Exposure Calculations
Number of Workers Exposed Per Site: Up to 29 workers per site (USCB, 2002).
Exposure from Unloading Transport Containers into Mixing Vessel: *Inhalation* *EPA/OPPT Mass Balance Inhalation Model* (see Section 5.3) *Dermal* $EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_oil}$ (Eqn. 5-1) This exposure will occur over the lesser of $N_{container_unload_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.5), up to [250] days per year.
Exposure During Transport Container Cleaning: *Inhalation* *EPA/OPPT Mass Balance Inhalation Model* (see Section 5.4) *Dermal* $EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_oil}$ (Eqn. 5-2) This exposure will occur over the lesser of $N_{container_unload_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.4), up to [250] days per year.
Exposure During Product Sampling: *Inhalation* *EPA/OPPT Mass Balance Inhalation Model* (see Section 5.5) *Dermal* $EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_final}$ (Eqn. 5-3) This exposure will occur over the lesser of $N_{container_unload_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.8), up to [250] days per year.

Occupational Exposure Calculations

Exposure During Equipment Cleaning:

Inhalation

EPA/OPPT Mass Balance Inhalation Model (see Section 5.6)

Dermal

$$EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_final} \quad \text{(Eqn. 5-4)}$$

This exposure will occur over $TIME_{working\ days}$ (consistent with Section 4.9), up to [250] days per year.

Exposure from Packaging of *Liquid* Commercial and Consumer Products:

Inhalation

EPA/OPPT Mass Balance Inhalation Model (see Section 5.7)

Dermal

$$EXP_{dermal} = Q_{liquid_skin} \times AREA_{surface} \times N_{exp_incident} \times F_{chem_final} \quad \text{(Eqn. 5-9)}$$

This exposure will occur over the lesser of $N_{container_load_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.11), up to [250] days per year.

Exposure from Packaging of *Solid* Commercial and Consumer Products:

Inhalation

$$Q_{final_site_day} = \frac{Q_{chem_site_day}}{F_{chem_final}} \quad \text{(Eqn. 5-6)}$$

If $Q_{final_site_day}$ is *greater than* 54 kg/site-day:

$$EXP_{inhalation} = C_{particulate} \times RATE_{breathing} \times TIME_{exposure} \times F_{chem_final} \quad \text{(Eqn. 5-7)}$$

This exposure will occur over the lesser of $N_{container_load_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.11), up to [250] days/year.

Or if $Q_{final_site_day}$ is *less than or equal to* 54 kg/site-day:

$$EXP_{inhalation} = Q_{final_site_day} \times F_{chem_final} \times F_{exposure} \quad \text{(Eqn. 5-8)}$$

This exposure will occur over the lesser of $N_{container_load_site_yr}$ or $TIME_{working_days}$ (consistent with Section 4.11), up to [250] days/year.

Dermal

$$EXP_{dermal} = \text{up to } 3{,}100\ \text{mg/day} \times F_{chem_final} \quad \text{(Eqn. 5-10)}$$

Table A-4. Parameter Declaration and Documentation Summary

Variable	Variable Description	Default Value	Data Source
$AREA_{opening}$	Surface area of the static pool or opening (cm^2)	Calculated	Appendix B
$AREA_{surface}$	Surface area of contact (cm^2)	840 cm2 (2 hands)	CEB, 2000
C_{chem_mass}	Mass concentration of the chemical vapor in air (mg/m^3)	Calculated	Section 6.3
$C_{chem_volumetric}$	Volumetric concentration of the chemical vapor in air (ppm)	Calculated	Section 6.3
$C_{particulate}$	Concentration of particulate in workers' breathing zone (OSHA Total PNOR PEL (8-hr TWA) (mg/m^3)	15	29 CFR 1910.1000
$D_{opening}$	Diameter of the mixing vessel opening (cm/vessel)	Calculated	Section 4.6
Efficiency	Efficiency of air pollution control device	0.85	EPA, 1993
$Elocal_{air}$	Daily release of the chemical vapor to air from the activity (kg/site-day)	Calculated	Appendix B
$Elocal_{container_residue_disp}$	Daily release of aroma chemical from container residue (kg aroma chemical/site-day)	Calculated	Section 4.3
$Elocal_{dust_generation}$	Daily release of aroma chemical from dust generation (kg aroma chemical/site-day)	Calculated	Section 4.12
$Elocal_{equipment_residue_disp}$	Daily release of aroma chemical from equipment residue (kg aroma chemical/site-day)	Calculated	Section 4.9
EXP_{dermal}	Potential dermal exposure to the aroma chemical per day (mg aroma chemical/day)	Calculated	Section 5.0
$EXP_{inhalation}$	Inhalation exposure to the aroma chemical per day (mg aroma chemical/day)	Calculated	Section 5.0
F_{APCD}	Air pollution control device efficiency	0.85	EPA, 1993
F_{chem_final}	Weight fraction of aroma chemical in final commercial and consumer product	Calculated	Section 3.3
F_{chem_oil}	Weight fraction of aroma chemical in fragrance oil	0.2	Kirk-Othmer, 2005
$F_{container_residue}$	Fraction of the aroma chemical remaining in the emptied container (kg aroma chemical remaining/kg aroma chemical in full container)	0.03	CEB, 2002
$F_{correction\ factor}$	Vapor pressure correction factor	0.2	Section 4.2
$F_{products}$	Fraction of days fragrance oil is formulated into commercial and consumer products	1	EPA assumption
$F_{dust\ generation}$	Fraction of final product released as dust	0.045	EPA, 1993

Variable	Variable Description	Default Value	Data Source
$F_{equipment_residue}$	Fraction of aroma chemical remaining in the equipment as residue (kg aroma chemical released/kg aroma chemical used in the process)	0.02	CEB, 1992
$F_{exposure}$	Weight fraction of total solid in workers' breathing zone (mg chemical/kg handled)	0.0477 (typical) 0.161 (worst case)	CEB, 1992
$F_{mixing\ factor}$	Mixing factor (dimensionless)	Varies	Appendix B
F_{oil_final}	Weight fraction of fragrance oil in final commercial and consumer product	0.02	Kirk-Othmer, 2005
MW_{chem}	Molecular weight of the aroma chemical (g/mol)	Chemical Specific	Manufacturer
$N_{container_load_site_yr}$	Number of transport containers unloaded at each site per year (containers/site-yr)	Calculated	Section 3.7
$N_{container_unload_site_yr}$	Number of transport containers unloaded at each site per year (containers/site-yr)	Calculated	Section 3.6
$N_{exp_incident}$	Number of exposure incidents per day (incidents/day)	1	CEB, 2000
N_{sites}	Number of sites using the fragrance oil containing the aroma chemical (sites)	Calculated	Section 3.5
$P_{ambient}$	Ambient pressure (atm)	1	CEB, 1991
$Q_{chem_site_day}$	Daily use rate of aroma chemical (kg aroma chemical/site-day)	Calculated	Section 3.4
Q_{chem_yr}	Annual production volume of aroma chemical (kg aroma chemical/yr)	Chemical Specific	Manufacturer
Q_{final_batch}	Mass of final product formulated per batch (kg product/batch)	500	Sigma, 2002
$Q_{final_site_day}$	Daily amount of final product that is transferred into transport containers (kg product/site-day)	Calculated	Section 5.7
Q_{liquid_skin}	Quantity of liquid remaining on skin (mg/cm^2-incident)	0.7 (low end) 2.1 (high end)	CEB, 2000
$Q_{oil_site_day}$	Daily use of fragrance oil (kg fragrance oil/site-day)	Calculated	Section 3.4
$Q_{oil_site_year}$	Quantity of fragrance oil used at each site (kg/site-yr)	20,500	USCB, 2005
$Q_{vapor_generation}$	Average vapor generation rate (g aroma chemical/sec)	Calculated	Section 6.0
$RATE_{air\ speed}$	Air speed (ft/min)	100	CEB, 1991
$RATE_{breathing}$	Typical worker breathing rate (m^3/hr)	1.25	CEB, 1991
$RATE_{fill}$	Fill rate (containers/hr)	Varies	Appendix B
$RATE_{ventilation}$	Ventilation rate (ft^3/min)	Varies	Appendix B

Variable	Variable Description	Default Value	Data Source
RHO_{final}	Density of the final product (kg product/L product)	1	EPA assumption
RHO_{oil}	Density of the fragrance oil (kg fragrance oil/L fragrance oil)	1	EPA assumption
$TEMP_{ambient}$	Ambient temperature (K)	298	CEB, 1991
$TIME_{activity_hours}$	Operating hours for the release activity per day (hrs)	Varies	Appendix B
$TIME_{exposure}$	Duration of exposure (hours/day)	Varies	Section 5.0
$TIME_{operating\ days}$	Total facility operating days (days/yr)	250	CEB, 1991
$TIME_{working_days}$	Number of operating days fragrance oil is formulated into commercial and consumer products (days/yr)	Calculated	Section 3.2
$V_{container_final}$	Volume of final product container (L/container)	3.78 (1-gallon container)	EPA assumption
$V_{container_oil}$	Volume of fragrance oil container (L/container)	208 (55-gallon drum)	EPA assumption
V_{molar}	Molar volume (L/mol)	24.45	Appendix B
VP_{chem}	Vapor pressure of the aroma chemical (torr)	Chemical Specific	Manufacturer

APPENDIX B
BACKGROUND INFORMATION AND EQUATIONS/DEFAULTS FOR THE STANDARD EPA ENVIRONMENTAL RELEASE AND WORKER EXPOSURE MODELS

B.1. INTRODUCTION

This appendix provides background information and a discussion of the equations, variables, and default assumptions for each of the standard release and exposure models used by EPA in estimating environmental releases and worker exposures. The models described in this appendix are organized into the following five sections:

- Section B.2: Chemical Vapor Releases & Associated Inhalation Exposures;
- Section B.3: Container Residue Release Models (non-air);
- Section B.4: Process Equipment Residue Release Models (non-air);
- Section B.5: Dust Emissions from Transferring Solids Model;
- Section B.6: Chemical Particle Inhalation Exposure Models; and
- Section B.7: Dermal Exposure Models.

Please refer to the guidance provided in the ESD for estimating environmental releases and worker exposures using these standard models, as it may suggest the use of certain overriding default assumptions to be used in place of those described for each model within this appendix.

This appendix includes a list of the key reference documents that provide the background and rationale for each of the models discussed. These references may be viewed in their entirety through the ChemSTEER Help System. To download and install the latest version of the ChemSTEER software and Help System, please visit the following EPA web site:

http://www.epa.gov/opptintr/exposure/docs/chemsteer.htm

B.2. CHEMICAL VAPOR RELEASES & ASSOCIATED INHALATION EXPOSURES

This section discusses the models used by EPA to estimate chemical vapor generation rates and the resulting volatile releases to air and worker inhalation exposures to that chemical vapor. The volatile air release models (discussed in B.2.1) calculate both a vapor generation rate ($Q_{vapor_generation}$; g/sec) and the resulting daily release rate of the chemical vapors to air. The *EPA/OPPT Mass Balance Inhalation Model* (discussed in Section B.2.2) uses the value of $Q_{vapor_generation}$, calculated by the appropriate release model, to estimate the resulting inhalation exposure to that released vapor.

B.2.1 Vapor Generation Rate and Volatile Air Release Models

The following models utilize a series of equations and default values to calculate a chemical vapor generation rate ($Q_{vapor_generation}$; g/sec) and the resulting daily volatile air release rate ($Elocal_{air}$; kg/site-day):

- *EPA/OPPT Penetration Model* – evaporative releases from an exposed liquid surface located indoors;
- *EPA/OPPT Mass Transfer Coefficient Model* – evaporative releases from an exposed liquid surface located outdoors; and

- *EPA/OAQPS AP-42 Loading Model* – releases of volatile chemical contained in air that is displaced from a container being filled.

Each of these models is described in greater detail in the following sections:

B.2.1.1 EPA/OPPT Penetration Model

Model Description and Rationale:

The *EPA/OPPT Penetration Model* estimates releases to air from evaporation of a chemical from an open, exposed liquid surface. This model is appropriate for determining volatile releases from activities that are performed *indoors*[1] or when air velocities are expected to be *less than or equal to 100 feet per minute*.

A draft paper (Arnold and Engel, 1999) evaluating the relative performance of this model and the *Mass Transfer Coefficient Model* against experimentally measured evaporation rates described laminar airflow conditions existing up to 100 feet per minute. The paper compared the *Penetration Model* to experimental evaporation rate data measured under laminar (less than 100 feet per minute) and turbulent (above 100 feet per minute) airflow conditions. While the *Penetration Model* did not provide accurate estimates of evaporation rates under turbulent air flow conditions (relative to the *Mass Transfer Coefficient Model*), the results modeled under laminar flow conditions were found to more closely approximate the experimental data (usually within 20 percent). It is assumed that the conditions of an indoor work area most closely approximate laminar airflow conditions.

The model was originally developed using Fick's second law of diffusion. Model results were tested against experimental results of a study on evaporation rates for 15 compounds studied at different air velocities and temperatures in a test chamber. The experimental data confirmed the utility and accuracy of the model equation. Sample activities in which the *Penetration Model* may be used to estimate volatile releases to air are sampling liquids and cleaning liquid residuals from smaller transport containers (e.g., drums, bottles, pails).

Model Equations:

The model first calculates the average vapor generation rate of the chemical from the exposed liquid surface using the following equation:

[B-1]

$$Q_{vapor_generation} = \frac{(8.24 \times 10^{-8}) \times MW_{chem}^{0.835} \times F_{correction_factor} \times VP_{chem} \times \left(1/29 + 1/MW_{chem} \right)^{0.25} \times RATE_{air_speed}^{0.5} \times AREA_{opening}}{TEMP_{ambient}^{0.05} \times D_{opening}^{0.5} \times P_{ambient}^{0.5}}$$

Where:

$Q_{vapor_generation}$ = Average vapor generation rate (g of chemical/sec)
MW_{chem} = Molecular weight of the chemical of interest (g/mol)

[1]Similar air releases from surfaces located at *outdoor* locations (air speeds > 100 ft/min) are calculated using the *Mass Transfer Coefficient Model* (see the description provided in this section of Appendix B).

$F_{correction_factor}$ = Vapor pressure correction factor (EPA default =1)[1]
VP_{chem} = Vapor pressure of the chemical of interest (torr)
$RATE_{air_speed}$ = Air speed (EPA default = 100 feet/min; value must be ≤ 100 feet/min for this model)
$AREA_{opening}$ = Surface area of the static pool or opening (cm^2; $B \times D_{opening}^2 / 4$)
$TEMP_{ambient}$ = Ambient temperature (EPA default = 298 K)
$D_{opening}$ = Diameter of the static pool or opening (cm; See Table B-1 for appropriate EPA default values)
$P_{ambient}$ = Ambient pressure (EPA default = 1 atm)

Note: The factor 8.24×10^{-8} in Equation B-1 accounts for various unit conversions. See Arnold and Engel, 1999, for the derivation of this constant.

Using the vapor generation rate ($Q_{vapor_generation}$) calculated in Equation B-1, the model then estimates the daily release to air for the activity using the following equation:

$$Elocal_{air} = Q_{vapor_generation} \times TIME_{activity_hours} \times \frac{3600 \text{ sec/hour}}{1000 \text{ g/kg}} \quad [B\text{-}2]$$

Where:

$Elocal_{air}$ = Daily release of the chemical vapor to air from the activity (kg/site-day)
$Q_{vapor_generation}$ = Average vapor generation rate (g of chemical/sec; see Equation B-1)
$TIME_{activity_hours}$ = Operating hours for the release activity per day (hours/site-day; See Table B-1 for appropriate EPA default values)

References:

Arnold, F.C. and Engel, A.J. Pre-publication draft article entitled, *Evaporation of Pure Liquids from Open Surfaces*. U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington DC. October 1999.

U.S. EPA. Chemical Engineering Branch. *CEB Manual for the Preparation of Engineering Assessment*, Volume 1 (Equation 4-24 and Appendix K). U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington DC. Contract No. 68-D8-0112. February 1991.

[1]The default vapor pressure correction factor, $F_{correction_factor}$, assumes that the chemical-containing material in the evaporating pool exhibits the vapor pressure of the chemical of interest, as a worst case (i.e., effective VP of the evaporating material = $F_{correction_factor} \times VP_{chem}$). Alternatively, Raoult's Law may be assumed (i.e., effective VP = mole fraction of the chemical in the material × VP_{chem}), thus the $F_{correction_factor}$ may be set equivalent to the chemical's mole fraction in the material, if known. Note: in the absence of more detailed data, the chemical's weight fraction within the material formulation may be used to approximate its mole fraction.

B.2.1.2 EPA/OPPT Mass Transfer Coefficient Model

Model Description and Rationale:

The *EPA/OPPT Mass Transfer Model* estimates releases to air from the evaporation of a chemical from an open, exposed liquid surface. This model is appropriate for determining this type of volatile release from activities that are performed *outdoors*[1] or when air velocities are expected to be *greater than 100 feet per minute*. A draft paper (Arnold and Engel, 1999) evaluating the relative performance of this and the *Penetration Model* against experimentally measured evaporation rates, described laminar airflow conditions existing up to 100 feet per minute. It is assumed that the conditions of an indoor process area most closely approximate laminar air flow conditions, while outdoor conditions approximate turbulent airflow conditions above 100 feet per minute.

As discussed in the draft paper, the model is predicated on the solution of the classical mass transfer coefficient model with the gas-phase mass transfer coefficient estimated by the correlation of Mackay and Matsugu. Results were tested against experimental results on 19 compounds generated by four different experimenters over a wide range of experimental conditions. While the *Mass Transfer Coefficient Model* matched the data well (usually within 20 percent), it was found that the *Penetration Model* (see description in previous section) outperformed the *Mass Transfer Coefficient Model* under laminar flow (i.e., "indoor") conditions. Therefore, the *Penetration Model* is used as a default for estimating indoor evaporation rates, while the *Mass Transfer Coefficient Model* is used for outdoor rates. Sample activities in which the *Mass Transfer Coefficient Model* may be used to estimate volatile releases to air are cleaning liquid residuals from process equipment and bulk transport containers (e.g., tank trucks, rail cars).

Model Equations:

The model first calculates the average vapor generation rate of the chemical from the shallow pool using the following equation:

[B-3]

$$Q_{vapor_generation} = \frac{(1.93\times10^{-7})\times MW_{chem}^{0.78}\times F_{correction_factor}\times VP_{chem}\times\left(1/29+1/MW_{chem}\right)^{0.33}\times RATE_{air_speed}^{0.78}\times AREA_{opening}}{TEMP_{ambient}^{0.4}\times D_{opening}^{0.11}\times\left(TEMP_{ambient}^{0.5}-5.87\right)^{2/3}}$$

Where:

$Q_{vapor_generation}$	=	Average vapor generation rate (g of chemical of interest/sec)
MW_{chem}	=	Molecular weight of the chemical of interest (g/mol)
$F_{correction_factor}$	=	Vapor pressure correction factor (EPA default =1)[2]
VP_{chem}	=	Vapor pressure of the chemical of interest (torr)

[1]Similar air releases from surfaces located at *indoor* locations (air speeds ≤ 100 ft/min) are calculated using the *Penetration Model* (see the description provided in this section of Appendix B).

[2]The default vapor pressure correction factor, $F_{correction_factor}$, assumes that the chemical-containing material in the evaporating pool exhibits the vapor pressure of the chemical of interest, as a worst case (i.e., effective VP of the evaporating material = $F_{correction_factor} \times VP_{chem}$). Alternatively, Raoult's Law may be assumed (i.e., effective VP = mole fraction of the chemical in the material × VP_{chem}), thus the $F_{correction_factor}$ may be set equivalent to the chemical's mole fraction in the material, if known. Note: in the absence of more detailed data, the chemical's weight fraction within the material formulation may be used to approximate its mole fraction.

$RATE_{air_speed}$ = Air speed (EPA default = 440 feet/min; value must be > 100 feet/min for this model)

$AREA_{opening}$ = Surface area of the static pool or opening (cm^2; $B \times D_{opening}^2 / 4$)

$TEMP_{ambient}$ = Ambient temperature (EPA default = 298 K)

$D_{opening}$ = Diameter of the static pool or opening (cm; See Table B-1 for appropriate EPA default values)

Note: The factor 1.93×10^{-7} in Equation B-3 accounts for various unit conversions. See Arnold and Engel, 1999, for the derivation of this constant.

Using the vapor generation rate ($Q_{vapor_generation}$) calculated in Equation B-3, the model then estimates the daily release to air for the activity using the following equation:

$$Elocal_{air} = Q_{vapor_generation} \times TIME_{activity_hours} \times \frac{3600 \text{ sec/hour}}{1000 \text{ g/kg}} \quad [B\text{-}4]$$

Where:

$Elocal_{air}$ = Daily release of the chemical vapor to air from the activity (kg/site-day)

$Q_{vapor_generation}$ = Average vapor generation rate (g of chemical/sec; see Equation B-3)

$TIME_{activity_hours}$ = Operating hours for the release activity per day (hours/site-day; See Table B-1 for appropriate EPA default values)

References:

Arnold, F.C. and Engel, A.J. Pre-publication draft article entitled, *Evaporation of Pure Liquids from Open Surfaces*. U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington DC. October 1999.

U.S. EPA. Chemical Engineering Branch. *CEB Manual for the Preparation of Engineering Assessment*, Volume 1. U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington DC. Contract No. 68-D8-0112. February 1991.

B.2.1.3 EPA/OAQPS AP-42 Loading Model

Model Description and Rationale:

The EPA's Office of Air Quality Planning and Standards (OAQPS) *AP-42 Loading Model* estimates releases to air from the displacement of air containing chemical vapor as a container/vessel is filled with a liquid. This model assumes that the rate of evaporation is negligible compared to the vapor loss from the displacement.

This model is used as the default for estimating volatile air releases during both loading activities and unloading activities. This model is used for unloading activities because it is assumed while one vessel is being unloaded another is assumed to be loaded. The *EPA/OAQPS AP-42 Loading Model* is used because it provides a more conservative estimate than either the *EPA/OPPT Penetration Model* or the *Mass Transfer Coefficient Model* for unloading activities.

Model Equations:

The model first calculates the average vapor generation rate of the chemical from the displacement during loading/filling operation using the following equation:

[B-5]

$$Q_{vapor_generation} = \frac{F_{saturation_factor} \times MW_{chem} \times \left(V_{cont_empty} \times \frac{3785.4 cm^3}{gal} \right) \times \left(\frac{RATE_{fill}}{3600 sec/hour} \right) \times F_{correction_factor} \times \left(\frac{VP_{chem}}{760 torr/atm} \right)}{R \times TEMP_{ambient}}$$

Where:

$Q_{vapor_generation}$	=	Average vapor generation rate (g of chemical/sec)
$F_{saturation_factor}$	=	Saturation factor (See Table B-1 for appropriate EPA default values)
MW_{chem}	=	Molecular weight of the chemical of interest (g/mol)
V_{cont_empty}	=	Volume of the container (gallons; see Table B-1 for appropriate EPA default values)
$RATE_{fill}$	=	Fill rate (containers/hour; see Table B-1 for appropriate EPA default values)
$F_{correction_factor}$	=	Vapor pressure correction factor (EPA default =1)[1]
VP_{chem}	=	Vapor pressure of the chemical of interest (torr)
R	=	Universal Gas Constant (82.05 atm-cm^3/mol-K)
$TEMP_{ambient}$	=	Ambient temperature (EPA default = 298 K)

Using the vapor generation rate ($Q_{vapor_generation}$) calculated in Equation B-5, the model then estimates the daily release to air for the activity using the following equation:

$$Elocal_{air} = Q_{vapor_generation} \times TIME_{activity_hours} \times \frac{3600 \text{ sec/hour}}{1000 \text{ g/kg}} \quad [B\text{-}6]$$

Where:

$Elocal_{air}$	=	Daily release of the chemical vapor to air from the activity (kg/site-day)
$Q_{vapor_generation}$	=	Average vapor generation rate (g of chemical/sec; see Equation B-5)
$TIME_{activity_hours}$	=	Operating hours for the release activity per day (hours/site-day; see Table B-1 for appropriate EPA default values)

[1]The default vapor pressure correction factor, $F_{correction_factor}$, assumes that the chemical-containing material in the evaporating pool exhibits the vapor pressure of the chemical of interest, as a worst case (i.e., effective VP of the evaporating material = $F_{correction_factor} \times VP_{chem}$). Alternatively, Raoult's Law may be assumed (i.e., effective VP = mole fraction of the chemical in the material × VP_{chem}), thus the $F_{correction_factor}$ may be set equivalent to the chemical's mole fraction in the material, if known. Note: in the absence of more detailed data, the chemical's weight fraction within the material formulation may be used to approximate its mole fraction.

Reference:

U.S. EPA. Chemical Engineering Branch. *CEB Manual for the Preparation of Engineering Assessment*, Volume 1 (Equation 4-21). U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington DC. Contract No. 68-D8-0112. February 1991.

Table B-1. Standard EPA Default Values Used in Vapor Generation Rate/Volatile Air Release Models

Activity Type (Location)	$V_{cont\ empty}$ (gallons)	$D_{opening}$ (cm)	$RATE_{fill}$ (containers/hour)	$F_{saturation\ factor}$	$TIME_{activity\ hours}$ (hours/site-day)
Container-Related Activities (e.g., filling, unloading, cleaning, open surface/evaporative losses):					
Bottles (Indoors)	1 (Range: <5)	5.08 (<5,000 gals)	60	Typical: 0.5 Worst Case: 1	Number of containers handled per site-day / $RATE_{fill}$
Small Containers (Indoors)	5 (Range: 5 to <20)				
Drums (Indoors)	55 (Range: 20 to <100)		20		
Totes (Indoors)	550 (Range: 100 to <1,000)				
Tank Trucks (Outdoors)	5,000 (Range: 1,000 to <10,000)	7.6 (≥5,000 gals)	2	1	
Rail Car (Outdoors)	20,000 (Range: 10,000 and up)		1		
Equipment Cleaning Activities:					
Multiple Vessels (Outdoors)	Not applicable	92	Not applicable	1	4
Single, Large Vessel (Outdoors)					1
Single, Small Vessel (Outdoors)					0.5
Sampling Activities:					
Sampling Liquids (Indoors)	Not applicable	Typical: 2.5[a] Worst Case: 10	Not applicable	1	1

Activity Type (Location)	$V_{cont\ empty}$ (gallons)	$D_{opening}$ (cm)	$RATE_{fill}$ (containers/hour)	$F_{saturation\ factor}$	$TIME_{activity\ hours}$ (hours/site-day)
Other Activities:					
Continuous Operation	If other scenario-specific activities are identified that use one of the vapor generation rate/air release models described in this section, the ESD will describe the model and provide appropriate default values for the model parameters.			1	24
Batch Operation					Lesser of: (Hours/batch × Batches/site-day) or 24

a - The "typical" diameter default value of 2.5 cm was adopted as a policy decision in 2002, which supersedes the previous default value of 7 cm shown in the 1991 U.S. EPA reference document.

B.2.2 Chemical Vapor Inhalation Model

The following sections describe the EPA standard model for estimating worker inhalation exposures to a chemical vapor, utilizing a vapor generation rate ($Q_{vapor_generation}$).

B.2.2.1 EPA/OPPT Mass Balance Model

Model Description and Rationale:

The *EPA/OPPT Mass Balance Model* estimates a worker inhalation exposure to an estimated concentration of chemical vapors within the worker's breathing zone. The model estimates the amount of chemical inhaled by a worker during an activity in which the chemical has volatilized and the airborne concentration of the chemical vapor is estimated as a function of the source vapor generation rate ($Q_{vapor_generation}$). This generation rate may be calculated using an appropriate standard EPA vapor generation model (see Equation B-1, Equation B-3, or Equation B-5) or may be an otherwise known value.

The *EPA/OPPT Mass Balance Model* also utilizes the volumetric ventilation rate within a given space and includes simplifying assumptions of steady state (i.e., a constant vapor generation rate and a constant ventilation rate) and an assumed mixing factor for non-ideal mixing of air. The default ventilation rates and mixing factors provide a typical and worst case estimate for each exposure. The airborne concentration of the chemical cannot exceed the level of saturation for the chemical.

An evaluation of the model was performed against collected monitoring data for various activities (see the 1996 AIHA article). This evaluation confirmed that the Mass Balance Model is able to conservatively predict worker inhalation exposures within one order of magnitude of actual monitoring data and is an appropriate model for screening-level estimates.

Model Equations:

The model first calculates the volumetric concentration of the chemical vapor in air using the following equation:

$$C_{chem_volumetric} = \frac{(1.7 \times 10^5) \times TEMP_{ambient} \times Q_{vapor_generation}}{MW_{chem} \times RATE_{ventilation} \times F_{mixing_factor}} \quad [B\text{-}7]$$

Where:

$C_{chem_volumetric}$ = Volumetric concentration of the chemical vapor in air (ppm)
$Q_{vapor_generation}$ = Average vapor generation rate (g of chemical/sec; see Equation B-1, Equation B-3, or Equation B-5, as appropriate)
$TEMP_{ambient}$ = Ambient temperature (EPA default = 298 K)
MW_{chem} = Molecular weight of the chemical of interest (g/mol)
$RATE_{ventilation}$ = Ventilation rate (ft^3/min; see Table B-2 for appropriate EPA default values)
F_{mixing_factor} = Mixing factor (dimensionless; see Table B-2 for appropriate EPA default values)

Note: The factor 1.7×10^5 in Equation B-7 accounts for various unit conversions. See Fehrenbacher and Hummel, 1996, for the derivation of this constant.

Note that the airborne concentration of the chemical vapor cannot exceed the saturation level of the chemical in air. Equation B-8 calculates the volumetric concentration at the saturation level based on

Raoult's Law. Use the lesser value for the volumetric concentration of the chemical vapor ($C_{chem_volumetric}$) calculated in either Equation B-7 or Equation B-8 in calculating the mass concentration of the chemical of interest in the air (see Equation B-9).

$$C_{chem_volumetric} = F_{correction_factor} \times VP_{chem} \times \frac{10^6 \text{ ppm}}{P_{ambient}} \quad [B\text{-}8]$$

Where:

$C_{chem_volumetric}$ = Volumetric concentration of the chemical of interest in air (ppm)

$F_{correction_factor}$ = Vapor pressure correction factor (EPA default =1)[1]

VP_{chem} = Vapor pressure of the chemical of interest (torr)

$P_{ambient}$ = Ambient pressure (Default = 760 torr)

Note: Raoult's law calculates the airborne concentration as a mole fraction. The factor 10^6 in Equation B-8 accounts for the unit conversion from mole fraction to ppm.

The volumetric concentration of the chemical of interest in air (calculated in either Equation B-7 or Equation B-8) is converted to a mass concentration by the following equation:

$$C_{chem_mass} = \frac{C_{chem_volumetric} \times MW_{chem}}{V_{molar}} \quad [B\text{-}9]$$

Where:

C_{chem_mass} = Mass concentration of the chemical vapor in air (mg/m^3)

$C_{chem_volumetric}$ = Volumetric concentration of the chemical vapor in air (ppm, see Equation B-7 or B-8, as appropriate)

MW_{chem} = Molecular weight of the chemical of interest (g/mol)

V_{molar} = Molar volume (Default = 24.45 L/mol at 25ºC and 1 atm)

Assuming a constant breathing rate for each worker and exposure duration for the activity, the inhalation exposure to the chemical vapor during that activity can be estimated using the following equation:

$$EXP_{inhalation} = C_{chem_mass} \times RATE_{breathing} \times TIME_{exposure} \quad [B\text{-}10]$$

Where:

$EXP_{inhalation}$ = Inhalation exposure to the chemical vapor per day (mg chemical/worker-day)

C_{chem_mass} = Mass concentration of the chemical vapor in air (mg/m^3; see Equation B-9]

$RATE_{breathing}$ = Typical worker breathing rate (EPA default = 1.25 m^3/hr)

[1]The default vapor pressure correction factor, $F_{correction_factor}$, assumes that the chemical-containing material in the evaporating pool exhibits the vapor pressure of the chemical of interest, as a worst case (i.e., effective VP of the evaporating material = $F_{correction_factor} \times VP_{chem}$). Alternatively, Raoult's Law may be assumed (i.e., effective VP = mole fraction of the chemical in the material × VP_{chem}), thus the $F_{correction_factor}$ may be set equivalent to the chemical's mole fraction in the material, if known. Note: in the absence of more detailed data, the chemical's weight fraction within the material formulation may be used to approximate its mole fraction.

$TIME_{exposure}$	=	Duration of exposure for the activity (hours/worker-day; see Table B-2 for appropriate EPA default values ($\leq$ 8 hours/worker-day))

References:

Fehrenbacher, M.C. and Hummel, A.A[1]. "Evaluation of the Mass Balance Model Used by the EPA for Estimating Inhalation Exposure to New Chemical Substances". *American Industrial Hygiene Association Journal*. June 1996. 57: 526-536.

U.S. EPA. Chemical Engineering Branch. *CEB Manual for the Preparation of Engineering Assessment*, Volume 1 (Equation 4-21). U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington DC. Contract No. 68-D8-0112. February 1991.

[1]Note: This reference is currently not available for viewing in the ChemSTEER Help System.

Table B-2. Standard EPA Default Values Used in the *EPA/OPPT Mass Balance Inhalation* Model

Activity Type (Location)	$V_{cont\ empty}$ (gallons)	$RATE_{fill}$ (containers/hour)	$RATE_{air\ speed}$ (feet/min)	$RATE_{ventilation}$ [a]	$F_{mixing\ factor}$	$TIME_{exposure}$ (hours/day)
Container-Related Activities (e.g., filling, unloading, cleaning, open surface/evaporative losses):						
Bottles (Indoors)	1 Range: <5	60	100 (Indoors)	Typical: 3,000 Worst Case: 500 (Indoors)	Typical: 0.5 Worst Case: 0.1	Lesser of: (Number of containers handled per site-day)) $RATE_{fill}$ or 8
Small Containers (Indoors)	5 Range: 5 to <20					
Drums (Indoors)	55 Range: 20 to <100	20				
Totes (Indoors)	550 Range: 100 to <1,000					
Tank Trucks (Outdoors)	5,000 Range: 1,000 to <10,000	2	440 (Outdoors)	Average: 237,600 Worst Case: 26,400 × (60 × $RATE_{air_speed}$) 5,280)^3 (Outdoors)		
Rail Car (Outdoors)	20,000 Range: 10,000 and up	1				
Equipment Cleaning Activities:						
Multiple Vessels (Outdoors)	Not applicable		440 (Outdoors)	Average: 237,600 Worst Case: 26,400 × (60 × $RATE_{air_speed}$) 5,280)^3 (Outdoors)	Typical: 0.5 Worst Case: 0.1	4
Single, Large Vessel (Outdoors)						1
Single, Small Vessel (Outdoors)						0.5
Sampling Activities:						
Sampling Liquids (Indoors)	Not applicable		100 (Indoors)	Typical: 3,000 Worst Case: 500 (Indoors)	Typical: 0.5 Worst Case: 0.1	1

Activity Type (Location)	$V_{cont\ emptv}$ (gallons)	$RATE_{fill}$ (containers/hour)	$RATE_{air\ speed}$ (feet/min)	$RATE_{ventilation}$ [a]	$F_{mixing\ factor}$	$TIME_{exposure}$ (hours/day)
Other Activities:						
Continuous Operation	If other scenario-specific activities are identified that use one of the vapor generation rate models with the *Mass Balance Inhalation Model* described in this section, the ESD will describe the models and provide appropriate default values for the model parameters.				Typical: 0.5 Worst Case: 0.1	≤8
Batch Operation						

a - If the appropriate vapor generation rate model is the *EPA/OAQPS AP-42 Loading Model* (see Equation B-5) for an outdoor activity, the $RATE_{air_speed}$ should be set to 440 feet/min, as a default in determining the worst case $RATE_{ventilation}$.

B.3. CONTAINER RESIDUE RELEASE MODELS (NON-AIR)

Model Description and Rationale:

EPA has developed a series of standard models for estimating the quantity of residual chemical remaining in emptied shipping containers that is released to non-air media (e.g., water, incineration, or landfill) when the container is either rinsed or disposed. All of the residue models assume a certain portion or fraction of the chemical remains in the emptied container to be later rinsed or discarded with the empty container.

The default parameters of model are defined based upon the particular size/type of container (e.g., small containers, drums, or large bulk), as well as the physical form of the chemical residue (e.g., liquid or solid). These defaults are based upon data collected during a 1988 EPA-sponsored study of residuals in containers from which materials have been poured or pumped.

Model Equation:

All of the models discussed in this section utilize the following common equation for calculating the amount of chemical residue:

$$Elocal_{container_residue_disp} = F_{container_residue} \times Q_{total_daily_container} \quad [B\text{-}11]$$

Where:

$Elocal_{container_residue_disp}$ = Daily release of the chemical residue to water, incineration, or landfill from the cleaning or disposal of empty shipping containers (kg/site-day)

$F_{container_residue}$ = Fraction of the amount of the total chemical in the shipping container remaining in the emptied container (dimensionless; see Table B-3 for appropriate EPA default values)

$Q_{total_daily_container}$ = Total (daily) quantity of the chemical contained in the shipping containers prior to emptying (kg of chemical/site-day; see Table B-4 for appropriate EPA default values)

Each model, however, utilizes unique default values within that equation based upon the relative size of the container and the physical form of the chemical residue. These default values are summarized in Table B-3 and Table B-4. The following models are the standard EPA models for estimating container residues:

- *EPA/OPPT Small Container Residual Model*;
- *EPA/OPPT Drum Residual Model*;
- *EPA/OPPT Bulk Transport Residual Model*; and
- *EPA/OPPT Solid Residuals in Transport Containers Model*.

The default frequency with which the container residues are released ($TIME_{days_container_residue}$, days/site-year) must be appropriately "paired" with the total daily quantity of chemical contained in the containers ($Q_{total_daily_container}$) used in calculating the daily release. Thus, Table B-4 also contains the appropriate EPA default values for $TIME_{days_container_residue}$.

References:

U.S. EPA. Chemical Engineering Branch. Memorandum: *Standard Assumptions for PMN Assessments*. From the CEB Quality Panel to CEB Staff and Management. October 1992.

U.S. EPA. Office of Pesticides and Toxic Substances. *Releases During Cleaning of Equipment.* July 1988.

Table B-3. Standard EPA Default Values for Use in the Container Residual Release Models

Chemical Form	Container Type	$V_{cont\ empty}$ (gallons)	Model Title	$F_{container_residue}$ [a]
Liquid	Bottle	1 Range: <5	*EPA/OPPT Small Container Residual Model*	Central Tendency: 0.003 High End: 0.006
	Small Container	5 Range: 5 to <20		
	Drum	55 Range: 20 to <100	*EPA/OPPT Drum Residual Model*	Central Tendency: 0.025 High End[b]: 0.03 (for pumping liquid out of the drum) Alternative defaults: Central Tendency: 0.003 High End: 0.006 (for pouring liquid out of the drum)
	Tote	550 Range: 100 to <1,000	*EPA/OPPT Bulk Transport Residual Model*	Central Tendency: 0.0007 High End: 0.002
	Tank Truck	5,000 Range: 1,000 to <10,000		
	Rail Car	20,000 Range: 10,000 and up		
Solid	Any	Any	*EPA/OPPT Solid Residuals in Transport Containers Model*	0.01

a - These defaults are based on the 1988 EPA study investigating container residue and summarized in the 1992 internal EPA memorandum (see *References* in this section for the citations of these sources).

b - The 1992 EPA memorandum reference document contains the previous default of 0.04 for the high-end loss fraction ($F_{container_residue}$) for the *Drum Residual Model*; however, this value was superseded by an internal policy decision in 2002. Per 40 CFR 261.7(b)(1) of the Resource Conservation and Recovery Act (RCRA), "a container or an inner liner removed from a container that has held any hazardous wastes, except waste that is a compressed gas or that is identified as an acute hazardous waste…is empty if…(ii) no more than 2.5 centimeters (1 inch) remain on the bottom of the container or liner or (iii)(A) no more than 3 percent by weight of the total capacity of the container remains in the container or inner liner if the container is equal to or less than 110 gallons in size…". The 3 percent high-end default is consistent with the range of experimental results documented in the 1988 EPA study (see *References* in this section for a citation of this study).

Table B-4. Standard EPA Methodology for Calculating Default $Q_{total_daily_container}$ and $TIME_{days_container_residue}$ Values for Use in the Container Residual Models

Number of Containers Emptied per Day	$Q_{total\ daily\ container}$ (kg/site-day)	$TIME_{days\ container\ residue}$ (days/year)
1 or more	(Mass quantity of chemical in each container (kg/container)) × (Number of containers emptied per day)	Total number of operating days for the facility/operation
Less than 1	Mass quantity of chemical in each container (kg/container)	Total number of containers emptied per site-year

B.4. PROCESS EQUIPMENT RESIDUE RELEASE MODELS (NON-AIR)

Model Description and Rationale:

EPA has developed two standard models for estimating the quantity of residual chemical remaining in emptied process equipment that is released to non-air media (e.g., water, incineration, or landfill) when the equipment is periodically cleaned and rinsed. The residue models assume a certain portion or fraction of the chemical remains in the emptied vessels, transfer lines, and/or other equipment and is later rinsed from the equipment during cleaning operations and discharged with the waste cleaning materials to an environmental medium.

The default parameters of the model are defined based upon whether the residues are being cleaned from a *single* vessel or from *multiple* pieces of equipment. These defaults are based upon data collected during an EPA-sponsored study of residuals in process equipment from which materials have pumped or gravity-drained.

Model Equation:

The models discussed in this section utilize the following common equation for calculating the amount of chemical residue:

$$Elocal_{equip_cleaning} = F_{equip_residue} \times Q_{total_chem_capacity} \quad [B\text{-}12]$$

Where:

$Elocal_{equip_cleaning}$ = Daily release of the chemical residue to water, incineration, or landfill from cleaning of empty process equipment (kg/site-day)

$F_{equip_residue}$ = Fraction of the amount of the total chemical in the process equipment remaining in the emptied vessels, transfer lines, and/or other pieces (dimensionless; see Table B-5 for appropriate EPA default values)

$Q_{equip_chem_capacity}$ = Total capacity of the process equipment to contain the chemical in question, prior to emptying (kg of chemical/site-day; see Table B-6 for appropriate EPA default values)

Each model, however, utilizes unique default values within that equation based upon whether the residues are cleaned from a single vessel or from multiple equipment pieces. These default values are summarized in Table B-5 and Table B-6. The following models are the standard EPA models for estimating process equipment residues:

- *EPA/OPPT Single Process Vessel Residual Model; and*
- *EPA/OPPT Multiple Process Vessel Residual Model.*

The default frequency with which the equipment residues are released ($TIME_{days_equip_residue}$, days/site-year) must be appropriately "paired" with the total capacity of the equipment to contain the chemical of interest ($Q_{equip_chem_capacity}$) used in calculating the daily release. Thus, Table B-6 also contains the appropriate EPA default values for $TIME_{days_equip_residue}$.

References:

U.S. EPA. Chemical Engineering Branch. Memorandum: *Standard Assumptions for PMN Assessments*. From the CEB Quality Panel to CEB Staff and Management. October 1992.

U.S. EPA. Office of Pesticides and Toxic Substances. *Releases During Cleaning of Equipment.* July 1988.

Table B-5. Standard EPA Default Values for Use in the Process Equipment Residual Release Models

Model Title	$F_{equip\ residue}$[a]
EPA/OPPT Single Process Vessel Residual Model	Conservative: 0.01 (for pumping process materials from the vessel) *Alternative defaults: Central Tendency: 0.0007 High End to Bounding: 0.002 (alternative defaults for gravity-draining materials from the vessel)
EPA/OPPT Multiple Process Vessel Residual Model	Conservative: 0.02

a - These defaults are based on the 1988 EPA study investigating container residue and summarized in the 1992 internal EPA memorandum (see *References* in this section for the citations of these sources).

Table B-6. Standard EPA Methodology for Calculating Default $Q_{equip_chem_capacity}$ and $TIME_{days_equip_residue}$ Values for Use in the Process Equipment Residual Models

Process Type	Number of Batches per Day	$Q_{equip\ chem.\ capacity}$ (kg/site-day)	$TIME_{days\ equip\ residue}$ (days/year)
Batch	1 or more	(Mass quantity of chemical in each batch (kg/batch)) × (Number of batches run per day)	Total number of operating days for the facility/operation
	Less than 1	Mass quantity of chemical in each batch (kg/batch)	Total number of batches run per site-year
Continuous	Not applicable	Daily quantity of the chemical processed in the equipment (kg/site-day)	Total number of operating days for the facility/operation

Note: Please refer to the ESD for any overriding default assumptions to those summarized above. Equipment cleaning may be performed periodically throughout the year, as opposed to the default daily or batch-wise cleaning frequencies shown above. For example, facilities may run dedicated equipment for several weeks, months, etc within a single campaign before performing equipment-cleaning activities, such that residuals remaining in the emptied are released less frequently than the standard default $TIME_{days_equip_residue}$ summarized above in Table B-6. Care should be given in defining the appropriate $Q_{total_daily_container}$ and $TIME_{days_container_residue}$ to be used in either of the standard EPA process equipment residue models.

B.5. DUST EMISSIONS FROM TRANSFERRING SOLIDS MODEL

EPA has developed the *EPA/OPPT Dust Emissions from Transferring Solids Model* to estimate the releases from dust generation during the unloading/transferring of solid powders. While there are multiple potential industrial sources of dust (e.g., grinding, crushing), the scope of this model is limited to transferring/unloading of solids. Specifically, this can be defined as activities where packaging/transport materials are opened and contents are emptied either into a feed system and conveyed or directly added into a process tank (e.g., reactor, mixing tank).

Model Description and Rationale:

The EPA/OPPT Dust Emissions from Transferring Solids Model estimates that 0.5% of the solid powder transferred may be released from dust generation. This model is based on 13 sources, including site visit reports, Organisation for Economic Co-operation and Development (OECD) Emission Scenario Documents (ESD), EPA's AP-42 Emission Factors, and Premanufacture Notice submissions (EPA's new chemicals review program). Each source contained estimates of the quantity of solid powder that may be lost during transfers for a specific industry. The different sources contained dust loss data or loss fraction estimates from a variety of industries including paint and varnish formulation, plastic manufacturing, printing ink formulation, rubber manufacturing, and chemical manufacturing. These estimates ranged from negligible to 3% of the transferred volume. The mean of the upper bound from each data set was 0.5%.

Additionally, dust generation test data were reviewed. A study by Plinke, et al. investigated key parameters for developing a theoretical approach for estimating dust losses based on moisture content, particle size, drop height, and material flow (Plinke, 1995). Dust generation rates during unloading and transfers were measured for four materials. The highest measured dust generation rate was 0.5%. These data further justified the adoption of a 0.5% loss fraction as a conservative estimate.

For the media of release of the dust generated, most facilities utilize some type of control device(s) to collect fugitive emissions. Many facilities collect fugitive dust emissions from these operations in filters and dispose of the filters in landfills or by incineration. Wet scrubbers may also be utilized by industry. However, in some cases, uncontrolled/uncollected particulates may be small enough to travel several miles from the facility, resulting in environmental and human exposures to the chemical of interest beyond the boundaries of the site. Fugitive dust emissions may also settle to facility floors and are disposed of when floors are cleaned (water if the floors are rinsed or land or incineration if the floors are swept). Therefore, as a conservative assumption the model assumes an uncontrolled release to air, water, incineration, or landfill.

If facility-specific information states a control technology is employed, the release may be partitioned to the appropriate media. If the control technology efficiency information is not available, the *CEB Engineering Manual* may be utilized for control technology efficiencies. Table B-7 provides estimated efficiencies for common control technologies.

Table B-7. Default Control Technology Efficiencies

Control Technology	Default Control Technology Capture Efficiency (%)	Notes/Source	Default Media of Release for Controlled Release
None (default)	0	No control technology should be assumed as conservative.	N/A

Control Technology	Default Control Technology Capture Efficiency (%)	Notes/Source	Default Media of Release for Controlled Release
Filter (such as a baghouse)	99	For particles > 1 um. CEB Engineering Manual.	Incineration or Land
Cyclone/Mechanical Collectors	80	For particles > 15 um CEB Engineering Manual.	Incineration or Land
Scrubber	Varies 95 may be assumed	Consult Table 7-1 of the CEB Engineering Manual.	Water

Model Equation:

Based on these data, the model estimates the portion of the release that is not captured or the uncontrolled release using the following equation. As a default this material is assumed released to air, water, incineration, or land.

$$Elocal_{dust_fugitive} = Q_{transferred} \times F_{dust_generation} \times (1 - F_{dust_control}) \qquad [B\text{-}13]$$

Where:

$Elocal_{dust_fugitive}$ = Daily amount not captured by control technology from transfers or unloading (kg/site-day)

$Q_{transferred}$ = Quantity of chemical transferred per day (kg chemical/site-day)

$F_{dust_generation}$ = Loss fraction of chemical during transfer/unloading of solid powders (Default: 0.005 kg released/kg handled)

$F_{dust_control}$ = Control technology capture efficiency (kg captured/kg processed) (Default: If the control technology is unknown, assume capture efficiency = 0 kg captured/kg processed, see Table B-7).

The following equation estimates the portion of dust release captured by the control technology. The default media of release for this material should be selected based on the information presented in Table B-7.

$$Elocal_{dust_captured} = Q_{transferred} \times F_{dust_generation} \times F_{dust_control} \qquad [B\text{-}14]$$

Where:

$Elocal_{dust_captured}$ = Daily amount captured by control technology from transfers or unloading (kg/site-day)

$Q_{transferred}$ = Quantity of chemical transferred per day (kg chemical/site-day)

$F_{dust_generation}$ = Loss fraction of chemical during transfer/unloading of solid powders (Default: 0.005 kg released/kg handled)

$F_{dust_control}$ = Control technology capture efficiency (kg captured/kg processed) (Default: If the control technology is unknown, assume capture efficiency = 0 kg captured/kg processed, see Table B-7).

References:

U.S. EPA. Chemical Engineering Branch. "Generic Model to Estimate Dust Releases from Transfer/Unloading Operations of Solid Powders". November 2006.

U.S. EPA. Chemical Engineering Branch. *CEB Manual for the Preparation of Engineering Assessment*, Volume 1 (page 4-11). U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington DC. Contract No. 68-D8-0112. February 1991.

Plinke, Marc A.E., et al. "Dust Generation from Handling Powders in Industry." *American Industrial Hygiene Association Journal*. Vol. 56: 251-257, March 1995.

B.6. CHEMICAL PARTICLE INHALATION EXPOSURE MODELS

The following EPA standard models may be used to estimate worker inhalation exposures to particles containing the chemical of interest:

- *EPA/OPPT Small Volume Solids Handling Inhalation Model*; and
- *OSHA Total Particulates Not Otherwise Regulated (PNOR) Permissible Exposure Limit (PEL)-Limiting Model.*

Each of these models is an alternative default for calculating worker inhalation exposures during the following particulate-handling activities, based upon the relative daily amount of particulate material being handled:

- Unloading and cleaning solid residuals from transport containers/vessels;
- Loading solids into transport containers/vessels; and
- Cleaning solid residuals from process equipment.

For amounts up to (and including) 54 kg/worker-shift, the *EPA/OPPT Small Volume Solids Handling Inhalation Model* is used, as it more accurately predicts worker exposures to particulates within this range than the *OSHA Total PNOR PEL-Limiting Model*. The *Small Volume Solids Handing Inhalation Model* is based on exposure monitoring data obtained for workers handling up to 54 kg of powdered material. Beyond this data-supported limit, EPA assumes that exposures within occupational work areas are maintained below the regulation-based exposure limit for "particulates, not otherwise regulated".

The *EPA/OPPT Small Volume Solids Handling Model* is also the exclusive model used for any solids sampling activity. Each of these models is described in detail in the following sections.

B.6.1 EPA/OPPT Small Volume Solids Handling Inhalation Model

Model Description and Rationale:

The *EPA/OPPT Small Volume Solids Handling Inhalation Model* utilizes worst case and typical exposure factors to estimate the amount of chemical inhaled by a worker during handling of *small volumes*[1] (i.e., ≤54 kg/worker-shift) of solid/powdered materials containing the chemical of interest. The

[1]Worker inhalation exposures to particulates handled in amounts *greater than 54 kg/worker-shift* are calculated using the *OSHA Total PNOR PEL-Limiting Model* (see the description provided in this section of Appendix B).

handling of these small volumes is presumed to include scooping, weighing, and pouring of the solid materials.

The worst case and typical exposure factor data were derived from a study of dye weighing and adapted for use in situations where workers are presumed to handle small volumes of solids in a manner similar to the handling in the study. The maximum amount of dye handled in the study was 54 kg/worker-shift, so the *Small Volume Solids Handling Inhalation Model* is presumed to be valid for quantities up to and including this amount. In the absence of more specific exposure data for the particular activity, EPA uses these data to estimate inhalation exposures to solids transferred at a rate up to and including 54 kg/worker-shift. This model assumes that the exposure concentration is the same as the concentration of the chemical of interest in the airborne particulate mixture.

Note that the amount handled per worker per shift is typically unknown, because while the throughput may be known, the number of workers and the breakdown of their activities are typically unknown. For example, while two workers may together handle 100 kg of material/day, one worker may handle 90 kg of material/day and the other may only handle 10 kg of material/day. Therefore, as a conservative estimate EPA assumes that the total throughput ($Q_{facility_day}$; kg/site-day) is equal to the amount handled per worker ($Q_{shift_handled}$; kg/worker-shift), if site-specific information is not available.

Model Equation:

The model calculates the inhalation exposure to the airborne particulate chemical using the following equation:

$$EXP_{inhalation} = (Q_{shift_handled} \times N_{shifts}) \times F_{chem} \times F_{exposure} \quad [B\text{-}15]$$

Where:

$EXP_{inhalation}$	=	Inhalation exposure to the particulate chemical per day (mg chemical/worker-day)
$Q_{shift_handled}$	=	Quantity of the solid/particulate material containing the chemical of interest that is handled by workers each shift (kg/worker-shift; see Table B-8 for appropriate EPA default values; must be ≤ 54 kg/worker-shift for this model to be valid)
N_{shifts}[1]	=	Number of shifts worked by each worker per day (EPA default = 1 shift/day)
F_{chem}	=	Weight fraction of the chemical of interest in the particulate material being handled in the activity (dimensionless; refer to the ESD discussion for guidance on appropriate default value)
$F_{exposure}$	=	Exposure factor; amount of total particulate handled that is expected to be inhaled (EPA defaults: 0.0477 mg/kg (typical) and 0.161 mg/kg (worst case))

[1]Note that this value is the number of shifts worked by *each worker* per day. This value would only be greater than one if a worker worked for over eight hours in a given day.

Table B-8. Standard EPA Default Values for $Q_{daily_handled}$ in the *EPA/OPPT Small Volume Solids Handling Inhalation Model*

Activity Type	Default $Q_{shift\ handled}$[1] (kg/worker-day)
Loading and Unloading Containers	Quantity of material in each container (kg/container) × Number of containers/worker-shift
Container Cleaning	Quantity of residue in each container (kg/container) × Number of container/worker-shift
Process-Related Activity (equipment cleaning, sampling):	
Continuous process:	Daily throughput of material / Number of shifts per day
Batch process (<1 batch per day):	Quantity of material per batch
Batch process (>1 batch per day):	Quantity of material per batch × Number of batches per shift

References:

U.S. EPA. Chemical Engineering Branch. Generic Scenario: *Textile Dyeing*. October 15, 1992.

U.S. EPA. Chemical Engineering Branch. *CEB Manual for the Preparation of Engineering Assessment*, Volume 1 (page 4-11). U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington DC. Contract No. 68-D8-0112. February 1991.

U.S. EPA Economics, Exposure and Technology Division[2]. *Textile Dye Weighing Monitoring Study*. U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington D.C., EPA 560/5-90-009. April 1990.

B.6.2 OSHA Total PNOR PEL-Limiting Model

Model Description and Rationale:

The *OSHA Total Particulates Not Otherwise Regulated (PNOR) Permissible Exposure Limit (PEL)-Limiting Model* estimates the amount of chemical inhaled by a worker during handling of solid/powdered materials containing the chemical of interest. The estimate assumes that the worker is exposed at a level no greater than the OSHA PEL for *Particulate, Not Otherwise Regulated*, total particulate. Operations are generally expected to comply with OSHA's federal regulation regarding total particulate exposures. This model assumes that the exposure concentration is the same as the concentration of the chemical of interest in the airborne particulate mixture.

The *OSHA Total PNOR PEL-Limiting Model* is used in cases where workers are handling quantities of solid/powdered materials *in excess of 54 kg/worker-shift*[1]. As stated in Section B.6.1, the *Small*

[1]The appropriate quantity of material handled by each worker on each day may vary from these standard CEB defaults, per the particular scenario. Be sure to consult the discussion presented in the ESD activity description in determining the most appropriate default value for $Q_{daily_handled}$.

[2]Note: This reference is currently available for viewing in the ChemSTEER Help System.

Volume Solids Handling Model, based on monitoring data, provides a more realistic estimate of worker inhalation exposures to smaller quantities particulate material. The data used by the *Small Volume Solids Handling Model* are supported up to and including 54 kg solid material handled per worker-shift. Beyond this amount, EPA assumes the occupational exposures are maintained below the regulatory exposure limit contained in the *OSHA Total PNOR PEL-Limiting Model*, although the exposures provided by this model are considered to be worst-case, upper-bounding estimates.

Refer to Table B-8 for the standard EPA assumptions used in determining the appropriate quantity of particulate material handled to determine the applicability of this model to a given activity.

NOTE: The OSHA Total PNOR PEL (used as the basis for the model calculations) is an 8-hour time-weighted average (TWA); therefore, *worker exposures must be assumed to occur over an 8-hour period* for the *OSHA Total PNOR PEL-Limiting Model* estimate to be valid basis for the calculated inhalation exposure estimate.

Model Equations:

The model first calculates the mass concentration of the airborne particulate chemical using the following equation:

$$C_{chem_mass} = C_{total_mass} \times F_{chem} \quad [B\text{-}16]$$

Where:

C_{chem_mass} = Mass concentration of the chemical in air (mg/m^3)

C_{total_mass} = Mass concentration of total particulate (containing the chemical) in air (EPA default = 15 mg/m^3, based on the OSHA Total PNOR PEL, 8-hr TWA)

F_{chem} = Weight fraction of the chemical of interest in the particulate material being handled in the activity (dimensionless; refer to the ESD discussion for guidance on appropriate default value)

Similar to Equation B-10 in the *EPA/OPPT Mass Balance Inhalation Model*, the *OSHA Total PNOR PEL-Limiting Model* then uses the mass airborne concentration of the chemical (C_{mass_chem}) in Equation B-16, to calculate the inhalation exposure to the particulate chemical using the following equation:

$$EXP_{inhalation} = C_{chem_mass} \times RATE_{breathing} \times TIME_{exposure} \quad [B\text{-}17]$$

Where:

$EXP_{inhalation}$ = Inhalation exposure to the airborne particulate chemical per day (mg chemical/worker-day)

C_{chem_mass} = Mass concentration of the particulate chemical in air (mg/m^3; see Equation B-17)

$RATE_{breathing}$ = Typical worker breathing rate (EPA default = 1.25 m^3/hr)

[1] Worker inhalation exposures to particulates handled in amounts *up to and including 54 kg/worker-shift* are calculated using the *EPA/OPPT Small Volume Handling Inhalation Model* (see the description provided in this section of Appendix B).

$TIME_{exposure}$ = Duration of exposure for the activity (EPA default = 8 hours/worker-day[1])

References:

U.S. EPA. Chemical Engineering Branch. *CEB Manual for the Preparation of Engineering Assessment*, Volume 1 (Equations 4-1 and 4-11). U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington DC. Contract No. 68-D8-0112. February 1991.

B.7. DERMAL EXPOSURE MODELS

Model Description and Rationale:

EPA has developed a series of standard models for estimating worker dermal exposures to liquid and solid chemicals during various types of activities. All of these dermal exposure models assume a specific surface area of the skin that is contacted by a material containing the chemical of interest, as well as a specific surface density of that material in estimating the dermal exposure. The models also assume *no use of controls or gloves* to reduce the exposure. These assumptions and default parameters are defined based on the nature of the exposure (e.g., one hand or two hand, immersion in material, contact with surfaces) and are documented in the references listed in this section.

In the absence of data, the EPA/OPPT standard models for estimating dermal exposures from industrial activities described in this section can be used. The models for exposures to liquid materials are based on experimental data with liquids of varying viscosity and the amount of exposure to hands was measured for various types of contact. Similar assessments were made based on experimental data from exposure to solids.

Model Equation:

All of the standard EPA models utilize the following common equation for calculating worker dermal exposures:

$$EXP_{dermal} = AREA_{surface} \times Q_{remain_skin} \times F_{chem} \times N_{event} \quad [B\text{-}18]$$

Where:

EXP_{dermal} = Dermal exposure to the liquid or solid chemical per day (mg chemical/worker-day)

$AREA_{surface}$ = Surface area of the skin that is in contact with liquid or solid material containing the chemical (cm^2; see Table B-9 for appropriate EPA default values)

Q_{remain_skin} = Quantity of the liquid or solid material containing the chemical that remains on the skin after contact (mg/cm^2-event; see Table B-9 for appropriate EPA default values)

[1]Since the OSHA Total PNOR PEL is an 8-hr TWA, the exposure duration must be assumed as 8 hours/worker-day for the model defaults to apply.

F_{chem}	=	Weight fraction of the chemical of interest in the material being handled in the activity (dimensionless; refer to the ESD discussion for guidance on appropriate default value)
N_{event}[1]	=	Frequency of events for the activity (EPA default = 1 event/worker-day)

Each model, however, utilizes unique default values within that equation based upon the nature of the contact and the physical form of the chemical material. These default values are summarized in Table B-9. The following models are the standard EPA models for estimating worker dermal exposures:

- *EPA/OPPT 1-Hand Dermal Contact with Liquid Model*;
- *EPA/OPPT 2-Hand Dermal Contact with Liquid Model*;
- *EPA/OPPT 2-Hand Dermal Immersion in Liquid Model*;
- *EPA/OPPT 2-Hand Dermal Contact with Container Surfaces Model;* and
- *EPA/OPPT 2-Hand Dermal Contact with Solids Model*.

For several categories of exposure, EPA uses qualitative assessments to estimate dermal exposure. Table B-10 summarizes these categories and the resulting qualitative dermal exposure assessments.

References:

U.S. EPA. Chemical Engineering Branch. *Options for Revising CEB's Method for Screening-Level Estimates of Dermal Exposure – Final Report.* U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington DC. June 2000.

U.S. EPA. Chemical Engineering Branch. *CEB Manual for the Preparation of Engineering Assessment*, Volume 1. U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington DC. Contract No. 68-D8-0112. February 1991.

[1]Only one contact per day (N_{event} = 1 event/worker-day) is assumed because Q_{remain_skin}, with few exceptions, is not expected to be significantly affected either by wiping excess chemical material from skin or by repeated contacts with additional chemical material (i.e., wiping excess from the skin does not remove a significant fraction of the small layer of chemical material adhering to the skin and additional contacts with the chemical material do not add a significant fraction to the layer). Exceptions to this assumption may be considered for chemicals with high volatility and/or with very high rates of absorption into the skin.

Table B-9. Standard EPA Default Values for Use in the Worker Dermal Exposure Models

Default Model	Example Activities	$AREA_{surface}$[a] (cm^2)	$Q_{remain\ skin}$[b] (mg/cm^2-event)	Resulting Contact $AREA_{surface} \times Q_{remain\ skin}$ (mg/event)
Physical Form: Liquids				
EPA/OPPT 1-Hand Dermal Contact with Liquid Model	Liquid sampling activities Ladling liquid/bench-scale liquid transfer	420 (1 hand mean)	Low: 0.7 High: 2.1	Low: 290 High: 880
EPA/OPPT 2-Hand Dermal Contact with Liquid Model	Maintenance Manual cleaning of equipment and containers Filling drum with liquid Connecting transfer line	840 (2 hand mean)	Low: 0.7 High: 2.1	Low: 590 High: 1,800
EPA/OPPT 2-Hand Dermal Immersion in Liquid Model	Handling wet surfaces Spray painting	840 (2 hand mean)	Low: 1.3 High: 10.3	Low: 1,100 High: 8,650
Physical Form: Solids				
EPA/OPPT 2-Hand Dermal Contact with Container Surfaces Model	Handling bags of solid materials (closed or empty)	No defaults	No defaults	< 1,100[c]
EPA/OPPT 2-Hand Dermal Contact with Solids Model	Solid sampling activities Filling/dumping containers of powders, flakes, granules Weighing powder/scooping/mixing (i.e., dye weighing) Cleaning solid residues from process equipment Handling wet or dried material in a filtration and drying process	No defaults	No defaults	< 3,100[23]

a - These default values were adopted in the 2000 EPA report on screening-level dermal exposure estimates (see *References* in this section for the citations of this sources) and are the mean values for men taken from the EPA Exposure Factors Handbook, 1997.

b - These default values were adopted in the 2000 EPA report on screening-level dermal exposure estimates (see *References* in this section for the citation of this source). The report derived the selected ranges of values for liquid handling activities from: U.S. EPA. A Laboratory Method to Determine the Retention of Liquids on the Surface of Hands. U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Exposure Evaluation Division. EPA 747-R-92-003. September 1992.

c - These default values were adopted in the 2000 EPA report on screening-level dermal exposure estimates (see *References* in this section for the citation of this source). The report derived values for dermal contact for solids handling activities from: Lansink, C.J.M., M.S.C. Breelen, J. Marquart, and J.J. van Hemmen: Skin Exposure to Calcium Carbonate in the Paint Industry. Preliminary Modeling of Skin Exposure Levels to Powders Based on Field Data (TNO Report V 96.064). Rijswijk, The Netherlands: TNO Nutrition and Food Research Institute, 1996.

Table B-10. EPA Default Qualitative Assessments for Screening-Level Estimates of Dermal Exposure

Category	Dermal Assessment
Corrosive substances (pH>12, pH<2)	Negligible
Materials at temperatures >140°F (60°C)	Negligible
Cast Solids (e.g., molded plastic parts, extruded pellets	Non-Quantifiable (Some surface contact may occur if manually transferred)
"Dry" surface coatings (e.g., fiber spin finishes, dried paint)	Non-Quantifiable (If manual handling is necessary and there is an indication that the material may abrade from the surface, quantify contact with fingers/palms as appropriate)
Gases/Vapors	Non-Quantifiable (Some contact may occur in the absence of protective clothing)

Source: U.S. EPA. Chemical Engineering Branch. *CEB Manual for the Preparation of Engineering Assessment*, Volume 1. U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington DC. Contract No. 68-D8-0112. February 1991.

APPENDIX C
DATA RECEIVED FROM ENVIRONMENT CANADA

On January 18, 2006, Environment Canada forwarded to EPA comments on an early version of the Fragrances ESD. Data that are relevant to this industry were also submitted for EPA's consideration. These data, provided by the Existing Substances and New Substances Divisions of Environment Canada, are presented below.

Canadian Industry Census Data:

Canadian Census data from 1995-2004 were provided for EPA's consideration. These data show that, although the total number of product formulation sites and workers is less than those located in the United States, the number of employees per site is approximately equal to that of U.S. formulators.

NAICS 32561 - Soaps and cleaning compounds

These statistics are for the Soaps and cleaning compounds industry, based on the North American Industry Classification System (NAICS) code 32561.

Principal statistics**

	Establishments	Shipments, $M	Employment	Imports, $M	Exports, $M
1995	135	2 020	8 100	876	415
1996	159	1 904	8 150	923	530
1997	168	1 936	8 547	1 033	511
1998	164	1 895	10 143	1 159	530
1999	150	2 026	8 417	1 277	571
2000	255	2 226	6 631	1 368	554
2001	235	1 918	6 429	1 503	640
2002	241	1 824	6 407	1 644	708
2003	232	1 801	6 274	1 653	666
2004	241*	1 677*	6 270*	1 804	779

Source: Statistics Canada

* Industry Canada estimates

** Beginning in 2000, data includes very small establishments. This accounts for the large jump in establishments, and for part of the increase in shipments and employment.

NAICS 32562 - Toilet preparations

These statistics are for the Toilet preparations industry, based on the North American Industry Classification System (NAICS) code 32562.

Principal statistics**

	Establishments	Shipments, $M	Employment	Imports, $M	Exports, $M
1995	75	1 083	7 160	717	376
1996	77	1 112	7 586	855	422
1997	77	1 143	7 257	948	504
1998	81	1 106	8 122	1 099	581
1999	71	1 073	7 408	1 165	617
2000	174	1 150	6 287	1 259	742
2001	168	1 229	6 948	1 418	890
2002	173	1 280	6 836	1 561	994
2003	170	1 451	7 388	1 582	1 016
2004	173*	1 592*	7 390*	1 656	1 155

Source: Statistics Canada

* Industry Canada estimates

** Beginning in 2000, data includes very small establishments. This accounts for the large jump in establishments, and for part of the increase in shipments and employment.

APPENDIX D
DATA RECEIVED FROM RESEARCH INSTITUTE FOR FRAGRANCE MATERIALS

EPA submitted a previous version of the draft ESD to the OECD ESD Task Force with a request for review and comment. In response, CEB received the following document:

> *Review and Evaluation of Environmental Emission Scenarios for Fragrance Materials during Compounding of Perfume Oils and Formulation of Consumer Products.* Research Institute for Fragrance Materials (RIFM), dated January 30, 2009.

The RIFM document summarizes information related to the emission of fragrance ingredients based on five available scenarios. In addition, the document summarizes the responses received from a 2008 industry questionnaire. RIFM did not specify whether the questionnaire was distributed to European or U.S. companies. Therefore, it is unclear whether these responses are representative of U.S. industry practices. The RIFM document covers 1) the compounding[23] of aroma chemicals into fragrance oils, and 2) the blending of fragrance oils into commercial and consumer products. Note the scope of the OECD ESD only includes the second step in the lifecycle of fragrance ingredients. Relevant RIFM data are presented below for references.

Container Cleaning

Based on responses received from the 2008 RIFM questionnaire, empty containers are generally not cleaned at the formulation sites. They are either dedicated containers or they are recycled by an external company.

The RIFM document also indicates that solid waste and packaging may be incinerated or collected by waste companies. This information is based on two large and one medium size companies who formulate polycyclic musk[24] into cleaning products.

Release from Container Residue

The Fragrance Materials Association (FMA) estimated a container residual of less than 0.5% based on studies on two basic drum handling scenarios.

Equipment Cleaning

Several formulation sites responded to the 2008 RIFM questionnaire and indicated that wash water from equipment and process vessel cleaning is recycled back into the production process to reduce loss. Residues or samples of soap or powdered detergent are also reused in production. For some perfume alcoholic products, alcohol is used for cleaning. The alcohol is then recovered without any loss to water.

Number of Operating Days

The RIFM document provides the following information on the number of operating days for the fragrance industry:

- 345 working days per year for large formulators; or
- 250 working days per year for small formulators who formulate polycyclic musk into cleaning products; and

[23] The word "compounding" is used by RIFM to refer to the "formulation of fragrance oils".

[24] Polycyclic musks are one of the many common "aroma chemicals" used as ingredients in fragrance oils.

- Between 250 and 312 days based on 8 formulator's responses to the 2008 RIFM questionnaire.

The document does not further define "large" or "small" formulators.

Pollution Control Technology for Water Releases

Based on responses to the RIFM questionnaire received from 8 formulation sites, some type of on-site treatment is generally utilized prior to discharge of wastewater. The WWTP removal ranges from 70 to 96 percent in the responses received. However, there is insufficient detail on the type of wastewater treatment for all product types.

Recommended Scenario

The RIFM document recommends the following parameters for estimating overall releases to wastewater at large and small formulation sites.

Table D-1. RIFM Recommended Release Estimates during the Formulation of Fragrance Oil into Consumer Products

Parameter	
Number of emission days	250
Fraction released to wastewater during the formulation of:	
Soap	0.0005 (large)[1] 0.001 (small)
Granular Detergents	0.001 (large) 0.002 (small)
Liquid conditioners, cleaners, Shampoo, Shower gel	0.001 (large) 0.002 (small)
Creams, lotions	0.01
Fine fragrances (if not cleaned with alcohol)	0.015

[1]Large and small formulation sites