Consumer Exposure Model (CEM)

Appendices

Prepared for EPA Office of Pollution Prevention and Toxics

by ICF

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APPENDIX A: Output from E6-A_ING1-A_ING3-A_DER1 and Conversion to Dose

A simulation for the SVOC dust model was run for five years during beta testing to ensure the model reached steady state for all the different high, medium, and low combinations of input variables within five years. Because the model reached steady state, the following simplifying assumptions were made:

"Omnipresent article": An article or articles of similar size (i.e., emission rate) are present in the house throughout the life of the individual. Each of these consecutive articles contain the same SVOC and in similar amounts.

Constant Lifetime Concentrations: The steady-state air phase, air particulate, and dust concentrations simulated in the model during the 5 year simulation are the approximate concentrations for *each* consecutive article (i.e., the article in place from birth to age 5, the article in place from age 5 to age 10, etc.). Thus, these steady-state concentrations are the constant concentrations throughout the lifetime of the individual across all the different consecutive articles.

No Ramp Up/Ramp Down: After one article is removed and the next consecutive article is replaced, the SVOC concentration in dust from the old article decreases at approximately the same rate that the SVOC concentration in dust from the new article increases. Thus, these "ramp up" and "ramp down" phases can be neglected and the concentration can be treated as constant over the lifetime of the individual.

Steady State Conditions throughout Home: The nearly constant source of SVOCs from articles will continue over a period that will allow for the air and dust within the house to reach steady state. Exposure will be calculated considering the whole house to be one well-mixed zone.

Based on these assumptions, the outputs of the SVOC dust model will be:

1. The steady-state air phase SVOC concentration in mg/m^3,

The steady-state air particulate SVOC concentration in mg/g,

The steady-state air particulate concentration in g/m^3, and

The steady-state effective total dust SVOC concentration in mg/g.

The fourth item is estimated as

$$TotDustConcen = \frac{FloorDustConcen \times FloorDustMass + FloorTSPConcen \times FloorTSPMass}{FloorDustMass + FloorTSPMass} \quad \text{(A1)}$$

Where:

$TotDustConcen$ = Estimated total dust SVOC concentration, as output by the SVOC Dust model (mg/g)

$FloorDustConcen$ = Concentration of SVOC in the floor dust (mg/g)

$FloorDustMass$ = Mass of dust on the floor (g)

$FloorRPConcen$ = Concentration of SVOC in the floor RP (mg/g)

$FloorRPMass$ = Mass of RP on the floor (g)

These four different values will be used to estimate the inhalation, ingestion and dermal doses for the different age groups in the model. These are estimated as:

$$IngDose = TotDustConcen \times FracTime \times DustIngest \quad \text{(A2)}$$

Where:

$IngDose$ = Ingestion dose of SVOC, averaged for the age group (mg/day)

$TotDustConcen$ = Estimated total dust SVOC concentration, as output by the SVOC Dust model (mg/g)

$FracTime$ = Age-dependent fraction of time the individual spends at home

$DustIngest$ = Age-dependent daily ingestion rate of dust (g/day)

$$InhAirPhaseDose = AirPhaseConcen \times FracTime \times InhalRate \tag{A3}$$

Where:

$InhAirPhaseDose$ = Inhalation dose of SVOC in the gas phase, averaged for the age group (mg/day)

$AirPhaseConcen$ = Airphase SVOC concentration, as output by the SVOC Dust model (mg/m^3)

$FracTime$ = Age-dependent fraction of time the individual spends at home

$InhalRate$ = Age-dependent daily inhalation rate (m^3/day)

$$InhAirPartDose = AirPartConcen \times SVOCPartConcen \times FracTime \times InhalRate \tag{A4}$$

Where:

$InhAirPartDose$ = Inhalation dose of SVOC bound to particulate, averaged for the age group (mg/day)

$AirPartConcen$ = Particulate concentration in the air (g/m^3)

$SVOCPartConcen$ = SVOC concentration on airborne particulate (mg/g)

$FracTime$ = Age-dependent fraction of time the individual spends at home

$InhalRate$ = Age-dependent daily inhalation rate (m^3/day)

$$InhDose = InhAirPhaseDose + \ InhAirPartDose \tag{A5}$$

Where:

$InhDose$ = Total inhalation dose of SVOC, averaged for the age group (mg/day)

$InhAirPhaseDose$ = Inhalation dose of SVOC in the gas phase, averaged for the age group (mg/day)

$InhAirPartDose$ = Inhalation dose of SVOC bound to particulate, averaged for the age group (mg/day)

Dermal doses from vapor-to-skin exposure will be estimated as:

$$DerDose = \frac{DerFlux \times \frac{SA}{BW} \times \mathrm{FracTime} \times ED_{cr} \times CF_1}{AT_{cr} \times CF_2} \tag{A6}$$

Where:

$DerDose$ = Dermal dose of SVOC from vapor-to-skin exposure, averaged for the age group (mg/kg-day)

$DerFlux$ = Dermal flux (mg/m^2-hr)

$\frac{SA}{BW}$ = Surface area to body weight ratio (cm^2/kg)

$FracTime$ = Fraction of time in environment (unitless)

ED_{cr} = Exposure duration (years)

CF_1 = Conversion factor 1 (24 hrs/day)

AT_{cr} = Averaging time (years)

CF_2 = Conversion factor 2 (10000 cm^2/ m^2)

Dermal flux in the above equation is estimated as:

$$DerFlux = K_{p\_g} \times (BkgdAirConcen + AirPhaseConcen) \quad \text{(A7)}$$

Where:

$DerFlux$ = Dermal flux (mg/m^2-hr)

K_{p_g} = Transdermal permeability coefficient (m/hr)

$BkgdAirConcen$ = Background air phase SVOC concentration (mg/m^3)

$AirPhaseConcen$ = Air phase SVOC concentration (mg/m^3), as output by the SVOC Dust model

APPENDIX B: Default Inputs Tables

Default values used in CEM are provided below. Data sources for values are noted where available. Please note that professional expert judgment was also considered in default value determinations through comparison of available data.

Table B-1. Product and Article Designations, Relevant Routes of Exposure, and Relevant Models for Products and Articles

Product or Article Name	Product or Article?	Relevant Routes of Exposure			Relevant Exposure Models																	
		Inhalation	Ingestion	Dermal	E1	E2	E3	E4	E5	E6	A_INH1	P_ING1	P_ING2	A_ING1	A_ING2	A_ING3	P_DER1a	P_DER1b	P_DER2	A_DER1	A_DER2	A_DER3
Glues and Adhesives (small scale)	P	X		X	X												X	X				
Glues and Adhesives (large scale)	P	X		X	X												X	X				
Caulk (Sealant)	P	X		X	X												X	X				
Fillers and Putties	P	X		X	X												X	X				
Fertilizers	P		X	X									X						X			
Instant Action Air Fresheners	P	X					X															
Continuous Action Air Fresheners	P	X							X													
Crafting Paint (direct and incidental contact)	P		X	X								X					X	X				
Spray Fixative and Finishing Spray Coatings	P	X					X															
Liquid-based Concrete, Cement, Plaster (prior to hardening)	P	X		X	X												X	X	X			
Anti-freeze Liquids	P	X		X	X												X	X				
De-icing Liquids	P	X		X	X												X	X				
De-icing Solids	P		X										X						X			
Shoe Polish, Shoe wax	P			X													X	X				
Anti-static Spray Fabric Protector	P	X		X			X										X	X				
Textile and Leather Finishing Products (stain remover,	P	X		X			X										X	X				

Product or Article Name	Product or Article?	Relevant Routes of Exposure			Relevant Exposure Models																	
		Inhalation	Ingestion	Dermal	E1	E2	E3	E4	E5	E6	A_INH1	P_ING1	P_ING2	A_ING1	A_ING2	A_ING3	P_DER1a	P_DER1b	P_DER2	A_DER1	A_DER2	A_DER3
waterproofing agent, leather tanning)																						
Textile and Fabric Dyes	P	X		X				X									X	X				
Exterior Car Wax and Polish	P			X													X	X				
Exterior Car Wash and Soaps	P	X		X				X									X	X				
Interior Car Care Cleaning and Maintenance Products	P	X		X			X										X	X				
Touch up Auto Paint	P	X					X															
All-Purpose Spray Cleaner	P	X					X															
All-purpose Liquid Cleaner (note, diluted or not-diluted)	P	X		X	X												X	X				
All-purpose waxes and polishes (furniture, floor,etc)	P	X		X	X												X	X				
Abrasive Powder Cleaners	P			X															X			
Drain and Toilet Cleaners	P	X						X														
Vehicular or Appliance Fuels	P			X													X	X				
Liquid Fuels/Motor Oil	P			X													X	X				
Inks Applied to Skin	P		X	X								X					X	X				
Laundry Detergent (liquid)	P	X						X														
Laundry Detergent (solid/granule)	P	X		X				X											X			
Hand Dishwashing Soap/Liquid Detergent	P	X		X				X									X	X				
Machine Dishwashing Detergent (solid/granule)	P	X		X				X											X			
Machine Dishwashing Detergent (liquid/gel)	P	X						X														
Lubricants (non-spray)	P	X		X	X												X	X				
Lubricants (spray)	P	X		X			X										X	X				

Product or Article Name	Product or Article?	Relevant Routes of Exposure			Relevant Exposure Models																			
		Inhalation	Ingestion	Dermal	E1	E2	E3	E4	E5	E6	A_INH1	P_ING1	P_ING2	A_ING1	A_ING2	A_ING3	P_DER1a	P_DER1b	P_DER2	A_DER1	A_DER2	A_DER3
Degreasers	P	X		X			X										X	X				
Solid Bar Soap (body)	P			X													X	X				
Solid Bar Soap (hands)	P			X													X	X				
Liquid Hand Soap	P			X													X	X				
Bubble Solution	P		X	X								X					X	X				
Liquid Body Soap	P			X													X	X				
Aerosol Spray Paints	P	X		X			X										X	X				
Paint Strippers/Removers	P	X		X		X											X	X				
Varnishes and Floor Finishes	P	X		X		X											X	X				
Lacquers and Stains	P	X		X		X											X	X				
Water-based Wall Paint	P	X		X		X											X	X				
Solvent-based Wall paint	P	X		X		X											X	X				
Adhesive/Caulk Removers	P	X		X		X											X	X				
Paint Thinners	P	X		X		X											X	X				
Powder Based Coatings, Pastels, Crafts	P		X	X								X							X			
Liquid Photographic Processing Solutions	P	X		X		X											X	X				
Drinking Water Treatment Products	P	X	X					X				X										
Electronic Appliances	A	X	X	X						X	X			X	X	X				X	X	X
Drywall	A	X	X	X						X	X			X	X	X				X	X	X
Fabrics: Curtains, Rugs, Wall Coverings	A	X	X	X						X	X			X	X	X				X	X	X
Fabrics: Blanket, Comfort Object, Fabric Doll, Stuffed Animal	A	X	X	X						X	X			X	X	X				X	X	X
Fabrics: Furniture Covers, Car Seat Covers, Tablecloths	A	X	X	X						X	X			X	X	X				X	X	X

Product or Article Name	Product or Article?	Relevant Routes of Exposure			Relevant Exposure Models																			
		Inhalation	Ingestion	Dermal	E1	E2	E3	E4	E5	E6	A_INH1	P_ING1	P_ING2	A_ING1	A_ING2	A_ING3	P_DER1a	P_DER1b	P_DER2	A_DER1	A_DER2	A_DER3
Fabrics: Clothing	A	X	X	X						X	X			X	X	X				X	X	X
Leather Furniture	A	X	X	X						X	X			X	X	X				X	X	X
Leather Clothing	A	X	X	X						X	X			X	X	X				X	X	X
Metal Articles: Jewelry and Other Routine Contact Articles	A	X	X	X						X	X			X	X	X				X	X	X
Paper Articles: With Potential for Routine Contact (diapers, wipes, newspaper, magazine, paper towels)	A	X	X	X						X	X			X	X	X				X	X	X
Rubber Articles: Flooring, Rubber Mats	A	X	X	X						X	X			X	X	X				X	X	X
Rubber Articles: With Potential for Routine Contact (baby bottle nipples, pacifiers, toys)	A	X	X	X						X	X			X	X	X				X	X	X
Wood Articles: Hardwood Floors, Furniture	A	X	X	X						X	X			X	X	X				X	X	X
Wood Articles: With Potential for Routine Contact (toys, pencils)	A	X	X	X						X	X			X	X	X				X	X	X
Plastic Articles: Foam Insulation	A	X	X	X						X	X			X	X	X				X	X	X
Plastic Articles: Vinyl Flooring	A	X	X	X						X	X			X	X	X				X	X	X
Plastic Articles: Objects Intended by Mouthed (pacifiers, teethers, toy food)	A	X	X	X						X	X			X	X	X				X	X	X
Plastic Articles: Other Objects with Potential for Routine Contact (toys, foam blocks, tents)	A	X	X	X						X	X			X	X	X				X	X	X
Plastic Articles: Furniture (sofa, chairs, tables)	A	X	X	X						X	X			X	X	X				X	X	X
Plastic articles: Mattresses	A	X	X	X						X	X			X	X	X				X	X	X

Product or Article Name	Product or Article?	Relevant Routes of Exposure			Relevant Exposure Models																	
		Inhalation	Ingestion	Dermal	E1	E2	E3	E4	E5	E6	A_INH1	P_ING1	P_ING2	A_ING1	A_ING2	A_ING3	P_DER1a	P_DER1b	P_DER2	A_DER1	A_DER2	A_DER3
Generic Article	A	X	X	X						X	X			X	X	X				X	X	X
Generic Product 1	P	X	X	X	X							X					X	X				
Generic Product 2	P	X	X	X		X						X					X	X				
Generic Product 3	P	X	X	X			X					X					X	X				
Generic Product 4	P	X	X	X				X				X					X	X				
Generic Product 5	P	X	X	X					X			X					X	X				
Generic Product in Soil or Powder	P		X	X									X						X			

[a] P = Product, A = Article.

Table B-2. Default Variables for Dermal Exposure to Products

Product	Surface-Area-to-Body-Weight Ratio Type	Density (g/cm^3)[a]	Dilution Fraction (-)	Film Thickness (m)
Glues and Adhesives (small scale)	Inside of One Hand	1		0.00499
Glues and Adhesives (large scale)	Inside of One Hand	1		
Caulk (Sealant)	Inside of One Hand	1		
Fillers and Putties	10% of Hand	1		
Fertilizers	Both Hands	1		
Instant action air fresheners		1		
Continuous action air fresheners		1		
Crafting paint (direct and incidental contact)	Half Body	1		
Spray Fixative and finishing spray coatings	10% of Hand	1		
Liquid-based concrete, cement, plaster (prior to hardening)	Inside of Both Hands	1.59		4.6478E-05
Anti-Freeze liquids	Inside of One Hand	1		
De-icing liquids	Inside of One Hand	1		
De-icing solids	Inside of One Hand	1		
Shoe polish, shoe wax	Inside of One Hand	1		0.0021
Anti-static Spray Fabric Protector	10% of Hand	1		0.00325
Textile and Leather finishing products (stain remover, waterproofing agent, leather tanning)	Both Hands	1		
Textile and Fabric Dyes	Inside of Both Hands	1	0.1	
Exterior Car Wax and Polish	Inside of Both Hands	1.077		0.00325
Exterior Car Wash and Soaps	Inside of Both Hands	1	0.1	
Interior Car Care Cleaning and Maintenance Products	Inside of One Hand	1		
Touch up Auto Paint	10% of Hand	1		
All-Purpose Spray Cleaner	10% of Hand	1		
All-purpose Liquid Cleaner (note, diluted or not-diluted)	Inside of One Hand	1.09		0.00214
All-purpose waxes and polishes (furniture, floor,etc)	Inside of Both Hands	1.017		0.0021
Abrasive powder cleaners	Inside of One Hand	2		

Product	Surface-Area-to-Body-Weight Ratio Type	Density (g/cm^3)[a]	Dilution Fraction (-)	Film Thickness (m)
Drain and Toilet Cleaners	Inside of Both Hands	1		
Vehicular or appliance fuels	Inside of Both Hands	0.75		0.0000364
Liquid Fuels/Motor Oil	Both Hands	0.88		0.0159
Inks Applied to Skin	Face Hands & Arms	1		
Laundry Detergent (liquid)	10% of Hand	1		
Laundry Detergent (solid/granule)	10% of Hand	1		
Hand Dishwashing Soap/Liquid Detergent	Both Hands	1	0.1	0.01
Dishwashing Detergent (solid/granule)	10% of Hand	1		
Dishwashing Detergent (liquid/gel)	10% of Hand	1.077		
Lubricants (non-spray)	Inside of Both Hands	0.9		8.21111E-05
Lubricants (spray)	10% of Hand	1		0.0159
Degreasers	10% of Hand	1		
Solid Bar Soap (body)	Whole Body	1		
Solid Bar Soap (hands)	Both Hands	1		0.0159
Liquid Hand Soap	Both Hands	1	0.1	
Bubble Solution	Inside of Both Hands	1		
Liquid Body Soap	Whole Body	1	0.1	
Aerosol Spray Paints	10% of Hand	0.9		0.00655
Paint Strippers/Removers	Inside of Both Hands	1		0.00188
Varnishes and Floor Finishes	Inside of Both Hands	0.88		
Lacquers and Stains	Inside of Both Hands	1		
Water Based Wall Paint	Face Hands & Arms	1		0.00981
Solvent-based wall paint	Face Hands & Arms	1		0.00981
Adhesive/Caulk Removers	Inside of Both Hands	1		
Paint Thinners	Inside of Both Hands	0.78		0.000035
Powder based coatings, pastels, crafts	Face Hands & Arms	1.2		0.000253833
Liquid photographic processing solutions	Both Hands	1		

[a] default values from various sources.

Table B-3. Default Variables for Products (E1, E2, E4, E5)

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr^{-1})	Frequency Data Source	Chronic years of usage (years/lifetime)
Glues and Adhesives (small scale)	High	30	(Delmaar et al., 2005) (Isaacs et al., 2014)	60	(Isaacs et al., 2014) (U.S. EPA, 1986) (ECETOC, 2012)	73	(Isaacs et al., 2014) (U.S. EPA, 1986) (ECETOC, 2012)	12, 57
	Med	10		20		52		
	Low	5		10		12		
Glues and Adhesives (large scale)	High	5000	(Delmaar et al., 2005) (Isaacs et al., 2014)	240	(ECETOC, 2012) (Isaacs et al., 2014)	14	(Isaacs et al., 2014) (Delmaar et al., 2005) (ECETOC, 2012)	5, 12
	Med	500		120		3		
	Low	100		60		1		
Caulk (Sealant)	High	400	(Isaacs et al., 2014) (Delmaar et al., 2005) (ECETOC, 2012)	240	(Isaacs et al., 2014) (ECETOC, 2012) (Delmaar et al., 2005) (U.S. EPA, 1986)	14	(U.S. EPA, 1986) (Delmaar et al., 2005) (Isaacs et al., 2014)	5, 12
	Med	150		120		3		
	Low	75		60		1		
Fillers and Putties	High	1000	(Isaacs et al., 2014) (Delmaar et al., 2005) (ECETOC, 2012)	240	(Isaacs et al., 2014) (Delmaar et al., 2005) (ECETOC, 2012)	14	(ECETOC, 2012) (U.S. EPA, 1986) (Delmaar et al., 2005)	12, 57
	Med	100		60		3		
	Low	10		20		1		
Fertilizers	High	1500	(U.S. EPA, 2012b) (Better Homes and Gardens, 2015)	150	(Isaacs et al., 2014)	6	(Isaacs et al., 2014)	1, 5, 12, 57
	Med	1000		120		4		
	Low	500		90		2		
Instant action air fresheners	High	10	(AISE) (ECETOC, 2012) (Isaacs et al., 2014)	30	(Isaacs et al., 2014) (ECETOC, 2012) (AISE)	500	(Isaacs et al., 2014) (ECETOC, 2012) (AISE)	12, 57
	Med	8		20		365		
	Med	8		20		365		
Continuous action air fresheners	High	150	(U.S. EPA, 2007) (ECETOC, 2012)	1440	(U.S. EPA, 2007) (ECETOC, 2012) (AISE)	365		57
	Med	100		1440		358		
	Low	50		1440		351		
Spray Fixative and finishing spray coatings	High	40	(Isaacs et al., 2014)	20	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)	12, 57
	Med	20		15		7		
	Low	10		10		2		

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr^{-1})	Frequency Data Source	Chronic years of usage (years/lifetime)
Liquid-based concrete, cement, plaster (prior to hardening)	High	8000		120		3		5, 12
	Med	4000		90		2		
	Low	1000		60		1		
De-icing liquids	High	120	(Isaacs et al., 2014)	10	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)	12, 57
	Med	60		5		12		
	Low	20		2		3		
De-icing solids	High	1100	(Isaacs et al., 2014)	60	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)	1, 5, 12, 57
	Med	1000		30		12		
	Low	900		15		3		
Anti-static Spray Fabric Protector	High	75	Generic Scenario, (U.S. EPA, 2007)	10	(U.S. EPA, 2007) (U.S. EPA, 1986)	14	(U.S. EPA, 1986) (U.S. EPA, 2007) (AISE) (ECETOC, 2012)	12, 57
	Med	25		5		7		
	Low	10		3		2		
Textile and Leather finishing products (stain remover, waterproofing agent, leather tanning)	High	20	(U.S. EPA, 2011)	30		73		12, 57
	Med	10		10		24		
	Low	100		5		150		
Textile and Fabric Dyes	High	100	(Isaacs et al., 2014), Generic Scenario	20	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)	5, 12
	Med	75		10		12		
	Low	50		5		3		
Exterior Car Wax and Polish	High	200	(Isaacs et al., 2014)	45	(Isaacs et al., 2014)	14	(Isaacs et al., 2014) Generic Scenario	
	Med	150		30		12		
	Low	100		15		3		
Exterior Car Wash and Soaps	High	250	(Isaacs et al., 2014)	20	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)	12, 57
	Med	150		10		12		
	Low	50		5		3		
	High	40	Generic Scenario	30	(U.S. EPA, 1986)	5	(U.S. EPA, 1986) (ECETOC, 2012)	12, 57
	Med	10		20		3		

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr^{-1})	Frequency Data Source	Chronic years of usage (years/lifetime)
Interior Car Care Cleaning and Maintenance Products	Low	5		10		1		
Touch up Auto Paint	High	400	(Isaacs et al., 2014)	60	(Isaacs et al., 2014)	5	(Isaacs et al., 2014)	5, 12
	Med	300		45		3		
	Low	200		30		1		
All-Purpose Spray Cleaner	High	60	(Isaacs et al., 2014)	30	(Delmaar et al., 2005) (ACI, 2010) (U.S. EPA, 1986) (Isaacs et al., 2014)	365	(U.S. EPA, 1986) (U.S. EPA, 2011) (ECETOC, 2012) (AISE) (Isaacs et al., 2014)	57
	Med	30		15		300		
	Low	10		5		150		
All-purpose Liquid Cleaner (note, diluted or not-diluted)	High	300	(U.S. EPA, 2007) (ECETOC, 2012) (Delmaar et al., 2005)	30	(Delmaar et al., 2005) (U.S. EPA, 2007) (U.S. EPA, 1986) (U.S. EPA, 2011)	365	(Isaacs et al., 2014) (U.S. EPA, 1986) (U.S. EPA, 2011) (ECETOC, 2012)	57
	Med	1000		30		12		
	Med	200		15		300		
All-purpose waxes and polishes (furniture, floor, etc.)	High	80	(Isaacs et al., 2014)	60	(Delmaar et al., 2005) (U.S. EPA, 1986) (ECETOC, 2012) (U.S. EPA, 2011) (U.S. EPA, 1987)	14	(U.S. EPA, 1986) (Delmaar et al., 2005) (ECETOC, 2012) (Isaacs et al., 2014)	57
	Med	40		5		12		
	Med	50		30		12		
Drain and Toilet Cleaners	High	300	(U.S. EPA, 2011) (Delmaar et al., 2005)	15	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)	12, 57
	Med	60		10		12		
	Low	30		5		3		
Laundry detergent (liquid)	High	400	(Isaacs et al., 2014) (U.S. EPA, 2007) (U.S. EPA, 1986)	20	(Delmaar et al., 2005) (U.S. EPA, 2007) (U.S. EPA, 2011) (U.S. EPA, 1987) (Isaacs et al., 2014)	365	(Delmaar et al., 2005) (U.S. EPA, 2007) (ACI, 2010) (AISE) (U.S. EPA, 1986) (Isaacs et al., 2014)	57
	Med	50		5		3		
	Low	30		3		1		
Laundry detergent (solid/granule)	High	60	(Isaacs et al., 2014) (U.S. EPA, 2007) (U.S. EPA, 1986)	50	(U.S. EPA, 2007; Delmaar et al., 2005) (U.S. EPA, 2011) (U.S. EPA, 1987)	365	(Delmaar et al., 2005) (U.S. EPA, 2007) (ACI, 2010) (AISE) (U.S. EPA, 1986) (Isaacs et al., 2014)	57
	Med	25		5		7		
	Med	40		45		300		
	High	125	(Isaacs et al., 2014)	20	(Isaacs et al., 2014)	365	(Isaacs et al., 2014)	57

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr^{-1})	Frequency Data Source	Chronic years of usage (years/lifetime)
Hand Dishwashing Soap/Liquid Detergent	Med	100		10		300		
	Low	75		5		185		
Dishwashing detergent (solid/granule)	High	20	(Isaacs et al., 2014) (ECETOC, 2012) (U.S. EPA, 2011) (ACI, 2010), Generic Scenario, (Delmaar et al., 2005)	10	(Isaacs et al., 2014)		(Isaacs et al., 2014)	57
	Med	10		5				
	Low	5		3				
Dishwashing Detergent (liquid/gel)	High	40	(Isaacs et al., 2014), (ECETOC, 2012) (U.S. EPA, 2011) (ACI, 2010)	50	(Isaacs et al., 2014)	365	(Isaacs et al., 2014)	57
	Med	10		5		7		
	Med	20		45		300		
Lubricants (non-spray)	High	100		15		5		5, 12
	Med	50		10		3		
	Low	20		5		1		
Lubricants (spray)	High	300	(ECETOC, 2012) (U.S. EPA, 2011)	30	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)	5, 12
	Med	100		20		7		
	Low	50		10		2		
Degreasers	High	200	(U.S. EPA, 2011) (Isaacs et al., 2014)	60	(Isaacs et al., 2014)	52	(Isaacs et al., 2014) (U.S. EPA, 2011) (U.S. EPA, 1987) (ECETOC, 2012)	5, 12
	Med	100		30		14		
	Low	50		15		6		
Aerosol Spray Paints	High	800	(U.S. EPA, 2007), Generic Scenario, (U.S. EPA, 2011) (Delmaar et al., 2005) (Isaacs et al., 2014)	90	(Delmaar et al., 2005; U.S. EPA, 1986); (U.S. EPA, 2007); (U.S. EPA, 2011) /Abt (1992)	14	(U.S. EPA, 2007); (Delmaar et al., 2005) (U.S. EPA, 1986); (U.S. EPA, 2011) (U.S. EPA, 1987) (ECETOC, 2012)	12, 57
	Med	400		45		7		
	Low	200		15		2		
Varnishes and Floor Finishes	High	750	Generic Scenario, (Isaacs et al., 2014)	240	(Isaacs et al., 2014); (U.S. EPA, 2011) (U.S. EPA, 1986)	20	(Isaacs et al., 2014; U.S. EPA, 2011) (U.S. EPA, 1987) (U.S. EPA, 1986); (ECETOC, 2012)	5, 12
	Med	500		180		14		
	Low	250		120		7		
Lacquers and Stains	High	1000		120		20	(U.S. EPA, 1986) (ECETOC, 2012)	5, 12
	Med	500		60		14		

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr^{-1})	Frequency Data Source	Chronic years of usage (years/lifetime)
	Low	250	(U.S. EPA, 2011) Generic Scenario, (Isaacs et al., 2014)	30	(U.S. EPA, 2011, 1986)_ENREF_8 (U.S. EPA, 1987) (Isaacs et al., 2014)	7	(Isaacs et al., 2014)	
Water Based Wall Paint	High	10000	(U.S. EPA, 2007) Generic Scenario, (Delmaar et al., 2005) (ECETOC, 2012; U.S. EPA, 2011); (Isaacs et al., 2014); (ACI, 2010)	540	(Isaacs et al., 2014), (U.S. EPA, 2007); (ECETOC, 2012); (ACI, 2010); (Delmaar et al., 2005) (U.S. EPA, 1986); (U.S. EPA, 2011) (U.S. EPA, 1987)	73	(Isaacs et al., 2014); (ACI, 2010) (Delmaar et al., 2005) (U.S. EPA, 1986); (U.S. EPA, 2011) (U.S. EPA, 1987)	5, 12
	Med	4000		360		52		
	Low	2000		120		12		
Solvent-based wall paint	High	6000	(Isaacs et al., 2014); (ACI, 2010); (U.S. EPA, 2007) Generic Scenario, (Delmaar et al., 2005) (ECETOC, 2012); (U.S. EPA, 2011)	30	(Isaacs et al., 2014), (U.S. EPA, 2007); (ECETOC, 2012); (ACI, 2010); (Delmaar et al., 2005) (U.S. EPA, 1986) (U.S. EPA, 2011)	14	(Isaacs et al., 2014); (ACI, 2010); (Delmaar et al., 2005) (U.S. EPA, 1986); (U.S. EPA, 2011) (U.S. EPA, 1987)	5, 12
	Med	5000		20		7		
	Low	4000		10		2		
Adhesive/Caulk Removers	High	750	(Isaacs et al., 2014)	120	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)	5, 12
	Med	500		90		7		
	Low	100		60		2		
Paint Thinners	High	600		60		14		5, 12
	Med	500		40		7		
	Low	400		20		2		
Liquid photographic processing solutions	High	800	Generic Scenario	480	(U.S. EPA, 1986)	14	(U.S. EPA, 1986) (ECETOC, 2012)	
	Med	700		240		7		
	Low	600		120		2		
Drinking water treatment products	High	20		45		365		57
	Med	10		30		300		
	Low	5		15		185		

Table B-4. Default Variables Relevant to Products (E3) (Data source (Jayjock, 2012))

Product	Level	Aerosol Fraction (unitless)
Instant action air fresheners	High	0.06
	Low	0.01
Spray Fixative and finishing spray coatings	High	0.06
	Low	0.01
De-icing liquids	High	0.06
	Low	0.01
Anti-static Spray Fabric Protector	High	0.05
	Low	0.01
Textile and Leather finishing products (stain remover, waterproofing agent, leather tanning)	High	0.05
	Low	0.01
Interior Car Care Cleaning and Maintenance Products	High	0.05
	Low	0.01
Touch up Auto Paint	High	0.06
	Low	0.01
All-Purpose Spray Cleaner	High	0.05
	Low	0.01
Lubricants (spray)	High	0.06
	Low	0.01
Degreasers	High	0.06
	Low	0.01
Aerosol Spray Paints	High	0.06
	Low	0.01
Paint Strippers/Removers	High	0.06
	Low	0.01
Adhesive/Caulk Removers	High	0.06
	Low	0.01

Table B-5. Default Variables Relevant to Articles

Articles	Default Use Environment	Surface-Area-to-Body-Weight Ratio Type	Surface Area of Article (m^2)	Density of Article (g/cm^3)	Duration of article contact (hr)[c]
Electronic appliances	Residence - Kitchen	Inside of Both Hands	1.62	1	
Drywall	Residence - Garage	Inside of Both Hands	61	1	
Fabrics: Curtains, Rugs, Wall coverings	Residence - Bedroom	Inside of Both Hands	1.6025	1	
Fabrics: Blanket, comfort object, fabric doll, stuffed animal	Residence - Bedroom	Inside of Both Hands	0.278	1	
Fabrics: furniture covers, car seat covers, tablecloths	Residence - Living room	Half Body	3	1	
Fabrics: Clothing	Residence - Bedroom	Whole Body	1.1789	1	16
Leather furniture	Residence - Living room	Half Body	3	1	0.5
Leather clothing	Residence - Utility room	Inside of Both Hands	0.03	1	8
Metal articles: jewelry and other routine contact articles	Residence - Bedroom	10% of Hand	0.091	1	
Paper articles: with potential for routine contact (diapers, wipes, newspaper, magazine, paper towels)	Residence - Bathroom	Both hands	0.0929	1	
Rubber articles: flooring, rubber mats	Residence - Kitchen	Half Body	27.87	1	0.5
Rubber articles: with potential for routine contact (baby bottle nipples, pacifiers, toys)	Residence - Kitchen	Inside of Both Hands	0.005	1	
Wood articles: hardwood floors, furniture	Residence - Living room	Half Body	27.87	1	0.5
Wood articles: with potential for routine contact (toys, pencils)	Residence - Living room	Inside of Both Hands	0.005	1	
Plastic articles: Foam Insulation	Residence - Living room	Inside of One Hand	100	1	
Plastic articles: Vinyl Flooring	Residence - Kitchen	Half Body	27.87	1	0.5
Plastic articles: Objects intended by mouthed (pacifiers, teethers, toy food)	Residence - Kitchen	Inside of Both Hands	0.005	1	
Plastic articles: Other objects with potential for routine contact (toys, foam blocks, tents)	Residence - Kitchen	Face Hands & Arms	1	1	0.08
Plastic articles: Furniture (sofa, chairs, tables)	Residence - Living room	Half Body	3	1	0.5
Plastic articles: Mattresses	Residence - Living room	Whole Body	4	1	8

[a] (ECETOC, 2012)
[b] Isaacs et al. (2014)
[c] Delmaar et al. 2003

Table B-6. Chemical inputs Relevant to All Articles

Level	Area of Article Mouthed (cm^2)	Thickness of Article Surface Layer (m)	Thickness of Interior Surface (m)
High	22.5	0.01	0.005
Medium	10		
Low	1		

Table B-7. Migration Rates of Chemicals in Various Articles

EPA has compiled available measured data on migration rates into saliva from twenty-six studies. Most of the available data are for phthalates and plastic materials. The migration rate into saliva appears to have a relationship with chemical concentration in the material. EPA is considering additional available approaches to estimate the migration rate into salvia. Additional measured data and/or refined estimation approaches are of interest for this model parameter.

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate $ug/cm^2/hr$	Reference
Decabromodiphenyl oxide (DBDPO)	1163195	Textile	65,000.00	6.20E-01	Babich et al . 2001
Antimony trioxide (AT)	1309644	Textile	23,000.00	1.20E+00	Babich et al . 2001
Hexabromocyclododecane (HBCD)	25637994	Textile	92,000.00	1.30E+01	Babich et al . 2001
PA	21020336	Textile	93,000.00	8.50E+01	Babich et al . 2001
DINP	28553120	Bath toy 2-12	151,000.00	9.10E-02	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy book 2-11	175,000.00	1.27E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Soother 2-8	302,000.00	1.36E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Teether 2-9	256,000.00	1.45E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy car 3-5	427,000.00	2.18E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy book 1-2	275,000.00	2.25E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Teether 1-7	300,000.00	2.64E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy 3-3	271,000.00	2.64E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Squeeze toy 3-6	525,000.00	2.64E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Teether 2-10	193,000.00	2.73E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy bear 2-13	199,000.00	3.00E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy duck 2-1	408,000.00	3.27E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy turtle 2-13	354,000.00	3.36E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Teether 2-3	503,000.00	3.55E-01	Babich et al 1998, Danish EPA 2016

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm²/hr	Reference
DINP	28553120	Toy bear 3-2	412,000.00	4.09E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Teether 1-9	335,000.00	4.36E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Spoon 2-15	352,000.00	4.36E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Teether 1-10	544,000.00	4.45E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy block 3-4	430,000.00	5.00E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Ball 3-1	412,000.00	5.36E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Teether 1-8	433,000.00	5.82E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy fish 2-4	370,000.00	5.91E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Spoons 2-16	343,000.00	8.27E-01	Babich et al 1998, Danish EPA 2016
DINP	28553120	Teether 1-3	366,000.00	1.03E+00	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy tiger 1-5	481,000.00	1.05E+00	Babich et al 1998, Danish EPA 2016
DINP	28553120	Squeeze toy 2-7	326,000.00	1.21E+00	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy treehouse 2-5	361,000.00	1.26E+00	Babich et al 1998, Danish EPA 2016
DINP	28553120	Corner pads 1-11	440,000.00	1.38E+00	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy food 1-14	510,000.00	1.96E+00	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy Dolphin 1-6	437,000.00	2.70E+00	Babich et al 1998, Danish EPA 2016
DINP	28553120	Toy duck 2-2	427,000.00	4.40E+00	Babich et al 1998, Danish EPA 2016
THPC	124641	Textile	130,000.00	3.00E+01	Babich et al 2001
octyl tetrabromobenzoate (OTB)	4825869	Furniture foam	68,000.00	7.50E-03	Babich et al 2006
phenol isopropylated phosphate (PIP)	68937417	Furniture foam	68,000.00	7.50E-03	Babich et al 2006
triphenyl phosphate (TPP)	1145866	Furniture foam	68,000.00	7.50E-03	Babich et al 2006
tris(1,3-dichloro-2-propyl)phosphate (TDCP)	13674878	Furniture foam	51,000.00	2.50E-02	Babich et al 2006
DINP	28553120	Toys on keychains: plastics	416,000.00	5.76E+00	Bouma et al 2001
DINP	28553120	Toys on keychains: plastics	416,000.00	1.09E+01	Bouma et al 2001
DINP	28553120	Toys on keychains: plastics	416,000.00	1.48E+01	Bouma et al 2001
DINP	28553120	Rucksack: textile	230,000.00	1.50E+00	Bouma et al 2002, Danish EPA 2016
DEHP	117817	Doll 3	30,000.00	1.86E+00	Bouma et al 2002, Danish EPA 2016

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm^2/hr	Reference
DEHP	117817	Apron: textiles	70,000.00	3.48E+00	Bouma et al 2002, Danish EPA 2016
DEHP	117817	Can	340,000.00	3.78E+00	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Animal figure 2	270,000.00	4.20E+00	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Key ring figure 2	390,000.00	4.50E+00	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Rucksack: textile	270,000.00	4.68E+00	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Animal figure 1	160,000.00	5.52E+00	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Swimming tool 1	310,000.00	6.12E+00	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Inflatable cushion	340,000.00	7.08E+00	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Inflatable cushion	310,000.00	7.20E+00	Bouma et al 2002, Danish EPA 2016
DEHP	117817	Inflatable furniture	370,000.00	7.38E+00	Bouma et al 2002, Danish EPA 2016
DEHP	117817	Swimming tool 4	370,000.00	7.86E+00	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Inflatable ball	300,000.00	8.34E+00	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Doll 13	450,000.00	9.54E+00	Bouma et al 2002, Danish EPA 2016
DEHP	117817	Inflatable furniture	410,000.00	9.84E+00	Bouma et al 2002, Danish EPA 2016
DEHP	117817	Swimming tool 2	330,000.00	9.84E+00	Bouma et al 2002, Danish EPA 2016
DEHP	117817	Swimming tool 3	360,000.00	1.05E+01	Bouma et al 2002, Danish EPA 2016
DEHP	117817	Ball 1	340,000.00	1.06E+01	Bouma et al 2002, Danish EPA 2016
DEHP	117817	Swimming tool 5	370,000.00	1.09E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Teething ring	450,000.00	1.11E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Doll 1	290,000.00	1.13E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	standard disk	390,000.00	1.18E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Key ring figure 4	450,000.00	1.22E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Doll 2	300,000.00	1.27E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Animal figure 4	340,000.00	1.31E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Doll 3	320,000.00	1.33E+01	Bouma et al 2002, Danish EPA 2016
DEHP	117817	Doll 15	440,000.00	1.36E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Doll 15	480,000.00	1.36E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Animal figure 3	280,000.00	1.39E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Key ring figure 3	440,000.00	1.43E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Doll 7	370,000.00	1.54E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Bath toy 2	360,000.00	1.56E+01	Bouma et al 2002, Danish EPA 2016

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm^2/hr	Reference
DINP	28553120	Doll 9	380,000.00	1.60E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Doll 12	430,000.00	1.63E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Doll 6	370,000.00	1.69E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Doll 5	370,000.00	1.73E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Doll 14	450,000.00	1.73E+01	Bouma et al 2002, Danish EPA 2016
DEHP	117817	Doll 8	380,000.00	1.76E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Doll 4	330,000.00	1.85E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Doll 11	420,000.00	1.97E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Bath toy 3	400,000.00	2.08E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Ball 2	350,000.00	2.21E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Bath toy 4	420,000.00	2.70E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Bath toy 1	330,000.00	2.91E+01	Bouma et al 2002, Danish EPA 2016
DEHP	117817	Doll 10	390,000.00	3.13E+01	Bouma et al 2002, Danish EPA 2016
DINP	28553120	Rucksack: textile	250,000.00	1.50E+00	Bouma, K., & Schakel, D. J. (2002).
DEHP	117817	Apron: textiles	70,000.00	3.48E+00	Bouma, K., & Schakel, D. J. (2002).
DINP	28553120	Animal figure: plastics	262,500.00	4.20E+00	Bouma, K., & Schakel, D. J. (2002).
DINP	28553120	Key ring figure: plastic	410,000.00	4.50E+00	Bouma, K., & Schakel, D. J. (2002).
DINP	28553120	Rucksack: textile	250,000.00	4.68E+00	Bouma, K., & Schakel, D. J. (2002).
DINP	28553120	Animal figure: plastics	262,500.00	9.18E+00	Bouma, K., & Schakel, D. J. (2002).
DINP	28553120	Key ring figure: plastic	410,000.00	1.00E+01	Bouma, K., & Schakel, D. J. (2002).
DINP	28553120	Animal figure: plastics	262,500.00	1.39E+01	Bouma, K., & Schakel, D. J. (2002).
DINP	28553120	Key ring figure: plastic	410,000.00	1.43E+01	Bouma, K., & Schakel, D. J. (2002).
Irgafos 168	31570044	Polypropylene container: plastic food contact	175.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irgafos 168	31570044	Polypropylene container: plastic food contact	200.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1010	6683198	Polypropylene container: plastic food contact	415.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm^2/hr	Reference
Irganox 1010	6683198	Polypropylene container: plastic food contact	390.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1076	2082793	Polypropylene container: plastic food contact	17.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1076	2082793	Polypropylene container: plastic food contact	16.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irgafos 168	31570044	Polypropylene container: plastic food contact	175.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irgafos 168	31570044	Polypropylene container: plastic food contact	200.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irgafos 168	31570044	Polypropylene container: plastic food contact	175.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irgafos 168	31570044	Polypropylene container: plastic food contact	200.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1010	6683198	Polypropylene container: plastic food contact	415.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1010	6683198	Polypropylene container: plastic food contact	390.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1010	6683198	Polypropylene container: plastic food contact	415.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1010	6683198	Polypropylene container: plastic food contact	390.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm²/hr	Reference
Irganox 1076	2082793	Polypropylene container: plastic food contact	17.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1076	2082793	Polypropylene container: plastic food contact	16.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1076	2082793	Polypropylene container: plastic food contact	17.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1076	2082793	Polypropylene container: plastic food contact	16.00	2.08E-05	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irgafos 168	31570044	Polypropylene container: plastic food contact	175.00	1.04E-04	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irgafos 168	31570044	Polypropylene container: plastic food contact	200.00	1.04E-04	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1010	6683198	Polypropylene container: plastic food contact	415.00	2.08E-03	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1010	6683198	Polypropylene container: plastic food contact	390.00	2.71E-03	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1076	2082793	Polypropylene container: plastic food contact	17.00	2.71E-03	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
Irganox 1076	2082793	Polypropylene container: plastic food contact	16.00	2.92E-03	Castle, L., Mercer, A. J., & Gilbert, J. (1995)
BDE99	60348609	Hard plastic toy	0.06	6.60E-05	Chen et al 2009
BDE47	5436431	Hard plastic toy	0.20	7.92E-05	Chen et al 2009
BDE153	68631492	Hard plastic toy	1.08	1.11E-04	Chen et al 2009

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm^2/hr	Reference
BDE28	41318756	Hard plastic toy	0.01	1.34E-04	Chen et al 2009
BDE66	189084615	Hard plastic toy	0.02	1.34E-04	Chen et al 2009
BDE100	189084648	Hard plastic toy	0.01	1.52E-04	Chen et al 2009
BDE138	182677301	Hard plastic toy	4.56	2.06E-04	Chen et al 2009
BDE154	207122154	Hard plastic toy	0.12	4.88E-04	Chen et al 2009
BDE196	No data	Hard plastic toy	2.72	8.38E-04	Chen et al 2009
BDE197	119264594	Hard plastic toy	2.39	8.39E-04	Chen et al 2009
BDE203	337513721	Hard plastic toy	2.31	8.48E-04	Chen et al 2009
1,2-bis(2,4,6-tribromophenoxy)ethane	37853591	Hard plastic toy	6.84	1.03E-03	Chen et al 2009
BDE183	207122165	Hard plastic toy	15.91	1.30E-03	Chen et al 2009
BDE208	63936561	Hard plastic toy	2.13	1.61E-03	Chen et al 2009
BDE206	63387280	Hard plastic toy	9.17	2.43E-03	Chen et al 2009
BDE207	437701796	Hard plastic toy	16.60	2.76E-03	Chen et al 2009
Decabromodiphenyl ethane	84852539	Hard plastic toy	15.61	9.23E-03	Chen et al 2009
BDE209	1163195	Hard plastic toy	201.99	4.37E-02	Chen et al 2009
DEHP	117817	Plasticized polyvinyl chloride	600,000.00	3.60E-01	Corea-Tellez, K. S., Bustamante-Montes, P., Garcia-Fabila, M., Hernández-Valero, M. A., & Vazquez-Moreno, F. (2008)
DEHP	117817	Plasticized polyvinyl chloride	600,000.00	4.10E+00	Corea-Tellez, K. S., Bustamante-Montes, P., Garcia-Fabila, M., Hernández-Valero, M. A., & Vazquez-Moreno, F. (2008)
DEHP	117817	Plasticized polyvinyl chloride	600,000.00	6.04E+00	Corea-Tellez, K. S., Bustamante-Montes, P., Garcia-Fabila, M., Hernández-Valero, M. A., & Vazquez-Moreno, F. (2008)
DINP	28553120	PVC	385,000.00	1.43E+00	Earls, A. O., Axford, I. P., & Braybrook, J. H. (2003).
Disperse Yellow 3	2832408	Fabric, textile	480.00	2.50E-03	ETAD 1997. Manufacturers (ETAD) project G1033.

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm²/hr	Reference
Disperse Yellow 3	2832408	Fabric, textile	480.00	2.50E-03	ETAD 1997. Manufacturers (ETAD) project G1033.
Disperse Blue 3	2475469	Fabric, textile	400.00	6.00E-03	ETAD 1997. Manufacturers (ETAD) project G1033.
Disperse Blue 3	2475469	Fabric, textile	400.00	9.00E-03	ETAD 1997. Manufacturers (ETAD) project G1033.
Disperse Yellow 3	2832408	Fabric, textile	2,900.00	2.60E-02	ETAD 1997. Manufacturers (ETAD) project G1033.
Disperse Yellow 3	2832408	Fabric, textile	2,900.00	2.70E-02	ETAD 1997. Manufacturers (ETAD) project G1033.
Disperse Blue 3	2475469	Fabric, textile	2,400.00	3.00E-02	ETAD 1997. Manufacturers (ETAD) project G1033.
Disperse Blue 3	2475469	Fabric, textile	2,400.00	6.70E-02	ETAD 1997. Manufacturers (ETAD) project G1033.
Tris(2-chloro-1-methylethyl) phosphate	13674845	Polyurethane foam	100,000.00	2.78E+00	EU RAR. 2008b.
Tris(2-chloro-1-methylethyl) phosphate	13674845	Polyurethane foam	100,000.00	4.60E+00	EU RAR. 2008b.
Tris(2-chloro-1-methylethyl) phosphate	13674845	Polyurethane foam	100,000.00	1.30E+02	EU RAR. 2008b.
DEHP	117817	PVC Plate E	320,000.00	1.40E-01	Fiala et al 2000, Danish EPA 2016
DEHP	117817	PVC Plate F	320,000.00	3.70E-01	Fiala et al 2000, Danish EPA 2016
DEHP	117817	PVC Plate I	320,000.00	1.02E+00	Fiala et al 2000, Danish EPA 2016
DEHP	117817	PVC Plate G	320,000.00	1.06E+00	Fiala et al 2000, Danish EPA 2016
DEHP	117817	PVC Plate H	320,000.00	1.28E+00	Fiala et al 2000, Danish EPA 2016
DEHP	117817	PVC Plate J	320,000.00	2.64E+00	Fiala et al 2000, Danish EPA 2016
DINP	28553120	Yellow teether	360,000.00	8.33E+00	Fiala et al 2000, Danish EPA 2016
DINP	28553120	Yellow teether	360,000.00	1.33E+01	Fiala et al 2000, Danish EPA 2016
TCPP	13674845	Foam	65,000.00	1.59E+00	Ghanem 2015(a)
TCPP	13674845	Foam	65,000.00	2.17E+00	Ghanem 2015(a)
TCPP	13674845	Foam	65,000.00	2.74E+00	Ghanem 2015(a)
TCPP	13674845	Foam	65,000.00	3.03E+00	Ghanem 2015(a)
TCPP	13674845	Foam	65,000.00	3.03E+00	Ghanem 2015(a)
TCPP	13674845	Foam	65,000.00	3.61E+00	Ghanem 2015(a)
TCPP	13674845	Foam	65,000.00	3.90E+00	Ghanem 2015(a)

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm^2/hr	Reference
TCPP	13674845	Foam	65,000.00	4.19E+00	Ghanem 2015(a)
TCPP	13674845	Foam	65,000.00	4.48E+00	Ghanem 2015(a)
TCPP	13674845	Foam	65,000.00	6.79E+00	Ghanem 2015(a)
TCPP	13674845	Foam	65,000.00	7.08E+00	Ghanem 2015(a)
TCPP	13674845	Foam	52,000.00	8.67E+00	Ghanem 2015(a)
TCPP	13674845	Foam	52,000.00	9.24E+00	Ghanem 2015(a)
TCPP	13674845	Foam	52,000.00	9.24E+00	Ghanem 2015(a)
TCPP	13674845	Foam	65,000.00	1.07E+01	Ghanem 2015(a)
TCPP	13674845	Foam	85,000.00	1.32E+01	Ghanem 2015(a)
TCPP	13674845	Foam	52,000.00	1.39E+01	Ghanem 2015(a)
TCPP	13674845	Foam	85,000.00	2.36E+01	Ghanem 2015(a)
TCPP	13674845	Foam	85,000.00	2.46E+01	Ghanem 2015(a)
TCPP	13674845	Foam	85,000.00	3.12E+01	Ghanem 2015(a)
TCPP	13674845	Foam	52,000.00	3.47E+01	Ghanem 2015(a)
TCPP	13674845	Foam	52,000.00	3.81E+01	Ghanem 2015(a)
TCPP	13674845	Foam	52,000.00	3.93E+01	Ghanem 2015(a)
TCPP	13674845	Foam	52,000.00	4.51E+01	Ghanem 2015(a)
TCPP	13674845	Foam	52,000.00	4.62E+01	Ghanem 2015(a)
TCPP	13674845	Foam	52,000.00	4.62E+01	Ghanem 2015(a)
TCPP	13674845	Foam	85,000.00	4.91E+01	Ghanem 2015(a)
TCPP	13674845	Foam	85,000.00	5.10E+01	Ghanem 2015(a)
TCPP	13674845	Foam	52,000.00	5.43E+01	Ghanem 2015(a)
TCPP	13674845	Foam	85,000.00	5.86E+01	Ghanem 2015(a)
TCPP	13674845	Foam	85,000.00	6.23E+01	Ghanem 2015(a)
TCPP	13674845	Foam	85,000.00	6.61E+01	Ghanem 2015(a)
TCPP	13674845	Foam	52,000.00	7.05E+01	Ghanem 2015(a)
TCPP	13674845	Foam	85,000.00	7.18E+01	Ghanem 2015(a)
TCPP	13674845	Foam	85,000.00	7.18E+01	Ghanem 2015(a)
TCPP	13674845	Foam	85,000.00	9.16E+01	Ghanem 2015(a)
ATO-DBE 209	mixture	Textiles	43,000.00	4.33E-02	Ghanem 2015(b)
ATO-DBE 209	mixture	Textiles	43,000.00	4.98E-02	Ghanem 2015(b)

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm²/hr	Reference
ATO-DBE 209	mixture	Textiles	43,000.00	5.22E-02	Ghanem 2015(b)
ATO-HBCD	mixture	Textiles	36,000.00	5.44E-02	Ghanem 2015(b)
ATO-HBCD	mixture	Textiles	36,000.00	5.44E-02	Ghanem 2015(b)
ATO-HBCD	mixture	Textiles	36,000.00	5.71E-02	Ghanem 2015(b)
ATO-DBE 209	mixture	Textiles	43,000.00	5.78E-02	Ghanem 2015(b)
ATO-DBE 209	mixture	Textiles	43,000.00	5.86E-02	Ghanem 2015(b)
ATO-DBE 209	mixture	Textiles	43,000.00	6.02E-02	Ghanem 2015(b)
ATO-HBCD	mixture	Textiles	36,000.00	6.05E-02	Ghanem 2015(b)
ATO-HBCD	mixture	Textiles	36,000.00	6.12E-02	Ghanem 2015(b)
ATO-DBE 209	mixture	Textiles	43,000.00	6.90E-02	Ghanem 2015(b)
ATO-DBE 209	mixture	Textiles	43,000.00	7.14E-02	Ghanem 2015(b)
ATO-HBCD	mixture	Textiles	36,000.00	7.26E-02	Ghanem 2015(b)
ATO-HBCD	mixture	Textiles	36,000.00	7.39E-02	Ghanem 2015(b)
ATO-HBCD	mixture	Textiles	36,000.00	8.06E-02	Ghanem 2015(b)
ATO-HBCD	mixture	Textiles	36,000.00	8.06E-02	Ghanem 2015(b)
ATO-HBCD	mixture	Textiles	36,000.00	8.40E-02	Ghanem 2015(b)
ATO-DBE 209	mixture	Textiles	43,000.00	9.15E-02	Ghanem 2015(b)
ATO-DBE 209	mixture	Textiles	43,000.00	9.87E-02	Ghanem 2015(b)
ATO-HBCD	mixture	Textiles	36,000.00	1.11E-01	Ghanem 2015(b)
ATO-HBCD	mixture	Textiles	36,000.00	1.24E-01	Ghanem 2015(b)
ATO-DBE 209	mixture	Textiles	43,000.00	1.30E-01	Ghanem 2015(b)
ATO-DBE 209	mixture	Textiles	43,000.00	1.40E-01	Ghanem 2015(b)
BDE 99	60348609	Toy car (hard plastic)	0.05	5.00E-06	Ionas 2016
BDE 183	207122165	Toy car (hard plastic)	0.05	5.00E-06	Ionas 2016
BDE 183	207122165	Toy figurine (softer plastic)	0.26	1.00E-05	Ionas 2016
BDE 153	68631492	Toy car (hard plastic)	0.04	3.00E-05	Ionas 2016
BDE 209	1163195	Toy car (hard plastic)	19.10	5.00E-05	Ionas 2016
BDE 28	41318756	EC-591	2.50	5.00E-05	Ionas 2016
BDE 66	189084615	EC-591	4.60	6.50E-05	Ionas 2016
BDE 28	41318756	EC-591	2.50	8.00E-05	Ionas 2016

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm^2/hr	Reference
BDE 66	189084615	EC-591	4.60	8.00E-05	Ionas 2016
BDE 154	207122154	EC-591	26.00	8.00E-05	Ionas 2016
BDE 154	207122154	EC-591	26.00	9.00E-05	Ionas 2016
BDE 85	182346210	EC-591	19.10	1.40E-04	Ionas 2016
BDE 85	182346210	EC-591	19.10	1.60E-04	Ionas 2016
BDE 209	1163195	Toy car (hard plastic)	19.10	2.00E-04	Ionas 2016
BDE 153	68631492	EC-591	44.00	2.20E-04	Ionas 2016
BDE 153	68631492	EC-591	44.00	2.20E-04	Ionas 2016
BDE 183	207122165	EC-591	87.00	3.70E-04	Ionas 2016
BDE 100	189084648	EC-591	66.00	4.00E-04	Ionas 2016
BDE 209	1163195	Toy figurine (softer plastic)	14.50	4.10E-04	Ionas 2016
BDE 100	189084648	EC-591	66.00	4.10E-04	Ionas 2016
BDE 183	207122165	EC-591	87.00	4.80E-04	Ionas 2016
BDE 99	60348609	EC-591	320.00	1.88E-03	Ionas 2016
BDE 99	60348609	EC-591	320.00	2.00E-03	Ionas 2016
BDE 47	5436431	EC-591	245.00	2.50E-03	Ionas 2016
BDE 209	1163195	EC-591	780.00	2.70E-03	Ionas 2016
BDE 47	5436431	EC-591	245.00	2.84E-03	Ionas 2016
BDE 209	1163195	EC-591	780.00	4.80E-03	Ionas 2016
BDE 209	1163195	TV casing	7,000.00	1.52E-01	Ionas 2016
BDE 209	1163195	TV casing	7,000.00	1.86E-01	Ionas 2016
DBP	84742	Toy ball A	100,000.00	1.17E+00	Niino et al 2001, Danish EPA 2016
DBP	84742	Toy ball A	100,000.00	3.39E+00	Niino et al 2001, Danish EPA 2016
DINP	28553120	PVC: soft doll	160,000.00	3.80E+00	Niino et al 2002
DINP	28553120	PVC: ball	255,000.00	7.80E+00	Niino et al 2002
DINP	28553120	PVC: teether	389,000.00	1.25E+01	Niino et al 2002
DINP	28553120	PVC: pacifier	583,000.00	2.00E+01	Niino et al 2002
DINP	28553120	PVC: rattle	380,000.00	2.19E+01	Niino et al 2002
DINP	28553120	PVC: plate	462,000.00	3.26E+01	Niino et al 2002
DINP	28553120	Toy ball B	255,000.00	7.80E+00	Niino et al 2002, Danish EPA 2016

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm²/hr	Reference
DBP	84742	Ball A	100,000.00	1.20E+00	Niino et al 2003, Danish EPA 2016
DEHP	117817	Ball A	370,000.00	4.40E+00	Niino et al 2003, Danish EPA 2016
DEHP	117817	Plate F	132,000.00	6.40E+00	Niino et al 2003, Danish EPA 2016
DINP	28553120	Ball C	256,000.00	7.80E+00	Niino et al 2003, Danish EPA 2016
DINP	28553120	Plate E	141,000.00	8.00E+00	Niino et al 2003, Danish EPA 2016
DINP	28553120	Teether	389,000.00	1.28E+01	Niino et al 2003, Danish EPA 2016
DINP	28553120	Pacifier	583,000.00	2.00E+01	Niino et al 2003, Danish EPA 2016
DINP	28553120	Rattle: plastic	380,000.00	2.24E+01	Niino et al 2003, Danish EPA 2016
DINP	28553120	Soft doll A	160,000.00	2.96E+01	Niino et al 2003, Danish EPA 2016
DINP	28553120	Plate A	462,000.00	3.24E+01	Niino et al 2003, Danish EPA 2016
DINP	28553120	Ball C	256,000.00	3.36E+01	Niino et al 2003, Danish EPA 2016
DBP	84742	Plate D	135,000.00	3.48E+01	Niino et al 2003, Danish EPA 2016
DBP	84742	Plate G	129,000.00	3.48E+01	Niino et al 2003, Danish EPA 2016
DINP	28553120	Plate D	144,000.00	4.28E+01	Niino et al 2003, Danish EPA 2016
DEHP	117817	Plate D	147,000.00	4.56E+01	Niino et al 2003, Danish EPA 2016
DINP	28553120	Toy food: plastic	311,000.00	4.60E+01	Niino et al 2003, Danish EPA 2016
DINP	28553120	Teether	389,000.00	5.16E+01	Niino et al 2003, Danish EPA 2016
DEHP	117817	Soft Doll	311,000.00	5.28E+01	Niino et al 2003, Danish EPA 2016
DBP	84742	Ball A	100,000.00	5.80E+01	Niino et al 2003, Danish EPA 2016
DEHP	117817	Ball A	185,000.00	6.96E+01	Niino et al 2003, Danish EPA 2016
DINP	28553120	Pacifier	583,000.00	7.32E+01	Niino et al 2003, Danish EPA 2016
DBP	84742	Ball B	220,000.00	7.92E+01	Niino et al 2003, Danish EPA 2016
DINP	28553120	Rattle: plastic	380,000.00	8.36E+01	Niino et al 2003, Danish EPA 2016
DINP	28553120	soft doll B	290,000.00	8.36E+01	Niino et al 2003, Danish EPA 2016
DEHP	117817	Ball B	320,000.00	8.52E+01	Niino et al 2003, Danish EPA 2016
DEHP	117817	Plate B	477,000.00	1.18E+02	Niino et al 2003, Danish EPA 2016
DINP	28553120	Plate A	462,000.00	1.25E+02	Niino et al 2003, Danish EPA 2016
DBP	84742	Plate C	471,000.00	1.45E+02	Niino et al 2003, Danish EPA 2016
DINP	28553120	Rattle: plastic	380,000.00	2.24E+01	Niino T, Asakura T, Ishibashi T, Itho T, Sakai S, Ishiwata H, Yamada T, Onodera S, 2003.

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm²/hr	Reference
DINP	28553120	Toy food: plastic	311,000.00	4.60E+01	Niino T, Asakura T, Ishibashi T, Itho T, Sakai S, Ishiwata H, Yamada T, Onodera S, 2003.
DINP	28553120	Rattle: plastic	380,000.00	8.52E+01	Niino T, Asakura T, Ishibashi T, Itho T, Sakai S, Ishiwata H, Yamada T, Onodera S, 2003.
DEHP	117817	Plastic toy	5,100.00	1.00E-04	Ozer et al 2011
DEHP	117817	Plastic toy	379,000.00	1.78E+00	Ozer et al 2011
DEHP	117817	Plastic toy	339,000.00	1.83E+00	Ozer et al 2011
DEHP	117817	Plastic toy	278,000.00	2.60E+01	Ozer et al 2011
DINP	28553120	Plastic toy	380,000.00	8.28E+01	RIVM 1998
DINP	28553120	Plastic toy	380,000.00	9.80E+01	RIVM 1998
DINP	28553120	Plastic toy	430,000.00	1.46E+02	RIVM 1998
DINP	28553120	PVC disk	159,000.00	9.31E-01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DINP/DBP	Mixture	PVC disk	117,000.00	1.24E+00	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DINP/DBP	Mixture	PVC disk	42,000.00	1.24E+00	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DIDP	26761400	PVC disk	242,000.00	6.51E+00	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DINP	28553120	PVC disk	260,000.00	7.45E+00	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm²/hr	Reference
DINP/DBP	Mixture	PVC disk	199,000.00	7.76E+00	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DEHP	117817	PVC disk	256,000.00	8.69E+00	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DINP/DBP	Mixture	PVC disk	49,000.00	9.00E+00	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
BBP	85687	PVC disk	230,000.00	9.62E+00	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DIDP	26761400	PVC disk	387,000.00	1.40E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DINP/DBP	Mixture	PVC disk	322,000.00	1.64E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DINP/DBP	Mixture	PVC disk	85,000.00	1.71E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DIDP	26761400	PVC disk	526,000.00	1.80E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DEHP	117817	PVC disk	400,000.00	1.86E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm^2/hr	Reference
					math surface area of disk diamter 2.3 cm, Table 4
DEHP	117817	PVC disk	394,000.00	1.89E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
BBP	85687	PVC disk	344,000.00	2.26E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DINP/DBP	Mixture	PVC disk	93,000.00	2.54E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DINP/DBP	Mixture	PVC disk	365,000.00	2.61E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DINP	28553120	PVC disk	392,000.00	2.67E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DEHP	117817	PVC disk	508,000.00	2.73E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DINP	28553120	PVC disk	470,000.00	3.04E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
BBP	85687	PVC disk	455,000.00	3.04E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm²/hr	Reference
DBP	84742	PVC disk	206,000.00	5.24E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
BBP	85687	PVC disk	426,000.00	5.62E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DBP	84742	PVC disk	368,000.00	6.92E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DBP	84742	PVC disk	366,000.00	8.25E+01	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DBP	84742	PVC disk	411,000.00	1.46E+02	Simoneau C, Hannaert P and Sarigiannis D (editor) (2009). Check math surface area of disk diamter 2.3 cm, Table 4
DINP	28553120	PVC toy disk	405,000.00	5.34E+01	The Danish Veterinary and Food Administration, 2003. Human exposure to selected phthalates in Denmark. Institute of Food Safety Nutrition.
DINP	28553120	Baby book: textile	93,500.00	2.70E-01	TNO Nutrition and Food Research, 2001.
DEHP	117817	Bumper sheet: textile	85,000.00	7.20E-01	TNO Nutrition and Food Research, 2001.
DEHP	117817	Baby book: textile	85,900.00	1.74E+00	TNO Nutrition and Food Research, 2001.
DINP	28553120	Baby book: textile	93,500.00	1.80E+00	TNO Nutrition and Food Research, 2001.

Chemical Name	CAS	Material Type	Concentration of chemical in Material (ppm)	Migration Rate ug/cm²/hr	Reference
DINP	28553120	Baby book: textile	93,500.00	2.10E+00	TNO Nutrition and Food Research, 2001.
DEHP	117817	Baby book: textile	85,900.00	3.30E+00	TNO Nutrition and Food Research, 2001.
DEHP	117817	Baby book: textile	85,900.00	4.14E+00	TNO Nutrition and Food Research, 2001.
DEHP	117817	Backpack: textile	31,900.00	8.76E+00	TNO Nutrition and Food Research, 2001.
DEHP	117817	Backpack: textile	31,900.00	1.13E+01	TNO Nutrition and Food Research, 2001.
DEHP	117817	Backpack: textile	31,900.00	1.70E+01	TNO Nutrition and Food Research, 2001.
DINP	28553120	Bumper sheet: textile	351,500.00	2.20E+01	TNO Nutrition and Food Research, 2001.
DINP	28553120	Bumper sheet: textile	351,500.00	2.56E+01	TNO Nutrition and Food Research, 2001.
DINP	28553120	Bumper sheet: textile	351,500.00	3.05E+01	TNO Nutrition and Food Research, 2001.

Table B-8. Receptor Activity Patterns

Time	Activity Pattern 1: Person stays at home for most of the day	Activity Pattern 2: Person goes to school or work for part of the day	Activity Pattern 3: Person goes to school or work for most of the day
12:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
1:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
2:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
3:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
4:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
5:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
6:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
7:00 AM	Residence - Bathroom	Residence - Bathroom	Residence - Bathroom
8:00 AM	Automobile	Automobile	Automobile
9:00 AM	Work / School / COF	Work / School / COF	Work / School / COF
10:00 AM	Residence - Living Room	Work / School / COF	Work / School / COF
11:00 AM	Residence - Living Room	Work / School / COF	Work / School / COF
12:00 PM	Residence - Kitchen	Work / School / COF	Work / School / COF
1:00 PM	Outside	Outside	Work / School / COF
2:00 PM	Residence - Living Room	Residence - Living Room	Work / School / COF
3:00 PM	Residence - Living Room	Residence - Living Room	Work / School / COF
4:00 PM	Residence - Laundry/Utility/Garage	Residence - Laundry/Utility/Garage	Work / School / COF
5:00 PM	Outside	Outside	Outside
6:00 PM	Residence - Kitchen	Residence - Kitchen	Residence - Kitchen
7:00 PM	Residence - Living Room	Residence - Living Room	Residence - Living Room
8:00 PM	Residence - Living Room	Residence - Living Room	Residence - Living Room
9:00 PM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
10:00 PM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
11:00 PM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom

Table B-9. Surface Area to Body Weight Ratios for Receptors by Age and Area of Body Impacted[a]

Receptor	Level	Whole Body	Half Body	Face Hands & Arms	Both Hands	Inside of Both Hands	Inside of One Hand	10% of Hand
Adult (≥21 years)	5th%ile	292.0	146.0	18.7	14.7	7.35	3.68	1.47
	Mean	245.9	122.9	15.8	12.4	6.19	3.10	1.24
	95th%ile	208.1	104.0	13.0	10.5	5.23	2.61	1.05
Youth (16-20 years)	5th%ile	305.0	152.5	17.7	13.8	6.88	3.44	1.38
	Mean	257.0	128.5	14.9	11.6	5.80	2.90	1.16
	95th%ile	215.7	107.9	12.5	9.72	4.86	2.43	0.97
Youth (11-15 years)	5th%ile	350.0	175.0	20.5	15.8	7.92	3.96	1.58
	Mean	279.9	140.0	16.4	12.7	6.34	3.17	1.27
	95th%ile	232.0	116.0	13.6	10.5	5.24	2.62	1.05
Child (6-10 years)	5th%ile	411.2	205.6	25.5	19.4	9.71	4.85	1.94
	Mean	339.6	169.8	21.1	16.0	8.02	4.01	1.60
	95th%ile	281.9	141.0	17.5	13.3	6.67	3.33	1.33
Small Child (3-5 years)	5th%ile	451.9	225.9	30.3	22.0	11.0	5.50	2.20
	Mean	408.6	204.3	27.4	19.9	9.95	4.97	1.99
	95th%ile	362.6	181.3	24.3	17.6	8.78	4.39	1.76
Infant (1-2 years)	5th%ile	489.9	244.9	37.9	24.9	12.5	6.23	2.49
	Mean	452.4	226.2	35.0	23.0	11.5	5.75	2.30
	95th%ile	421.2	210.6	32.8	21.9	10.9	5.47	2.19
Infant (<1 year)	5th%ile	560.2	280.1	90.1	29.6	14.8	7.40	2.96
	Mean	509.6	254.8	81.9	26.9	13.5	6.73	2.69
	95th%ile	472.8	236.4	42.0	24.9	12.5	6.23	2.49

[a] U.S. EPA. (2011)

Table B-10. Receptor Inputs

Receptor	Body Weight (kg)	Inhalation Rate (m^3/day)		Mouthing Duration (min/hr)		Transfer Coefficient (cm^2/hr)		Dust Ingestion Rate (mg/day)	Soil Ingestion Rate (mg/day)	Averaging time			Exposure Duration		
		During Use	After Use	Mean	95th	Mean	95th			Acute (days)	Chronic (years)	Lifetime (years)	Acute (days)	Chronic (years)	Lifetime (years)
Adult (≥21 years)	80	0.74	0.61			6800	17000	30	20	1	1	78	1	1	1, 5, 12, 57[a]
Youth (16-20 years)	71.6	0.72	0.68			5576	13940	60	50	1	1		1	1	
Youth (11-15 years)	56.8	0.78	0.63			5576	13940	60	50	1	1		1	1	
Child (6-10 years)	31.8	0.66	0.5	1.1	1.1	3740	9350	60	50	1	1		1	1	
Small Child (3-5 years)	18.6	0.66	0.42	8.4	8.9	2652	6630	100	50	1	1		1	1	
Infant (1-2 years)	12.6	0.72	0.35	7	22	1972	4930	60	50	1	1		1	1	
Infant (<1 year)	7.8	0.46	0.23	10	22.5	1564	3910	30	30	1	1		1	1	

[a] See Table B-3

Table B-11. Environmental Inputs Relevant to all Models[a]

Environment	Zone 1 Volume (m^3)	Zone 1 Air Exchange Rate (per hr)	Zone 2 Air Exchange Rate (per hr)	Building Volume (m^3)
Residence - Whole house	492	0.45	0.45	492
Residence - Bedroom	36	0.45	0.45	492
Residence - Kitchen	24	0.45	0.45	492
Residence - Bathroom	15	0.45	0.45	492
Residence - Living room	50	0.45	0.45	492
Residence - Laundry room	8	0.45	0.45	492
Residence - Utility room	20	0.45	0.45	492
Residence - Garage		0.45	0.45	492
Office	50	1.5	1.5	1400
School	50	1.5	1.5	2800
Automobile	2.4	12.5	12.5	1E+11

[a] (U.S. EPA, 2011)

Table B-12. Environmental Inputs Relevant Only to P_ING2

Environment	Yard Area (m^2)	Soil Depth (m)	Soil Density (kg/m^3)	Soil Porosity (-)
Outdoors	1327	0.015	2600	0.2

Table B-13. Environmental Inputs Relevant Only to Model E6-A_ING3-A_ING1-A_DER1

Level	RP							Cleaning Periodicity (hr^{-1})	Cleaning Efficiency (unitless)
	Dep. Rate Constant (hr^{-1})[a]	Resus. Rate Constant (hr^{-1})[a]	Mass Gen. Rate to Indoor Air (mg/hr)	Mass Gen. Rate to Indoor Floor (mg/hr)	Filter Pen. Ratio (unitless)	Radius of Particle (m)[b]	Ambient Particle Conc. (mg/m^3)[c]		
Low			2.1				0.028	0.0015	0.05[d]
Med	1	0.000026	14.7	0	0.05	0.000005	0.052	0.006	0.46[e]
High			20.7				0.081	0.0119	0.95[f]
	Dust								
Low			84.6	7.7					
Medium	3.3	0.00021	117.9	25.3	0.8	0.0005			
High			156.9	82.7					
	Abraded Particles								
Low									
Medium	2.34	0.000129		0.00531		0.00007			
High									

[a] Thatcher and Layton (1995)
[b] Little et al. (2012)
[c] http://www.epa.gov/airtrends/pm.html
[d] Qian et al. (2008) (carpets)
[e] Yiin et al. (2002) (midpoint of range, carpets)
[f] Ewers et al. (1994) (wood floors)

Table B-14. Environmental Inputs Relevant Only to the Near Field – Far Field Model

Parameter	Value	Units
Near Field-Far Field Air Exchange Rate	402[a]	hr^{-1}
Near Field-Far Field Volume	0.204[a]	m^3

[a] Keil et al., 2009; Keil and Nicas, 2003

Table B-15. Partitioning Coefficient Values from the Literature

EPA has compiled available measured data on material air partition coefficients from fourteen studies. Most of the available data are for VOCs, rather than SVOCs. The material-air partition coefficient can vary based on the chemical properties such as vapor pressure and mass, but also by the type of product matrix. EPA is considering additional available approaches to estimate the material-air partition coefficient for chemicals without measured data to better inform which values could be selected for OPPT chemical assessments. Additional measured data and/or refined estimation approaches are of interest for this model parameter.

Chemical	Product Matrix	Partitioning coefficient (K)	Source[a]
Cyclohexane	Ceiling tile	6.8	Huang (2006)2
Toluene	Cellulose fibre and fibrous glass	83.2	Huang (2006)2
Rthyl acetate	Cellulose fibre and fibrous glass	239.3	Huang (2006)2
Isopropyl alcohol	Cellulose fibre and fibrous glass	239.3	Huang (2006)2
Methanol	Cellulose fibre and fibrous glass	3.12	Huang (2006)2
Benzene	Medium density board 1	190	Wang et al 2008
Benzene	Medium density board 2	430	Wang et al 2008
Toluene	Medium density board 1	260	Wang et al 2008
Toluene	Medium density board 2	470	Wang et al 2008
Xylene	Medium density board 1	330	Wang et al 2008
Xylene	Medium density board 2	580	Wang et al 2008
Toluene	Carpet backing	6171	Bodalal 2000
Nonane	Carpet backing	6216	Bodalal 2000
Nonane	Vinyl floor tile	2142	Bodalal 2000
Decane	Carpet backing	14617	Bodalal 2000
Decane	Plywood	6948	Bodalal 2000
Decane	Vinyl floor tile	13045	Bodalal 2000
Undecane	Carpet backing	24255	Bodalal 2000
Undecane	Vinyl floor tile	26647	Bodalal 2000
Cyclohexane	Plywood	348	Bodalal 2000
Ethylbenzene	Plywood	1636	Bodalal 2000
Ethylbenzene	Vinyl floor tile	1920	Bodalal 2000
Water	Vinyl flooring	78 ± 6.8	Cox 2001
n-Butanol	Vinyl flooring	810 ± 77	Cox 2001
Toluene	Vinyl flooring	980 ± 34	Cox 2001
Phenol	Vinyl flooring	1.2 (± 0.30) e5	Cox 2001
n-decane	Vinyl flooring	3000 ± 420	Cox 2001
n-dodecane	Vinyl flooring	1.7 (± 0.03) e4	Cox 2001
n-Tetradecane	Vinyl flooring	1.2 (± 0.13) e5	Cox 2001

Chemical	Product Matrix	Partitioning coefficient (K)	Source[a]
n-Pentadecane	Vinyl flooring	4.2 (± 0.38) e5	Cox 2001
Hexanal	Oriented strand board	6600 ± 400	Yuan, 2007
Styrene	Polystyrene foam	260 ± 17	Yuan, 2007
TVOC	Particle board	3300	Yang, 2001
Hexanal	Particle board	3300	Yang, 2001
α-Pinene	Particle board	5600	Yang, 2001
Ethyl acetate	Brick	186.6	Zhang, 2004
Ethyl acetate	Concrete	1186.4	Zhang, 2004
Ethyl acetate	Gypsum board	88.68	Zhang, 2004
Ethyl acetate	Carpet	43.91	Zhang, 2004
Ethyl acetate	Wall paper	3000	Zhang, 2004
n-Octane	Brick	23.14	Zhang, 2004
n-Octane	Concrete	61.4	Zhang, 2004
n-Octane	Gypsum board	70.02	Zhang, 2004
n-Octane	Carpet	98.42	Zhang, 2004
n-Octane	Wall paper	2000	Zhang, 2004
DEHP	Vinyl flooring	2.30E+11	Xu, 2006
Chlorobenzene	Carpet	80.34	Deng et al
Ethylbenzene	Carpet	57.05	Deng et al
123-Trimethylbenzene	Carpet	28.68	Deng et al
Diethyl-hexylphthalate	Vinyl flooring	2.75E+11	Holmgren et al 2012
Di-iso-nonyl phthalate	Vinyl flooring	1.88E+12	Holmgren et al 2013
Diethyl-hexyl isosorbate	Vinyl flooring	2.58E+10	Holmgren et al 2014
Diethyl-hexyladipate	Vinyl flooring	7.37E+09	Holmgren et al 2015
1,2-Cyclohexanedicarboxylic acid di-iso-nonyl ester	Vinyl flooring	5.66E+11	Holmgren et al 2016
TVOC	Wallpaper	3289	Kim et al 2012
TVOC	Laminate flooring	3289	Kim et al 2013
TVOC	Particle board	3289	Wang et al 2008
Naphthalene	Polyurethane foam	6400	Zhao et al 2004
1,2,4-Trimethylbenzene	Polyurethane foam	440	Zhao et al 2004
Styrene	Polyurethane foam	310	Zhao et al 2004
p-Xylene	Polyurethane foam	130	Zhao et al 2004
Ethylbenzene	Polyurethane foam	110	Zhao et al 2004
Chlorobenzene	Polyurethane foam	140	Zhao et al 2004
Toluene	Polyurethane foam	58	Zhao et al 2004
Benzene	Polyurethane foam	19	Zhao et al 2004

[a]Sources to be added in next iteration.

Table B-16. Diffusion Coefficient Values from the Literature

EPA has compiled available measured data on diffusion coefficients from sixteen studies. Most of the available data are for VOCs, rather than SVOCs. The diffusion coefficient can vary based on the chemical properties such as vapor pressure and mass, but also by the type of product matrix. EPA is considering additional available approaches to estimate the diffusion coefficient for chemicals without measured data to better inform which values could be selected for OPPT chemical assessments. Additional measured data and/or refined estimation approaches are of interest for this model parameter.

Chemical	Product	Diffusion Coefficient (m^2/s)	Source[a]
1,2- Propanediol	Carpet	6.50E-14	Little et al. (1994)
1,2,3-Trimethylbenzene	Carpet	6.00E-11	Deng et al
1,2,4-Trimethylbenzene	Polyurethane Foam	1.00E-13	Zhao et al 2004
1,2-Cyclohexanedicarboxylic acid di-iso-nonyl ester	Vinyl Flooring	1.18E-14	Holmgren et al 2012
1,2-Dichloroethane	HPDE Geomembrane	2.60E-12	Chao et al (2006)
2,2,4-Trimethylpentane	Carpet	6.00E-15	Little et al. (1994)
2,3,5,6-Tetramethyl-phenol	Low Density Polyethylene	1.60E-13	Piringer (2008)
2,3-Benzopyrrole	Low Density Polyethylene	5.50E-13	Piringer (2008)
2,6-Di-tert-butyl-4-methyl-phenol	Low Density Polyethylene	4.80E-14	Piringer (2008)
2-Ethyl-1-hexanol	Carpet	8.80E-14	Little et al. (1994)
2-Hydroxy-4-ethandiol methyl-thioacetic acid ester[b]	Low Density Polyethylene	9.00E-15	Piringer (2008)
2-Phenyl-ethanol	Low Density Polyethylene	4.30E-13	Piringer (2008)
3,7-Dimethyl-6-octene-1-al[b]	Low Density Polyethylene	1.00E-13	Piringer (2008)
3,7-Dimethyl-octene-3-ol [b]	Low Density Polyethylene	1.60E-13	Piringer (2008)
3-Octen-2-one	Low Density Polyethylene	7.30E-13	Piringer (2008)
3-Phenyl-1-propanol	Low Density Polyethylene	2.80E-13	Piringer (2008)
4-Ethenylcyclohexene [b]	Carpet (Nylon and polypropelyne w SBR adhesive)	2.10E-12	Little et al. (1994)
4-Ethenylcyclohexene [b]	Carpet (Nylon w SBR latex adhesive)	5.20E-12	Little et al. (1994)
4-Isopropyl-toluene	Low Density Polyethylene	5.40E-13	Piringer (2008)
4-Phenylcyclohexene (PCH)	Carpet (Nylon and polypropylene w SBR adhesive)	1.20E-12	Little et al. (1994)
4-Phenylcyclohexene (PCH)	Carpet (Nylon w SBR latex adhesive)	5.90E-13	Little et al. (1994)
4-Phenylcyclohexene (PCH)	Carpet (Nylon w SBR latex adhesive)	5.00E-13	Little et al. (1994)
7-Methyl-quinoline	Low Density Polyethylene	4.30E-13	Piringer (2008)
Acetaldehyde (ACE)	Carpet (Nylon w PVC backing)	6.40E-12	Little et al. (1994)
a-Pinene	Particle board	1.20E-10	Yang et al. (2001)
Benzene	HPDE Geomembrane	7.10E-12	Chao et al (2006)
Benzene	Low Density Polyethylene	1.10E-12	Piringer (2008)
Benzene	Low Density Polyethylene	4.00E-13	Piringer (2008)
Benzene	Polyurethane Foam	7.00E-13	Zhao et al 2004

Chemical	Product	Diffusion Coefficient (m^2/s)	Source[a]
Cedrylacetate	Low Density Polyethylene	4.10E-14	Piringer (2008)
Chlorobenzene	Carpet	1.24E-11	Deng et al
Chlorobenzene	Polyurethane Foam	3.30E-13	Zhao et al 2004
Chloroform	HPDE Geomembrane	7.90E-12	Chao et al (2006)
Cyclohexane	Ceiling Tile	2.15E-06	Farajollahi et al 2009
Cyclohexane	Plywood	1.55E-10	Bodalal et al (2000)
Decane	Carpet backing	5.42E-12	Bodalal et al (2000)
Decane	Plywood	1.28E-11	Bodalal et al (2000)
Decane	vinyl floor tile	2.09E-12	Bodalal et al (2000)
Decane	Vinyl flooring	2.10E-12	Bodalal et al (2000)
Dichloromethane	HPDE Geomembrane	1.02E-11	Chao et al (2006)
Didodecyl-3-3-thio-dipropionate	Low Density Polyethylene	2.00E-15	Piringer (2008)
Diethyl-hexyl isosorbate (isDEH) [b]	Vinyl Flooring	2.09E-14	Holmgren et al 2012
Diethyl-hexyladipate (DEHA)	Vinyl Flooring	4.48E-14	Holmgren et al 2012
Diethyl-hexylphthalate (DEHP)	Vinyl Flooring	1.75E-14	Holmgren et al 2012
Di-iso-nonyl phthalate (DINP)	Vinyl Flooring	1.33E-14	Holmgren et al 2012
Dimethyl-benzyl-carbinol	Low Density Polyethylene	7.50E-14	Piringer (2008)
Dimethyl-phthalate	Low Density Polyethylene	1.90E-13	Piringer (2008)
Diphenyl-oxide	Low Density Polyethylene	3.70E-13	Piringer (2008)
Docosane	Low Density Polyethylene	3.50E-14	Piringer (2008)
Eicosane	Low Density Polyethylene	6.30E-14	Piringer (2008)
Ethane	Low Density Polyethylene	5.40E-12	Piringer (2008)
Ethane	Low Density Polyethylene	4.80E-12	Piringer (2008)
Ethyl Acetate	Brick	2.42E-09	Zhang and Niu (2004)
Ethyl Acetate	Carpet	1.03E-08	Zhang and Niu (2004)
Ethyl Acetate	Ceiling Tile	2.01E-06	Farajollahi et al 2009
Ethyl Acetate	Concrete	4.33E-11	Zhang and Niu (2004)
Ethyl Acetate	Gypsum board	1.27E-08	Zhang and Niu (2004)
Ethyl Acetate	Wallpaper	2.78E-12	Zhang and Niu (2004)
Ethyl benzene	Carpet	1.85E-11	Deng et al
Ethyl benzene	Carpet (Nylon and polypropelyne w SBR adhesive)	1.50E-12	Little et al. (1994)
Ethyl benzene	Carpet (Nylon w SBR latex adhesive)	1.02E-11	Little et al. (1994)
Ethyl benzene	Carpet (Nylon w SBR latex adhesive)	4.30E-12	Little et al. (1994)
Ethyl benzene	HPDE Geomembrane	6.80E-12	Chao et al (2006)
Ethyl benzene	Plywood	4.04E-11	Bodalal et al (2000)
Ethyl benzene	Polyurethane Foam	3.70E-13	Zhao et al 2004

Chemical	Product	Diffusion Coefficient (m^2/s)	Source[a]
Ethyl benzene	vinyl floor tile	1.60E-11	Bodalal et al (2000)
Formaldehyde	Carpet (Nylon w PVC backing)	3.20E-12	Little et al. (1994)
Heptanol	Low Density Polyethylene	5.30E-13	Piringer (2008)
Hexanal	Oriented strand board	1.80E-12	Yuan et al. (2007)
Hexanal	Particle board	7.70E-11	Yang et al. (2001)
Limonene	Low Density Polyethylene	4.30E-13	Piringer (2008)
Methane	Low Density Polyethylene	1.90E-11	Piringer (2008)
Methane	Low Density Polyethylene	3.00E-11	Piringer (2008)
Methanol	Low Density Polyethylene	4.80E-12	Piringer (2008)
Methyl-octacosanoate	Low Density Polyethylene	3.00E-15	Piringer (2008)
Methyl-tricosanoate	Low Density Polyethylene	1.50E-14	Piringer (2008)
Naphthalene	Polyurethane Foam	6.60E-15	Zhao et al 2004
n-Butanol	Vinyl flooring	6.70E-13	Cox et al. (2001)
n-Decanal	Low Density Polyethylene	1.40E-13	Piringer (2008)
n-Decane	Vinyl flooring	4.50E-13	Cox et al. (2001)
n-Dodecane	Low Density Polyethylene	2.60E-13	Piringer (2008)
n-Dodecane	Vinyl flooring	3.40E-13	Cox et al. (2001)
n-Hexane	Ceiling Tile	1.95E-06	Farajollahi et al 2009
n-Hexane	Low Density Polyethylene	1.10E-12	Piringer (2008)
n-Hexane	Low Density Polyethylene	8.40E-13	Piringer (2008)
n-Nonanal	Low Density Polyethylene	1.80E-13	Piringer (2008)
n-Octanal	Low Density Polyethylene	2.30E-13	Piringer (2008)
n-octane	Brick	1.40E-09	Zhang and Niu (2004)
n-octane	Carpet	3.56E-08	Zhang and Niu (2004)
n-Octane	Carpet	1.69E-11	Zhang and Niu (2004)
n-octane	Concrete	1.69E-11	Zhang and Niu (2004)
n-octane	Gypsum board	1.20E-08	Zhang and Niu (2004)
n-octane	Wallpaper	4.17E-12	Zhang and Niu (2004)
Nonane	Carpet backing	2.83E-11	Bodalal et al (2000)
Nonane	Vinyl floor tile	1.48E-11	Bodalal et al (2000)
n-Pentadecane	Vinyl flooring	6.70E-14	Cox et al. (2001)
n-Pentane	Low Density Polyethylene	8.00E-13	Piringer (2008)
n-Tetradecane	Low Density Polyethylene	1.90E-13	Piringer (2008)
n-Tetradecane	Vinyl flooring	1.20E-13	Cox et al. (2001)
Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-propionate	Low Density Polyethylene	1.10E-15	Piringer (2008)
Octane	Ceiling Tile	1.75E-06	Farajollahi et al 2009

Chemical	Product	Diffusion Coefficient (m^2/s)	Source[a]
Phenol	Low Density Polyethylene	4.50E-13	Piringer (2008)
Phenol	Vinyl flooring	1.20E-13	Cox et al. (2001)
Propane	Low Density Polyethylene	5.20E-12	Piringer (2008)
p-Xylene	Polyurethane Foam	2.70E-13	Zhao et al 2004
Styrene	Carpet (Nylon and polypropelyne w SBR adhesive)	3.10E-12	Little et al. (1994)
Styrene	Carpet (Nylon w SBR latex adhesive)	4.10E-12	Little et al. (1994)
Styrene	Carpet (Nylon w SBR latex adhesive)	3.60E-12	Little et al. (1994)
Styrene	HPDE Geomembrane	2.50E-12	Chao et al (2006)
Styrene	polysterene foam	6.20E-12	Yuan et al. (2007)
Styrene	Polyurethane Foam	1.90E-13	Zhao et al 2004
Tetradecanol	Low Density Polyethylene	8.20E-14	Piringer (2008)
Tinuvin 326	Low Density Polyethylene	2.00E-14	Piringer (2008)
Toluene	Carpet backing	4.31E-11	Bodalal et al (2000)
Toluene	HPDE Geomembrane	9.60E-12	Chao et al (2006)
Toluene	Polyurethane Foam	4.20E-13	Zhao et al 2004
Toluene	Vinyl flooring	6.90E-13	Cox et al. (2001)
Trichloroethylene	HPDE Geomembrane	1.60E-11	Chao et al (2006)
TVOC	Laminate Flooring	3.10E-13	Kim et al 2012
TVOC	Particle board	7.65E-11	Wang et al 2008
TVOC	Particle board	7.70E-11	Yang (2001)
TVOC	Wallpaper	2.00E-13	Kim et al 2012
Undecane	Carpet backing	2.79E-12	Bodalal et al (2000)
Undecane	vinyl floor tile	8.55E-13	Bodalal et al (2000)
Water	Vinyl flooring	3.60E-12	Cox et al. (2001)

[a] Sources to be added in next iteration.

[b] Chemical CAS name may be reported incorrectly in original source.

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APPENDIX C: CEM Sensitivity Analysis

Overview

A sensitivity analysis was conducted to evaluate CEM version 1.5.[1] The sensitivity analysis was conducted on non-linear, continuous variables and categorical variables that were used in CEM models. Linear terms were excluded from the analysis since an incremental positive or negative change, such as +/-10%, in the given parameter would yield the same incremental change in the dose. Similarly, if an equation contained only linear terms then it was not included in this sensitivity analysis.

A base run of different models using the product or article categories in **Table D.1** along with CEM defaults was used. Individual variables were modified one at a time and the resulting Chronic Average Daily Dose (CADD) and Acute Dose Rate (ADR) were then compared to the CADD and ADR produced in the base run. In the version of CEM used for the sensitivity analysis, the article models were connected as one differential equation (SVOC Article Model). Therefore, the article models were run simultaneously. In the case of E6, CADD and ADR were calculated by the different media concentration (particulate phase and gas phase) instead of aggregated CADD/ADR. This was done because the aggregated CADD and ADR showed little variation, therefore, individual media concentrations were examined.

Table D.1. Product/Article categories used by model for sensitivity analysis.

Model Name	Chemical used	Product/Article Scenario Used
E1	benzyl alcohol	All-purpose Liquid Cleaner/Polish (neat)
E2	benzyl alcohol	Water-based Wall Paint
E3	benzyl alcohol	Aerosol Spray Paints
E4	benzyl alcohol	Laundry Detergent (liquid)
E5	benzyl alcohol	Continuous Action Air Fresheners
E6	bis(2-ethylhexyl) phthalate	Plastic Article Sofa
P_DER1a		NA[+]
P_DER1b[ǂ]	benzyl alcohol	All-purpose Liquid Cleaner/Polish (neat)
A_DER1	bis(2-ethylhexyl) phthalate	Plastic Article Sofa
A_DER2	bis(2-ethylhexyl) phthalate	Plastic Article Sofa
P_ING1		NA[+]
P_ING2	benzyl alcohol	Soil Amendments
A_ING2		NA[+]
A_ING3	bis(2-ethylhexyl) phthalate	Plastic Article Sofa
A_ING1	bis(2-ethylhexyl) phthalate	Plastic Article Sofa
E1 (UDER[++])	benzyl alcohol	All-purpose Liquid Cleaner/Polish (neat)
P_DER1a (UDER[++])	benzyl alcohol	All-purpose Liquid Cleaner/Polish (neat)
P_INH1 (Near Field-Far Field)	benzyl alcohol	All-purpose Liquid Cleaner/Polish (neat)

[ǂ] A previous version of CEM was used for the sensitivity analysis of this model, which did not contain revisions to the SVOC model however this would not have impacted the results for P_DER1b

[1] CEM was undergoing revisions at the time of the sensitivity analysis. The version that was used in the sensitivity analysis did not include models P_DER2 or A_DER3, the updated A_DER2 model, the latest fraction absorbed estimator for P_DER1a, no change to the absorption fraction P_DER1a model).

$^{+}$NA = Not applicable, model contained all linear terms and was not included in sensitivity analysis.
$^{++}$UDER = User defined

Two chemicals were used in the sensitivity analysis: bis(2-ethylhexyl) phthalate was selected for the SVOC Article model and benzyl alcohol for the other models. These were selected because bis(2-ethylhexyl) phthalate is a SVOC, which is better modeled by the Article model and benzyl alcohol is a VOC which is better modeled by the rest of the equations. Other variables that were held constant during the analysis of continuous variables were that the person stayed at home full time, the use was in the living room (except for P_ING2 and article models), the use was midnight (except for article models as this did not apply), and exposure factors were the same as the ones listed in the Exposure Factor Handbook.

For some values in CEM, users have the option of providing an estimate (for example saturation concentration) or using a built in estimator equation. EPA completed two different models runs in addition to the base run for those parameters in order to evaluate the sensitivity of the estimator equations. The first run was conducted by varying the input value only; the second was by varying the input value and using that value in the estimator equation for all the subsequent terms based on the changed input values. In the following analysis, results from parameters with an asterisk are from the second run using the estimator equations.

All model parameters were changed by a 10% increase, except for parameters in the SVOC Article model. Variables in the SVOC Article model were increased by 900%, since a 10% change in model parameters resulted in very small differences in CADD and ADR between the base run and sensitivity runs. Variables that would have yielded unrealistic results such as an ingestion fraction above one, were truncated to a realistic values. These variables were molecular weight, molecular weight*, dust ingestion fraction, abraded article ingestion fraction, cleaning efficiency, and cleaning frequency. Continuous variables were calculated as elasticity which was defined using Equation D-1.

$$Elasticity = \frac{\frac{Result_{sensitivity} - Result_{base}}{Result_{base}} x\ 100\%}{\%\ perturbation} \qquad [D\text{-}1]$$

Where,

$Result_{sensitivity}$ = Model results (either CADD or ADR) from sensitivity run

$Result_{base}$ = Model results (either CADD or ADR) from base run

% perturbation = 10% (or 900% for SVOC Article model)

A positive elasticity meant an increase in the model parameter resulted in an increase in the model output while a negative elasticity meant an increase in the model parameter resulted in a decrease in the model output. An elasticity of one meant the parameter had a linear relationship with the model result (either CADD or ADR).

Percent difference rather than elasticity was used to examine the sensitivity of model results to categorical variables (such as receptor and room type). One level of the category was used in the base run, then the level was changed in a subsequent run and the percent difference between the runs was calculated using Equation D-2. Near-field and far-field variables were modified in conjunction with selecting the "use near-field" option. An elasticity or percent difference was deemed to be noteworthy if the resulting elasticity or percent difference was above the absolute value of 0.05 (See Table D.11 at the end for all SVOC elasticities).

$$Percent\ difference = \frac{Result_{sensitivity} - Result_{base}}{Result_{base}} x\ 100\% \qquad [D\text{-}2]$$

The results of the sensitivity analysis are presented in three parts:

(1) The results by exposure pathway (inhalation, dermal, and ingestion) for product models;
(2) The results by exposure pathway (inhalation, dermal, and ingestion) for article models, and
(3) The results for user defined variables that affected multiple models (e.g. receptor, room type).

Product Inhalation Models

The first five inhalation models had similar trends, however each model had varying magnitudes across their elasticities. A negative elasticity was observed to different extents by increasing the use environment, building size, air zone exchange rates for Zone 1 and 2, and interzone ventilation rate. All of these variables decrease the concentration of the chemical either by increasing the volume the chemical fills or by replacing the air with cleaner air. Increasing the weight fraction, or the amount of product used had a positive elasticity. This is because this change increases the overall amount of chemical being added into the air and thus leads to a higher exposure.

Vapor pressure and molecular weight tended to have a positive elasticity. This could be due to the fact that an increase in vapor pressure means more of the chemical will be in the gas phase for exposure and an increase in molecular weight would result in a higher mass per particle in the air thus a higher dose by weight.

Except for E3, all models had an increase of dose with an increase of duration of use. Increasing this parameter increases the peak concentration of the product thus giving a higher overall exposure. The direction of elasticity was the same for both the CADD and the ADR for most product inhalation models. Finally, for all product inhalation models except E3, there was a change in CADD for duration of use (acute) and for mass of product used (acute) and there was a change in ADR for duration of use (chronic) and for mass of product used (chronic), however none of the parameters resulted in an elasticity greater than 0.05. At this time, it is unclear why CADD and ADR would have been affected by acute and chronic parameters, respectively.

E1: Product Applied to a Surface Incremental Source Model

For the first inhalation model, which is a single decay model, the trends match the general overall trends of the other models as seen in

Table D**.2** and **Figure 1**. Saturation concentration did not have a notable effect for this model for either ADR or CADD. Mass of product used and weight fraction had a positive linear relationship with dose. All the negative parameters had elasticities less than 0.4, indicating some terms mitigated the full effect of dilution (air exchange rates and volume of use/ building volume). This result may occur because even though the concentration is lower, the removal/dilution is not stronger than the rate of emitting or the period of time that a person is in the room being exposed.

Table D.2. E1 elasticity results using benzyl alcohol for all parameters (Parameters with an absolute elasticity ≥ 0.05 are shaded).

Parameter Name	Parameter	CADD Elasticity	ADR Elasticity
Air Exchange Rate Zone 1	AER_Zone1	-0.221340	-0.223345
Air Exchange Rate Zone 2	ZER_Zone2	-0.515567	-0.523298
Building Volume	Vol_Building	-0.623705	-0.612507
Duration Acute	Duration_Acute	-0.003215	-0.033826
Duration Chronic	Duration_Chronic	-0.026196	0.030472
Environment Volume	Vol_Zone1	-0.210045	-0.226720
Interzone Ventilation Rate	Qz12	-0.095139	-0.098124
Mass of Product Used Acute	M_Chronic	-0.003215	0.994940
Mass of Product Used Chronic	M_Acute	1.007954	0.030472
Molecular Weight	MW	0.075109	0.058947
Molecular Weight*	MW*	0.075109	0.058947
Saturation Concentration	CSATA	-0.003215	0.030472
Vapor Pressure	VP	0.075109	0.058947
Vapor Pressure*	VP*	0.075109	0.058947
Weight Fraction	WF	1.007954	0.994940

*Changes to parameters were carried through all estimator equations for the sensitivity run.

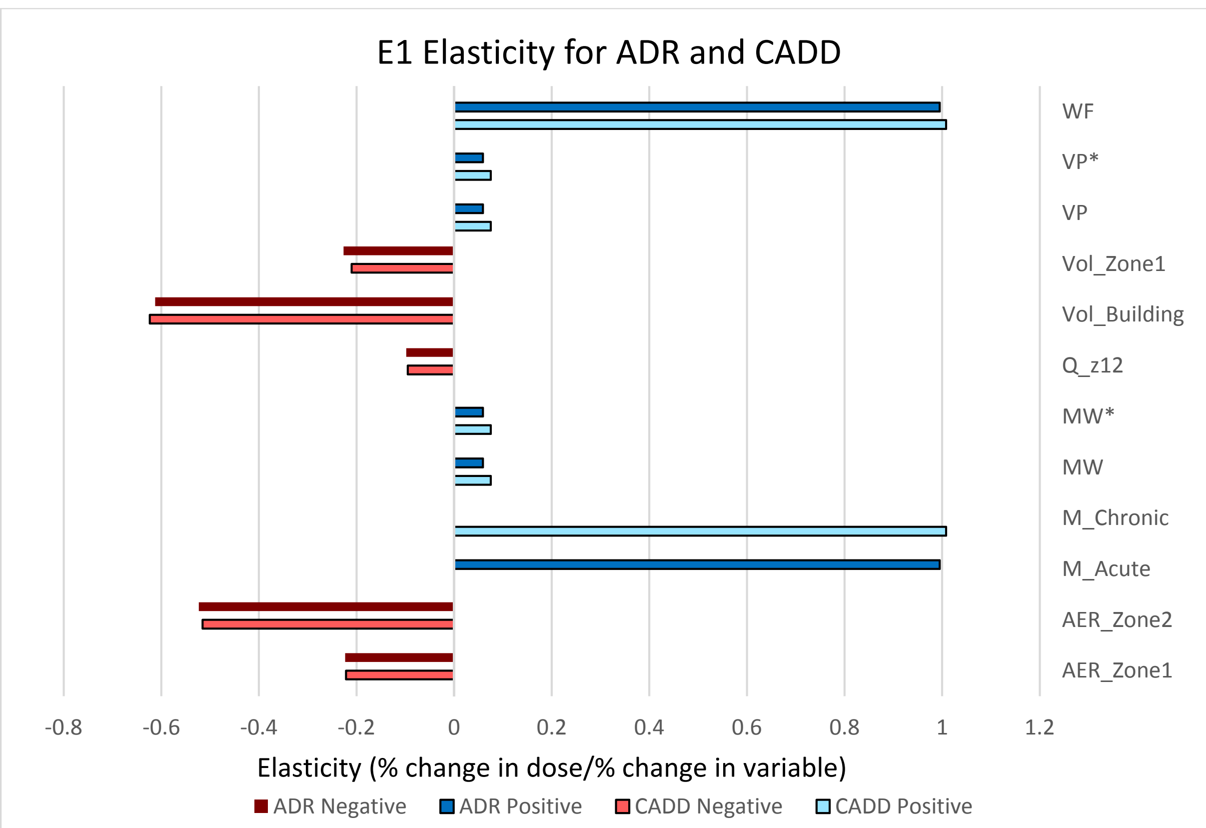

Figure 1. Tornado plot of parameters with an absolute elasticity ≥ 0.05 for E1 model. *Changes to parameters were carried through all estimator equations for the sensitivity run.

E2: Product Applied to a Surface Double Exponential Model

E2 is a double decay model. As with the trend across all product inhalation models, volume and air exchange rates had negative elasticities (**Table D.3** and **Figure D.2**). The normal trend of increasing use time resulted in an increased exposure. Contrary to the results from other product inhalation models, the elasticity of weight fraction was not close to 1 for either CADD or ADR. The elasticity for mass of product used was also smaller compared to other product inhalation models.

Compared to other models, increasing molecular weight and using it in the subsequent estimator equation had a notable positive elasticity for ADR, although it did not have a notable effect on CADD. The initial decay equation must reach near saturation, by increasing this, there is more chemical to be released in the initial decay. The initial decay releases far more chemical and in a rapid fashion compared to the second decay. This would explain why the CADD is not notable for either molecular weight or saturation concentration. The exposure window is larger than the initial peak. Thus since there will be less chemical released in subsequent days, the higher initial dose is averaged out.

The negative value for vapor pressure in ADR without using the estimator equations is that more of the chemical will be released because of the higher vapor pressure but will reach saturation concentration and start moving mass form the first decay to the second decay. This lower release of chemical would yield an overall lower dose because the sampling window would end before the same amount of chemical is released. This is further seen in the mass/weight fraction. Because most of the chemical is released in the second decay, ADR does not allow this enough time for the increased amount of chemical to be released.

Table D.3. E2 elasticity results using benzyl alcohol for all non-linear parameters. (Parameters with an absolute elasticity ≥ 0.05 are shaded).

Parameter Name	Parameter	CADD Elasticity	ADR Elasticity
Air Exchange Rate Zone 1	AER_Zone1	-0.199787	-0.063832
Air Exchange Rate Zone 2	ZER_Zone2	-0.220419	-0.174541
Building Volume	Vol_Building	-0.282315	-0.146864
Duration Acute	Duration_Acute	0.006533	0.545070
Duration Chronic	Duration_Chronic	0.542966	0.987907
Environment Volume	Vol_Zone1	-0.241051	-0.063832
Interzone Ventilation Rate	Qz12	-0.406107	-0.036155
Mass of Product Used Acute	M_Chronic	0.006533	0.240619
Mass of Product Used Chronic	M_Acute	0.687390	-0.008477
Molecular Weight	MW	0.027165	0.766488
Molecular Weight*	MW*	0.027165	2.952999
Saturation Concentration	CSATA	0.006533	0.711134
Vapor Pressure	VP	0.145187	-0.052181
Vapor Pressure*	VP*	0.151315	0.682864
Weight Fraction	WF	0.687390	0.240619

*Changes to parameters were carried through all estimator equations for the sensitivity run.

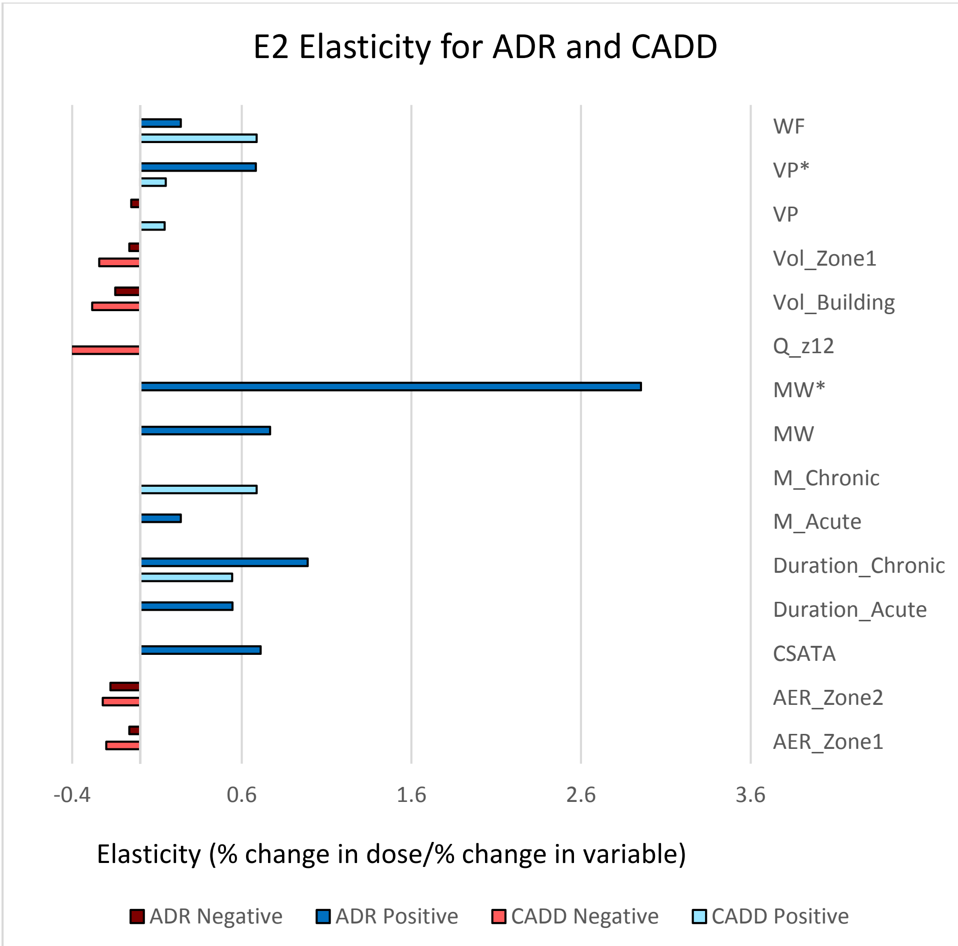

Figure D.2. Tornado plot of parameters with an absolute elasticity ≥0.05 for E2 model. *Changes to parameters were carried through all estimator equations for the sensitivity run.

E3: Product Sprayed

The E3 model is a single decay model with an additional equation for the aerosolized fraction. This model had a similar trend with the other models in that the air exchange rates and building volume had negative elasticities. In contrast, this model was the only model that had negative values for duration times as seen in **Table D.4** and Figure D.3. Additionally, the interzone ventilation rate had a positivity elasticity with respect to ADR. In all other models this parameter had a moderately negative elasticity. The aerosol fraction had only a slightly positive elasticity for CADD.

Another unique trend was that only ADR had positive notable elasticities for molecular weight*, vapor pressure*, and saturation concentration. In addition, this coupled with the negative elasticity with molecular weight and vapor pressure indicated that increasing these values without increasing saturation concentration reduced the amount of exposure which would explain the attenuated elasticity increases with the estimator equations used in conjunction with the increase of those parameters.

This indicates that the saturation concentration is reached within this model with the addition of the aerosol fraction. By increasing the duration of use, more of the product is removed before exposure occurs because of the increased rate to saturation. It would also explain why only the CADD had a notable elasticity for the aerosol fraction. Only after repeated exposure to a capped maximum exposure (saturation) will there be a strong enough signal to have increased exposure. This would also explain the attenuated increase in elasticity for ADR by increasing mass of product used. If the product is reaching saturation, using more will not increase exposure because it will have reached saturation. This could carry over until the sampling window ends and more of the product is taken away by ventilation into other compartments.

Table D.4. E3 elasticity results using benzyl alcohol for all non-linear parameters. (Parameters with an absolute elasticity ≥ 0.05 are shaded).

Parameter Full Name	Parameter	CADD Elasticity	ADR Elasticity
Aerosol Fraction	Aerosol_Fraction	0.079489	0.038801
Air Exchange Rate Zone 1	AER_Zone1	-0.215381	-0.168900
Air Exchange Rate Zone 2	ZER_Zone2	-0.496624	-0.491143
Building Volume	Vol_Building	-0.592108	-0.565973
Duration Acute	Duration_Acute	0.000000	-0.078236
Duration Chronic	Duration_Chronic	-0.061818	0.000000
Environment Volume	Vol_Zone1	-0.222127	-0.133730
Interzone Ventilation Rate	Qz12	-0.110418	0.046207
Mass of Product Used Acute	M_Chronic	0.000000	0.678305
Mass of Product Used Chronic	M_Acute	1.000000	0.000000
Molecular Weight	MW	0.036522	-0.215895
Molecular Weight*	MW*	0.036522	0.074425
Saturation Concentration	CSATA	0.000000	0.259764
Vapor Pressure	VP	0.036522	-0.215895
Vapor Pressure*	VP*	0.036522	0.074425
Weight Fraction	WF	1.021599	0.678305

*Changes to parameters were carried through all estimator equations for the sensitivity run.

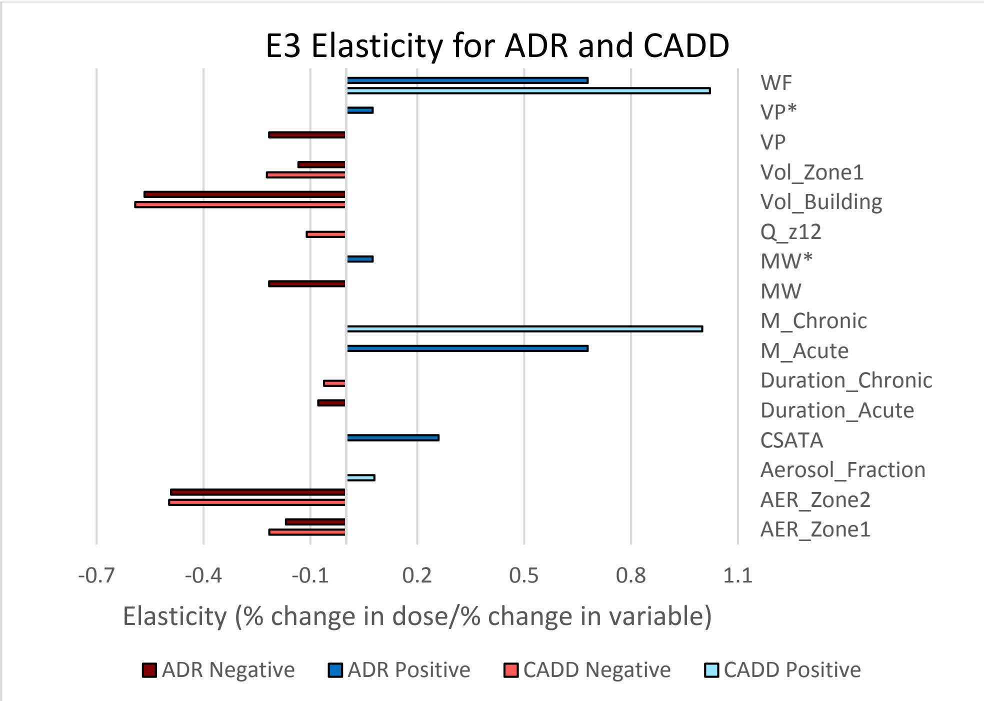

Figure D.3. Tornado plot of parameters with an absolute elasticity ≥ 0.05 for E3 model. *Changes to parameters were carried through all estimator equations for the sensitivity run.

E4: Product Added to Water

In the E4 model, the product is added to water which then evaporates. Though having a near linear elasticity for mass of product used was not unique to this model, what was unique to this and the next model was that increased use time, vapor pressure, and molecular weight had near linear positive elasticities as seen in

Table D.5 and Figure D.4. This is thought to be related to the increased amount of time the chemical needs move into the gaseous phase from water than from the other exposure scenarios described thus far.

Increasing the vapor pressure, would increase the fugacity of the chemical out of the aqueous phase thus increasing exposure. The increase from molecular weight comes more of an artifact that if all other parameters are held constant and there is a set transfer rate from the aqueous to gaseous phase, the heavier the molecule, the more exposure would occur because each molecule weighs more. The variable that had the strongest negative elasticity was increasing the environment of use with the air exchange rate of Zone 1 having the least effect. Since the highest exposure will occur in the initial use zone, then decreasing the initial exposure in this zone would reduce the overall exposure.

Table D.5. E4 elasticity results using benzyl alcohol for all non-linear parameters. (Parameters with an absolute elasticity ≥ 0.05 are shaded).

Parameter Full Name	Parameter	CADD Elasticity	ADR Elasticity
Air Exchange Rate Zone 1	AER_Zone1	-0.141741	-0.165904
Air Exchange Rate Zone 2	ZER_Zone2	-0.261964	-0.289603
Building Volume	Vol_Building	-0.261964	-0.289603
Duration Acute	Duration_Acute	-0.021518	0.947390
Duration Chronic	Duration_Chronic	1.000374	0.019645
Environment Volume	Vol_Zone1	-0.322075	-0.351453
Interzone Ventilation Rate	Qz12	-0.322075	-0.289603
Mass of Product Used Acute	M_Chronic	-0.021518	1.009240
Mass of Product Used Chronic	M_Acute	1.000374	0.019645
Molecular Weight	MW	0.952505	0.952505
Molecular Weight*	MW*	0.952505	0.952505
Saturation Concentration	CSATA	-0.021518	0.019645
Vapor Pressure	VP	0.952505	0.952505
Vapor Pressure*	VP*	0.952505	0.952505
Weight Fraction	WF	1.000374	1.009240

*Changes to parameters were carried through all estimator equations for the sensitivity run.

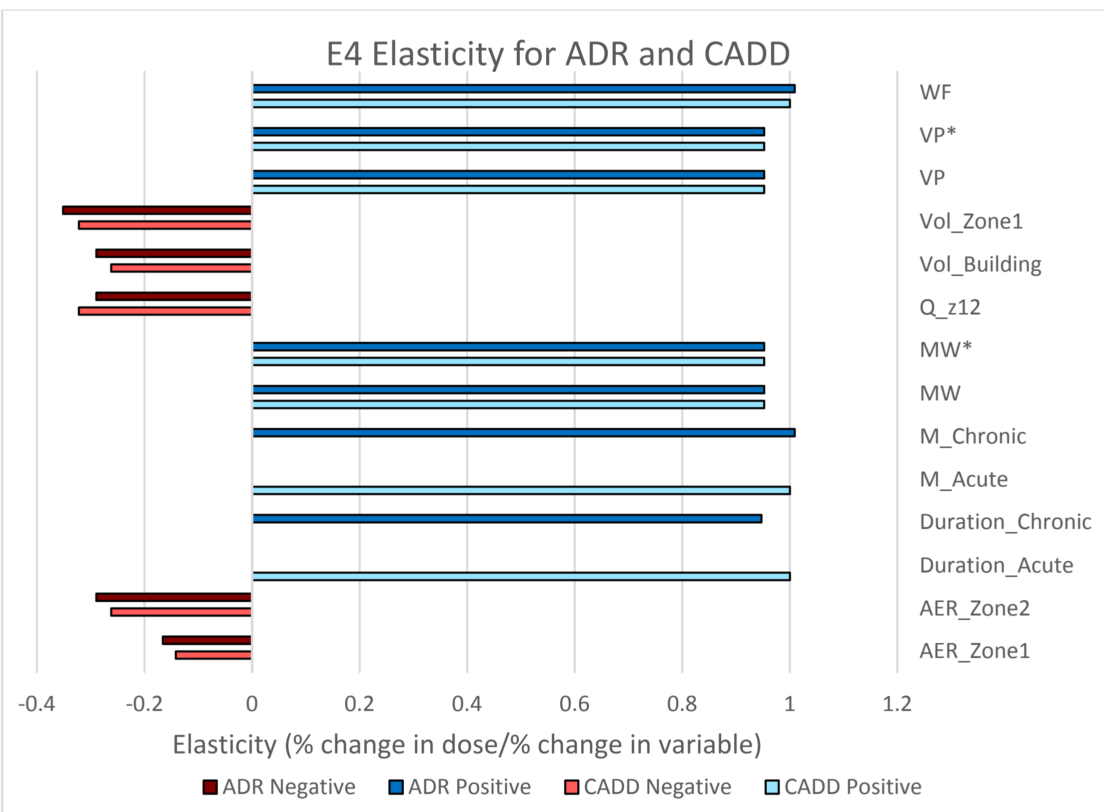

Figure D.4. Tornado plot of parameters with an absolute elasticity ≥ 0.05 for E4 model. *Changes to parameters were carried through all estimator equations for the sensitivity run.

E5: Product Placed in Environment

The E5 model is used for a continuous emitting source such as an air freshener. This model has a longer period of use time than the other inhalation models, which is not captured in **Table D.6**. Since the model has a steady emission, it reaches a steady state with air concentration for a longer period of time. The usual trend was seen with this model in that air transfer rates and increasing volume had a negative elasticity. The interzone ventilation rate had the largest negative elasticity, with the elasticity for ADR being -0.48 as seen in **Table D.6** and Figure D.5. This could reflect that the interzone ventilation rate has the strongest effect at steady state levels over long periods of time.

Similar to the previous models, vapor pressure, molecular weight, mass of product used, weight fraction, and duration of use all had positive elasticities. However, this model had a much higher elasticity for the chronic duration of use. With a longer period of time, it is likely that the user is exposed to the steady state concentration. The longer sampling time and more frequent use in the CADD scenario would lead to a higher background concentration than would be experienced with the ADR.

Table D.6. E5 elasticity results using benzyl alcohol for all non-linear parameters. (Parameters with an absolute elasticity ≥ 0.05 are shaded).

Parameter Full Name	Parameter	CADD Elasticity	ADR Elasticity
Air Exchange Rate Zone 1	AER_Zone1	-0.17144	-0.18477
Air Exchange Rate Zone 2	ZER_Zone2	-0.22825	-0.18477
Building Volume	Vol_Building	-0.28506	-0.25856
Duration Acute	Duration_Acute	-0.00100	1.069813
Duration Chronic	Duration_Chronic	1.476125	0.03663
Environment Volume	Vol_Zone1	-0.28506	-0.25856
Interzone Ventilation Rate	Q_z12	-0.39869	-0.47996
Mass of Product Used Acute	M_Chronic	-0.00100	0.996014
Mass of Product Used Chronic	M_Acute	1.021625	0.03663
Molecular Weight	MW	0.964812	0.922215
Molecular Weight*	MW*	0.964812	0.922215
Saturation Concentration	CSATA	-0.00100	0.03663
Vapor Pressure	VP	0.952505	0.952505
Vapor Pressure*	VP*	0.952505	0.952505
Weight Fraction	WF	1.021625	0.996014

*Changes to parameters were carried through all estimator equations for the sensitivity run.

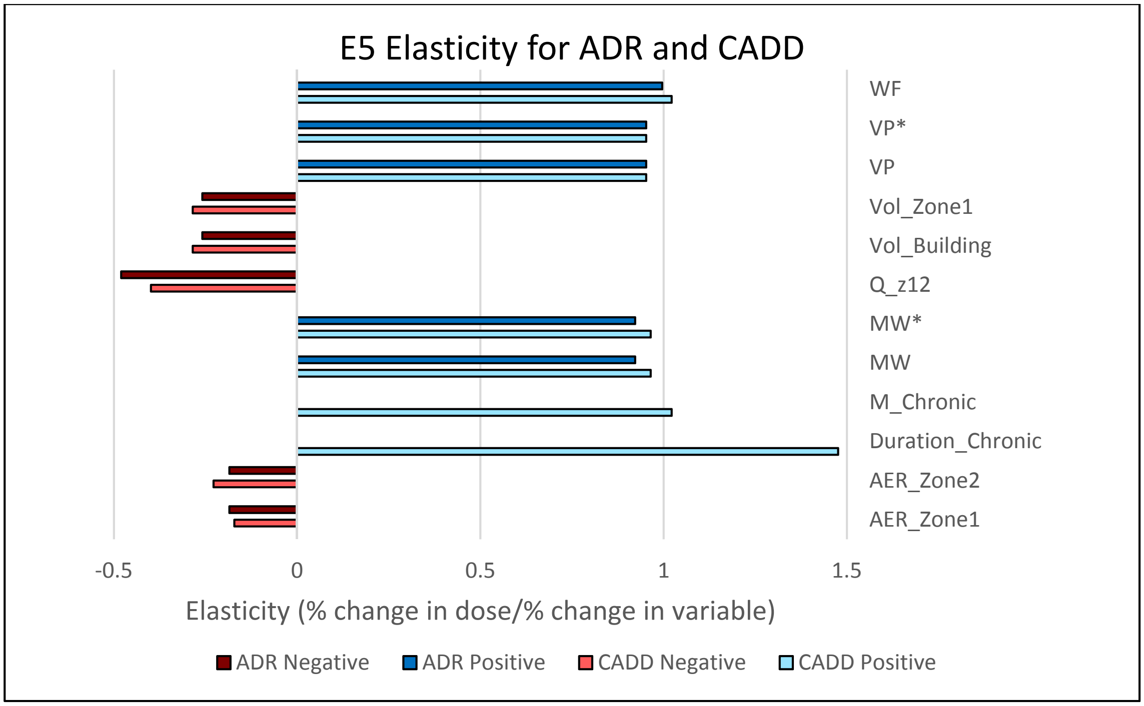

Figure D.5. Tornado plot of parameters with an absolute elasticity ≥ 0.05 for E5 model. *Changes to parameters were carried through all estimator equations for the sensitivity run.

Product Dermal Model

At the time of the sensitivity analysis, P_DER1b was the only product dermal model that contained non-linear terms. The P_DER1b model estimates exposure based on the ability of a chemical to penetrate the skin layer once contact occurs. As seen in

Table D.7 and Figure D.6, dermal permeability had a near linear elasticity, while log K_{OW} and molecular weight had zero elasticity. This means the permeability of the chemical has a larger effect than log K_{ow} and molecular weight. However, when the estimator equations were used, the resulting absolute elasticities were higher. Using the estimators for log K_{ow}* produced a positive elasticity of 2.65 for CADD and ADR while using the estimators with molecular weight produced a negative elasticity of -1.77 for CADD and ADR. This is reflected in that increasing K_{ow} drastically increases the ability of the molecule to penetrate the lipid heavy skin barrier, thus resulting in a higher CADD and ADR. In contrast, larger molecules will penetrate the skin at a lower rate compared to smaller molecules thus decreasing the CADD and ADR.

The results from this model were different from the inhalation models in that the elasticities for CADD and ADR were almost the same. This is consistent with the model structure, in that the chemical is placed on the skin so there is no time factor for a peak concentration to occur.

Table D.7. P_DER1b elasticity results using benzyl alcohol for all non-linear parameters. (Parameters with an absolute elasticity ≥ 0.05 are shaded).

Parameter Full Name	Parameter	CADD Elasticity	ADR Elasticity
Dermal Permeability Coefficient	Kp_g	0.993617	0.993617
log Kow	LogKow	0.000000	0.000000
log Kow*	LogKow*	2.648896	2.648896
Molecular Weight	MW	0.000000	0.000000
Molecular Weight*	MW*	-1.769600	-1.769600

*Changes to parameters were carried through all estimator equations for the sensitivity run.

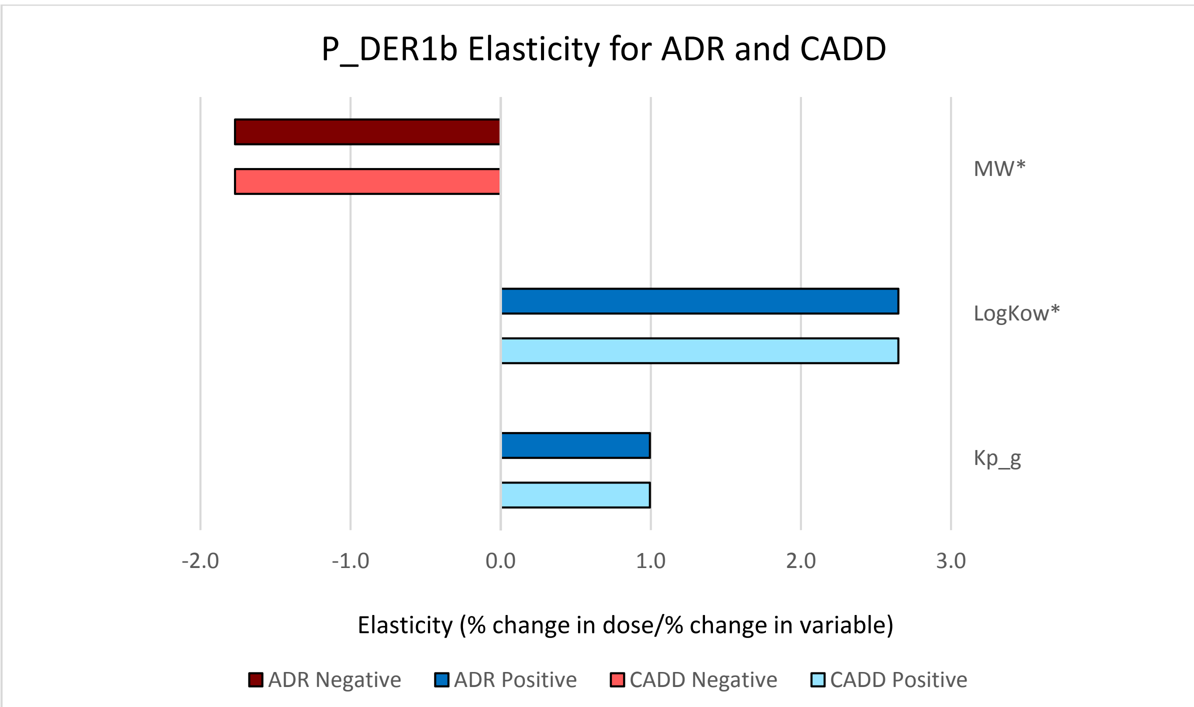

Figure D.6. Tornado plot of parameters with an absolute elasticity ≥ 0.05 for P_DER1b model.
*Changes to parameters were carried through all estimator equations for the sensitivity run.

Product Ingestion Models

P_ING2: Product Applied to Ground

There was only one product ingestion model, P_ING2, which contained non-linear parameters. In this model, the product is used outside and ingestion occurs when soil is transferred to a surface that then has contact with the mouth, resulting in ingestion. The half-life of the chemical in soil (Soil_hl) as seen in **Table D.8** and Figure D.7 had a positive, almost linear relationship. This would indicate that chemicals with longer half-lives in soil will result in higher chronic and acute doses.

Table D.8. P_ING2 elasticity results using benzyl alcohol for all non-linear parameters. (Parameters with an absolute elasticity ≥ 0.05 are shaded).

Parameter Full Name	Parameter	CADD Elasticity	ADR Elasticity
Half-Life in Soil	Soil_hl	1.013986	1.017964

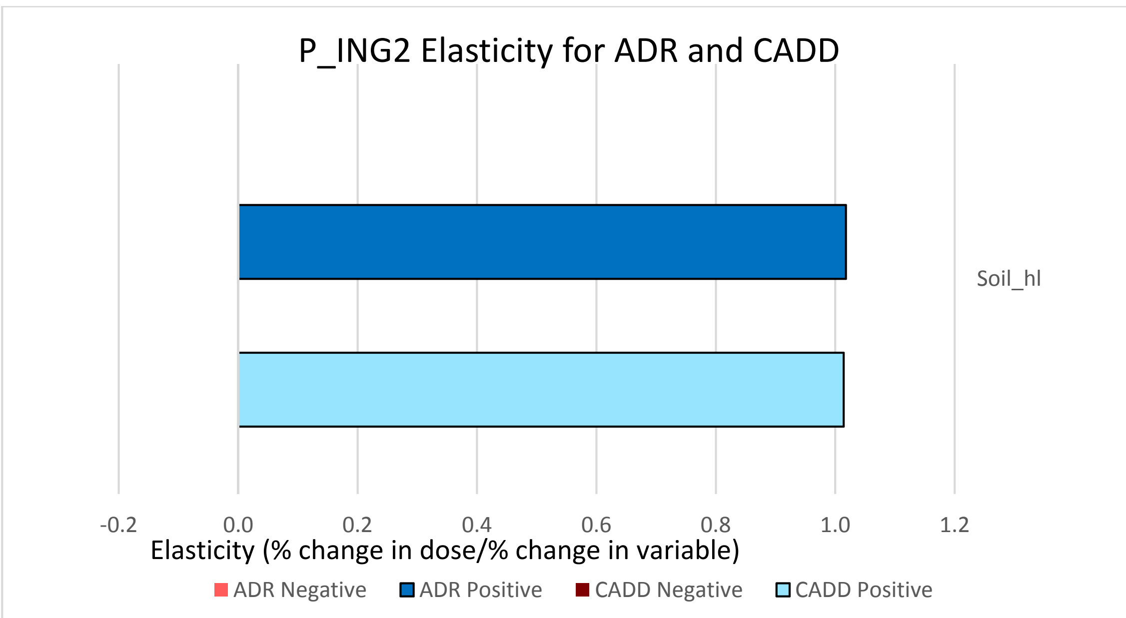

Figure D.7. Tornado plot of parameters with an absolute elasticity ≥ 0.05 for P_ING2 model.

Article models

For article models, the source of the chemical is not from the use of a product but from an article that is emitting the chemical. This would imply that at some point after the article has been placed in the room, equilibrium would be reached between the amount of chemical left in the article and the amount in the exposure mediums (gaseous, abraded particles, dust, and respirable particles). Second the concentration of the chemical is balanced across multiple mediums simultaneously unlike other models which examines one media at a time. Therefore, the article models were analyzed differently from the product models.

In addition, ingestion, dermal, and inhalation exposure rates were examined simultaneously. These models also have a finer scale for exposure since they model multiple mediums that the chemical is stored in and the method that a person may come into contact with it. When examining total exposure via multiple pathways, adjusting one parameter may have only affected one pathway the contributed the smallest to overall dose but if the largest contributor was unaffected then it would not appear to affect the total dose. Therefore while one media drove most of the exposure for a route, both mediums per exposure route were examined since changing one parameter may have only effected the smallest contributing exposure media. While for bis(2-ethylhexyl) phthalate (chemical used for the SVOC sensitivity analysis) these routes may be minor, for another chemical with different properties, these other mediums may be more important thus adding value for this finer scale differentiation.

The percent increase for most of the model parameters for the SVOC Article model were 900% (unless that would yield fractions above one or in the case of molecular weight give an unrealistic value for the mass of a SVOC). This was done for two reasons. First the concentrations in some of the mediums were so small that a 10% increase often did not produce a detectable difference in concentration. Second, even with the use of the estimator equations, there are many physical parameters of the chemical that are needed for the article models to run that are not estimated. These values are thus fixed, and do not reflect that a change in vapor pressure would change the value for Henry's Law coefficient or K_{oa}. As such, the model only investigates a parameter in an isolated case but not necessarily true to another chemical. Thus a higher level of perturbation would be needed because of the cascading effect of other physical parameters are not necessary captured. The complete results for parameters within the overall article model are listed in the in **Table**1.

Article Inhalation Model

E6: Inhalation from Article Placed in Environment

The inhalation model measures exposure to particles that are inhaled and deposited into the lungs and the amount of chemical inhaled from the gas phase. The results of the sensitivity analysis are described separately for the particulate and gas phases. The results show that in both phases, the initial concentration of SVOC in the article (C0_art) had a positive elasticity of one for ADR and CADD. The results also showed the interzone ventilation rate (Q_z12) had a negative elasticity for both phases as seen in Figure D.10 and D.11. The increased rate would mean there would be less of the chemical in the gaseous or particulate phase to inhale.

Particulate Phase

The resulting elasticities in the particulate phase had the same direction and magnitude for both ADR and CADD. The particulate phase is strongly influenced by the abraded particle phase. This is seen in the positive elasticities of the gas phase transfer (H_AbArt), the deposition rate (kdep_AbArt), and the amount of organic content of abraded particles (Fom_AbArt). Higher values of these three parameters indicate that there is a higher concentration of SVOC in this type of particle. Therefore, parameters that increase either the amount of SVOC in the particle or increase the amount of the particle had a strong effect on the resulting ADD and CADD. The inverse relationship was also demonstrated in that increasing the deposition rate resulted in an elasticity of -0.1. Finally the larger the room (Vol_Zone1), the lower the concentration of particles, which results in lower exposure.

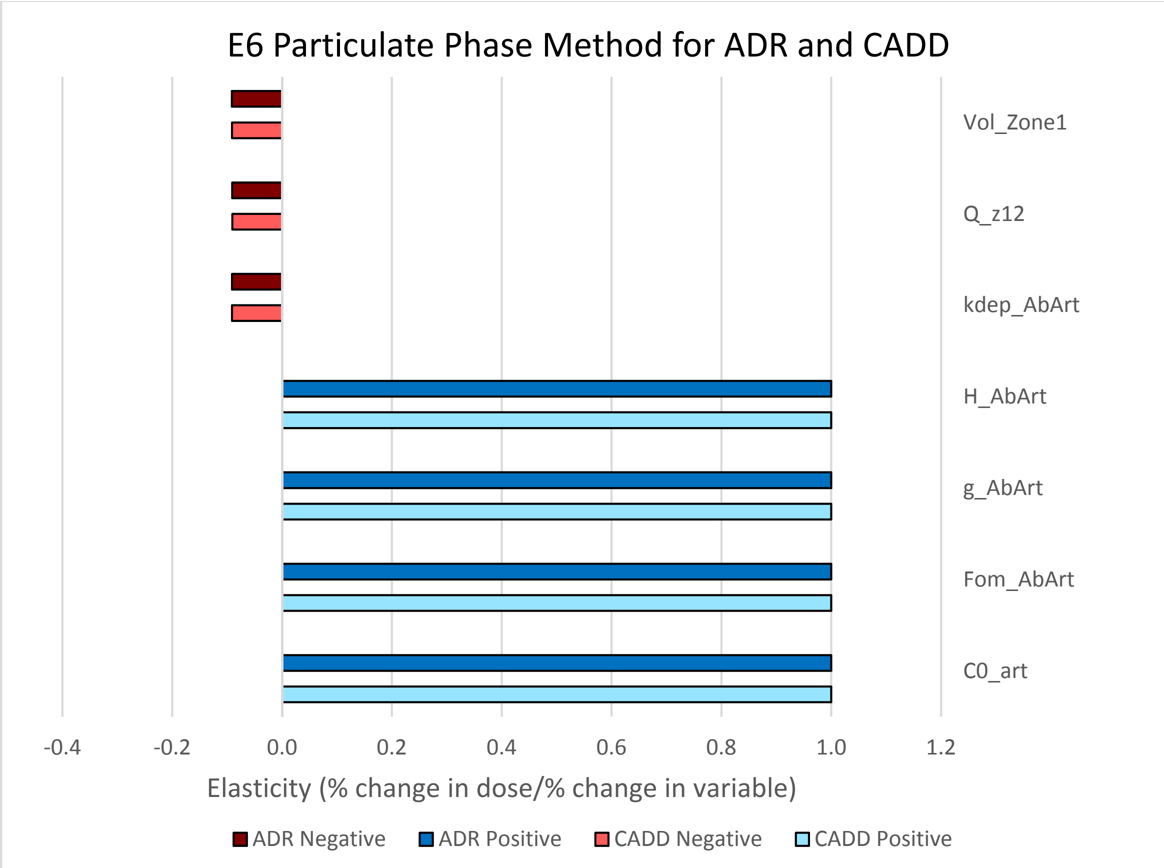

Figure D.10. Tornado plot of parameters with an absolute elasticity ≥ 0.05 for particulate phase in E6.

Gas Phase

The gas phase had similar directions for all the parameters except for the mass gas phase transfer coefficient (h). This was only seen to have a notable elasticity with CADD; the mass gas phase transfer coefficient that used the subsequent estimator equations was positive for both ADR and CADD. Vapor pressure (VP) had a positive elasticity as well but was less than for the other models. These all could be explained because these two parameters shift more of the SVOC to the gaseous phase but other factors attenuate the increase. Almost all of the negative elasticities can be connected to the solid phase variables:

- interior surface air partition coefficient, K_solid, with and without the estimator equation,
- area of the interior surface, A_Int,
- gas transfer into the solid phase, and
- interior surfaces overall mass transfer coefficient, H_Int.

These parameters relate to more of the SVOC being transferred to the solid phase out of the gaseous phase, which would lead to a lower exposure. The negative elasticity for molecular weight using the estimator equation (MW*) is likely due to reduced transfer out of the solid phase.

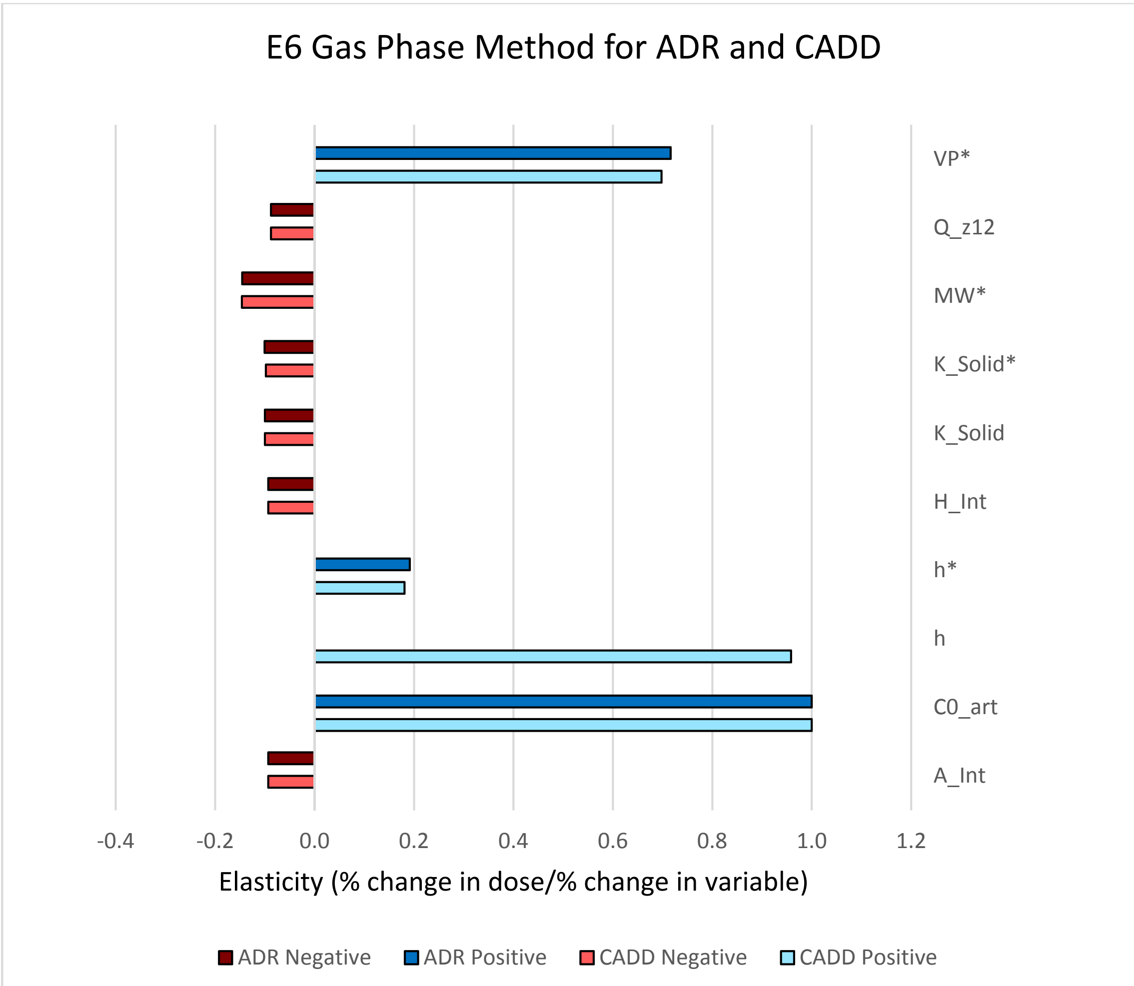

Figure D.11. Tornado plot of parameters with an absolute elasticity ≥ 0.05 for gas phase in E6.

Article Dermal Models

There are two article dermal models within CEM, the A_DER1 (A_DER1) which models the chemical in the gaseous phase sorbing onto the skin, and A_DER2 (A_DER2) which models dermal contact by direct contact with the article. Both models had negative elasticities of -0.11 in respect to internal area (A_Int) for ADR and CADD. The area of internal surfaces acts as a sink for the chemical, so the larger the area is, the more chemical can be stored. Finally both models for ADR and CADD had positive elasticities of one for area of emitting surface (As). The increased area of emitting surface would create a larger area of contact. This would lead to a higher probability of chemical transfer directly onto the body, in a linear relationship as seen in the elasticity of one in Figures D.12 and D.13.

A_DER1: Direct Transfer From Vapor Phase to Skin

The direction of the trends between CADD and ADR were the same for vapor to skin exposure with similar magnitudes. An increase in vapor pressure (VP), SVOC gas phase mass transfer coefficient (h, h*), area of emitting surface (As), Log Kow (LogKow*), transdermal permeability coefficient (Kp_g), and the initial concentration of chemical in the article (C0_art) had positive elasticities. Increase in vapor pressure would lead to more of the chemical going into the gas phase, which could then become deposited on the skin. Initial concentration of the chemical in the article and transdermal permeability coefficient had a positive linear relationship, meaning an increase in either would result in a higher CADD and ADR. This is due to the fact that higher chemical concentrations means more of the chemical will eventually absorb to the skin. For the same amount of chemical applied to the skin, an increase in permeability would lead to more of the chemical moving through the skin and thus a higher dose.

An increase in the SVOC interior surface air partition coefficient (K_Solid) or an increase in the SVOC dust air partition coefficient (K_DUST) resulted in a negative elasticity. Increasing either parameter leads to more of the chemical being removed from the air compartment which is where this exposure occurs. Since molecular weight (MW) was used to calculate the transdermal permeability coefficient (Kp_g), an increase in molecular weight (MW) led to a decrease in transdermal permeability coefficient. This led to an overall decrease in CADD and ADR which resulted in a negative elasticity (Figure D.12).

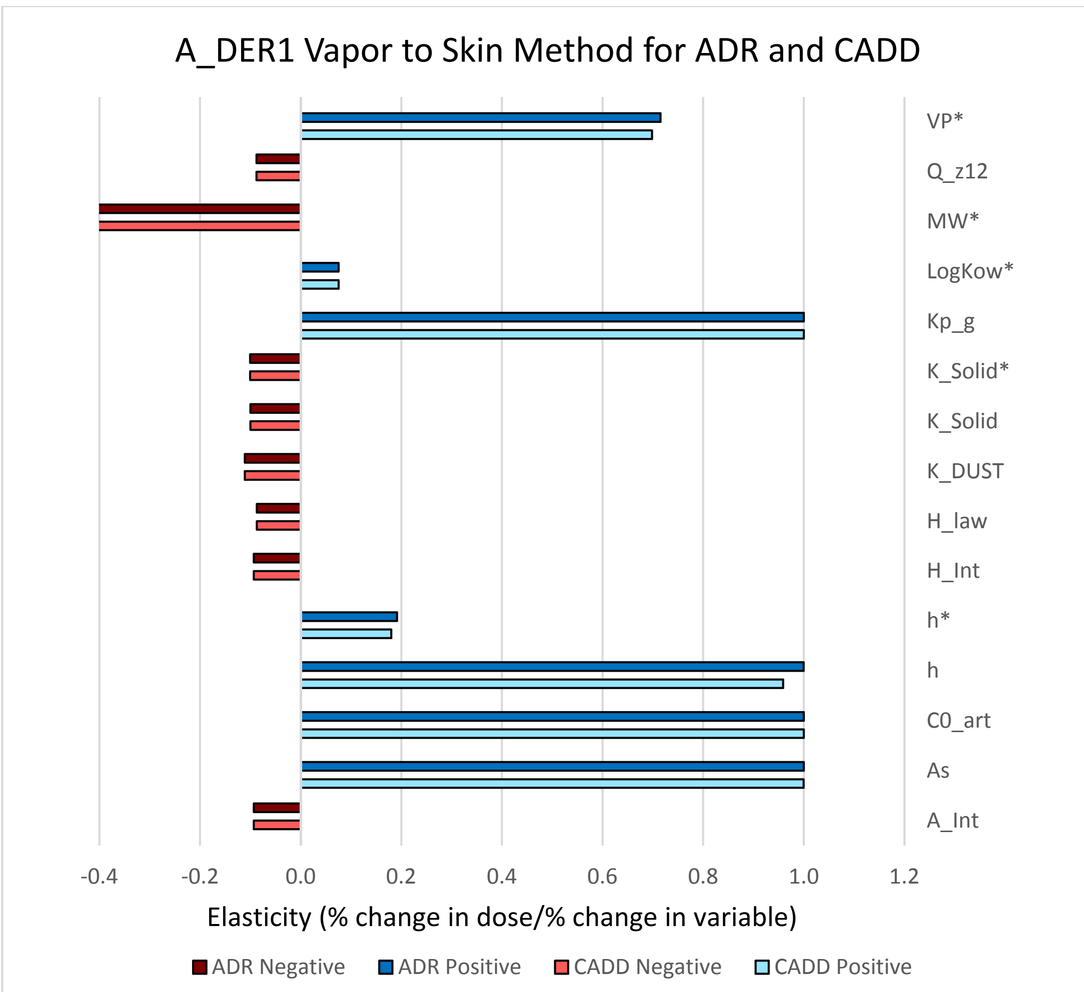

Figure D.12. Tornado plot of parameters with an absolute elasticity ≥ 0.05 for A_DER1 model.
*Changes to parameters were carried through all estimator equations for the sensitivity run.

A_DER2: Dermal Dose from Article where Skin Contact Occurs

This model was only affected by two variables used in the sensitivity analysis (Figure D.13). This is a result of this model being driven by direct contact to the article. As such, parameters that modulate the concentration in other media have no effect on this exposure route.

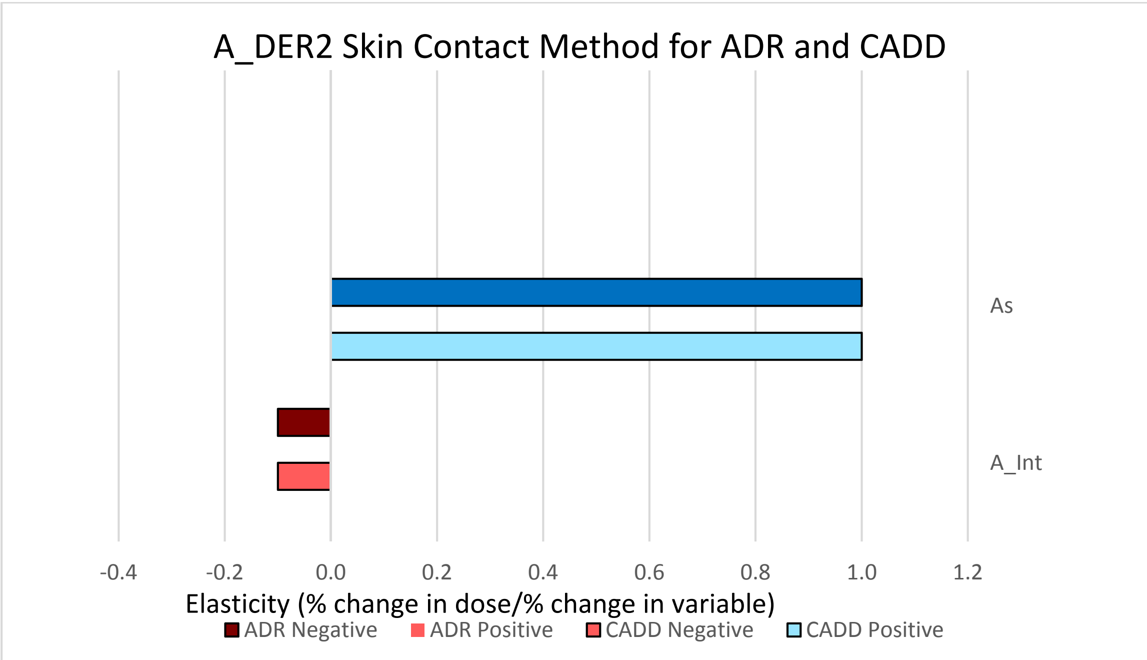

Figure D.13. Tornado plot of parameters with an absolute elasticity ≥ 0.05 for A_DER2 skin contact model.

Article Ingestion Models

Within CEM there are two article ingestion models with non-linear terms, (i) A_ING1 models ingestion after inhalation when the particles that are trapped in the mucus lining and swallowed at a later point in time after inhaling the particle and (ii) A_ING3 models incidental ingestion of settled dust, respirable particles, and abraded particles. The ingestion models had the fewest number of parameters with absolute elasticities greater than 0.05 as shown in Figures D.14 and D.15. The results for this exposure route were unique in that the direction and magnitude of the elasticities were the same for both ADR/CADD for the media concentration. This is thought to be a result of the exposure factors and the stability of media concentration results resulting in the same extent of change regardless of time period.

Both models were affected by the initial concentration of the SVOC in the article (C0_art) and the dust deposition rate (kdep_Dust). The initial concentration had a positive elasticity of one and the dust deposition rate had an elasticity of -0.111. Increasing the chemical in circulation would understandably increase the amount of chemical attached to dust thus resulting in an increase in the amount of exposure per dust particle ingested. As for the disposition rate, if the dust is settled, then the chance for exposure from respirable particles would be reduced.

A_ING1: Ingestion after Inhalation

This model unlike the incidental ingestion of dust, was affected by changes of abraded particle concentrations. This is the only model that was affected by a change in ingestion fraction of abraded particles (IF_Abr). This could be a result of the abraded particles having a higher concentration of the chemical than the dust or respirable particles. This would also explain the positive elasticity for the generation rate of abraded particles (G_AbArt), since more abraded particles would mean there are more to potentially breathe in. The deposition rates for dust and abraded particles (kdep_Dust and kdep_AbArt) and the interzone ventilation rate (Q_z12) had negative elasticities. This makes sense because these terms would lead to a reduction of particles in air or the room in which the user is located.

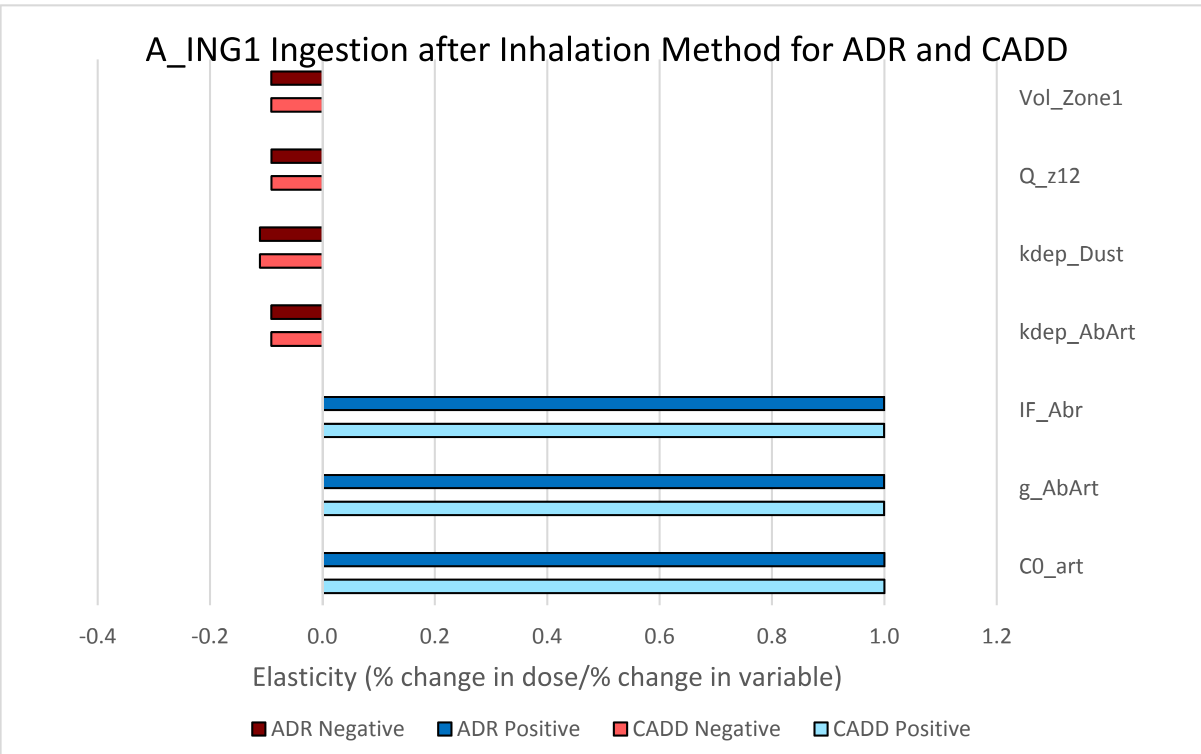

Figure D.14. Tornado plot of parameters with an absolute elasticity ≥ 0.05 for A_ING2 ingestion after inhalation model.

A_ING3: Incidental Ingestion of Dust

The incidental dust ingestion model was affected by fewer parameters than the other exposure mediums because it only measured ingestion of dust, not the other particles that may be on the skin. In addition, the adult receptor would have lower overall exposure because of the reduced rate of hand to mouth, mouthing incidents, and body size that could reduce the dose.

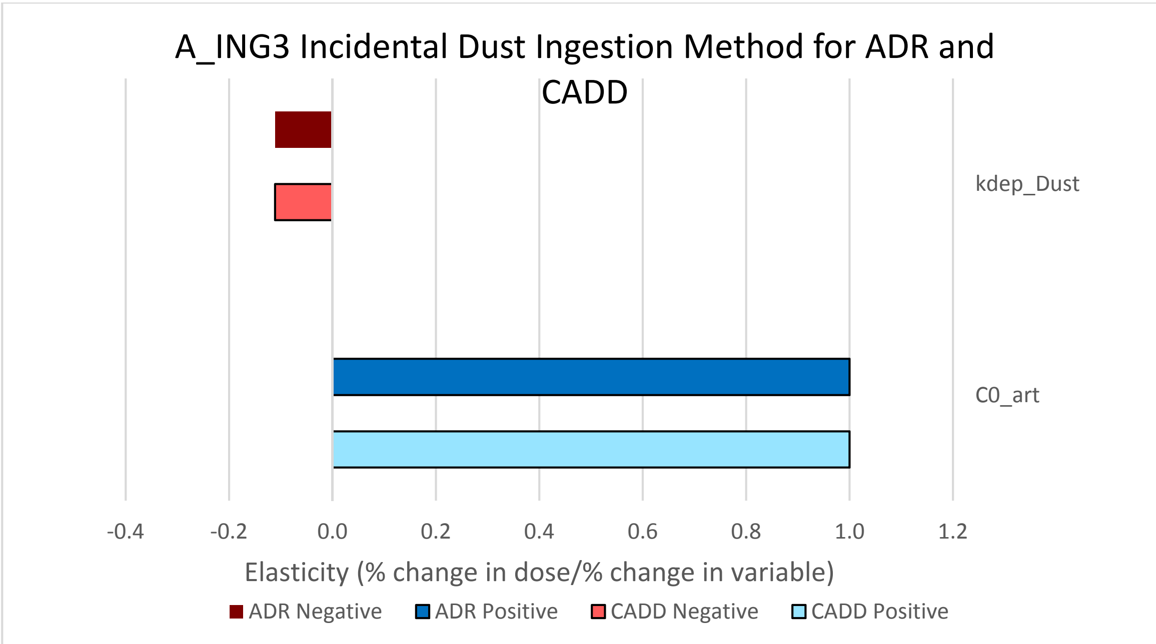

Figure D.15. Tornado plot of parameters with an absolute elasticity ≥ 0.05 for A_ING3 incidental ingestion model.

User Defined

The user defined variables that affected multiple models were separated into categorical and continuous variables. For the categorical variables there were multiple parameters that affected other parameters within the model. For example, varying the room type changed the ventilation rates, volume size and the amount of time per day that a person resided in the room. As such the results from different runs were calculated as percent difference from the base run (Table D.9). For the continuous variables that affected multiple models, the results were calculated as elasticity (Table D.10).

Categorical

User/Receptor

The inhalation model and dermal model results had a positive percent change when comparing an adult to a child and to a youth (Table D.9). Dermal had a smaller percent change between receptors than inhalation. The largest difference was between an adult and a child for both inhalation and dermal. Even though children have smaller surface area and smaller lungs, they are exposed at a higher dosage. Children have the largest surface area to volume ratio compared to youths and adults. As such each molecule that enters a child is diluted by less body which outweighs the lower rate of exposure a child experience resulting in a higher dose.

Work Schedule

The percent difference for working full and part-time might have been attenuated by the time of day that was selected and the type of exposure. For the sensitivity analysis, the time the product was used and the duration of use occurred while the person was at home. Therefore, there was no effect on the

ADR since the acute dose exposure period was too short to be affected by the work schedule. Similarly, the work schedule only had a slight effect on CADD.

Rooms

The general trend was that from the living room to the selected room caused a negative percent difference for inhalation. However, the one exception to that trend was the bedroom that had positive percent difference of about 70%. Since the receptor spent a large amount of time in the bedroom and it had a smaller volume than the living room it likely resulted in a higher ADR and CADD. The largest negative percent differences were changing the living room to the outside and to office/school as seen in **Table D.9** and Figure D.16. This is related to the time spent in microenvironments that are not in the house and have large volumes to dilute the concentration of VOC.

For dermal as seen in Figure D.17, the only room that resulted in a large percent difference was the office/school. This is because a person only spends half-hour at that location when specified since the stay-at- home activity pattern was selected. Therefore, any chemical used in the room will remain there and not migrate back to the house.

Near Field-Far Field (NFFF) base

Near field is calculated as two volumes in the first zone. The near field is the small area where the chemical is used and far field is the rest of the room. For inhalation, changing from a far field to a near field base resulted in a higher ADR and CADD. This is likely due to the fact that when a user is in the near field, it is a smaller volume than the total room which leads to less dilution and a larger exposure.

Table D.9. Percent difference for various exposure routes for user defined variables.

Parameter Category	Parameter Full Name	Parameter	INH % Difference CADD	INH % Difference ADR	DER % Difference CADD	DER % Difference ADR
Receptor	User Child	chk_Use_Child	80.74%	84.56%	38.12%	38.12%
	User Youth	chk_Use_Youth	45.48%	45.54%	13.84%	13.84%
Work Schedule	Part Time	chk_Part_Time	-0.01%	0.00%	0	0
	Full Time	chk_Full_Time	-0.01%	0.00%	0	0
Room	Whole House	Environment_ID_1	-18.57%	-19.31%	0	0
	Bedroom	Environment_ID_2	70.13%	72.55%	0	0
	Kitchen	Environment_ID_3	-12.80%	-13.31%	0	0
	Bathroom	Environment_ID_4	-10.16%	-10.56%	0	0
	Laundry Room	Environment_ID_6	-18.57%	-19.31%	0	0
	Utility Room	Environment_ID_7	-16.29%	-16.94%	0	0
	Garage	Environment_ID_8	-30.92%	-29.81%	0	0
	Office/School	Environment_ID_9	-90.33%	-90.13%	-9.96%	-9.96%
	Automobile	Environment_ID_11	-16.42%	-14.77%	0	0
	Outside	Environment_ID_12	-95.82%	-95.74%	0	0
Near Field-Far Field	NFFFbase	opt_CEM04	13.21%	12.87%	-	-

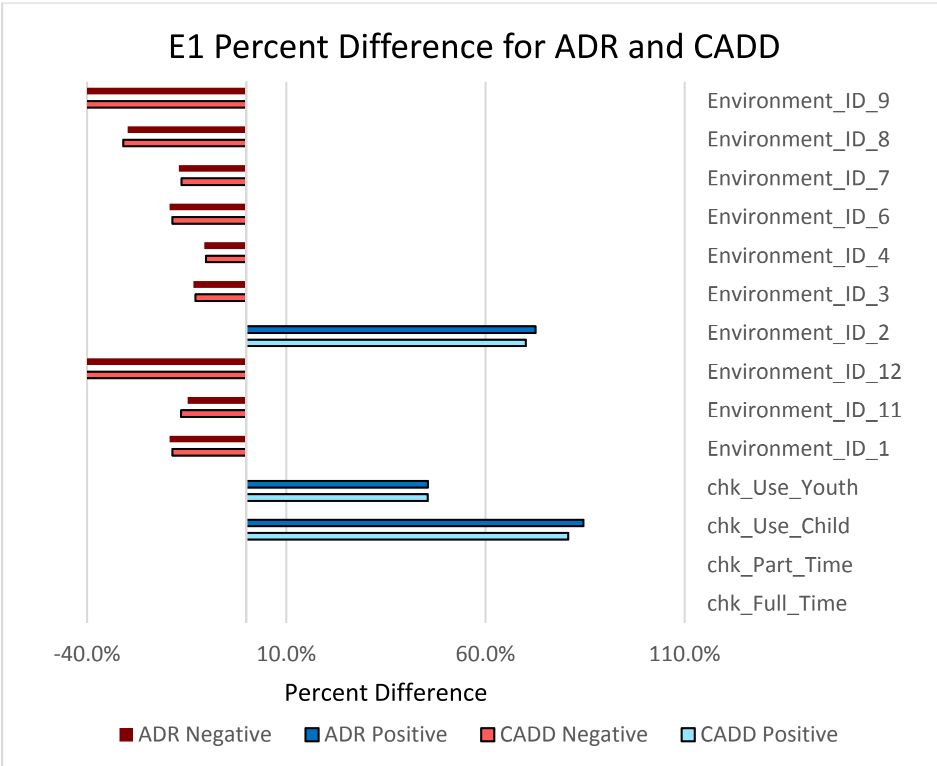

Figure D.16. Tornado plot of the inhalation percent change for user defined variables in E1.

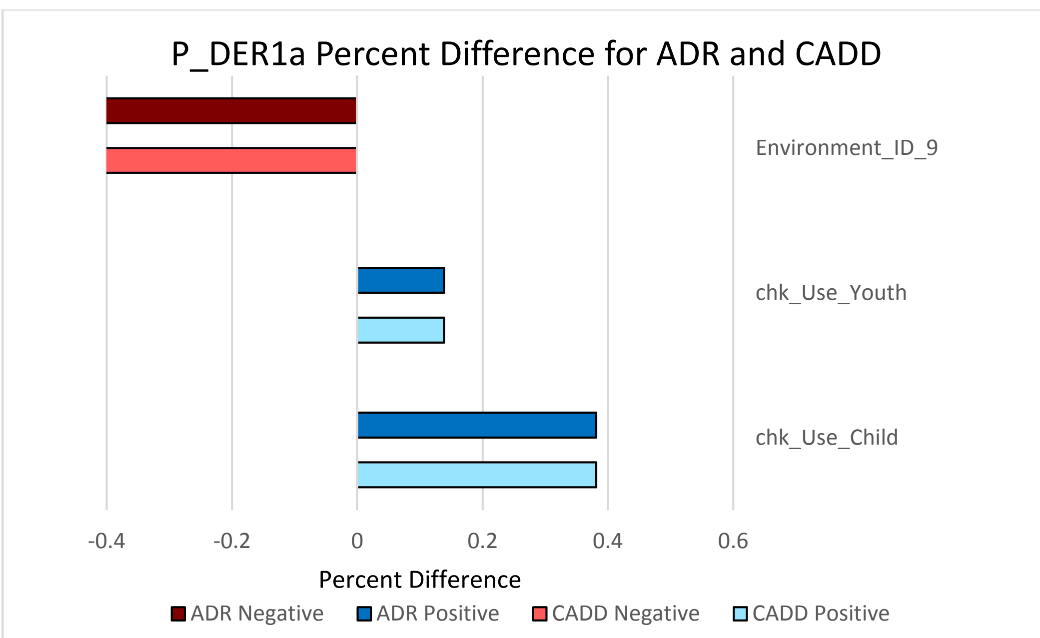

Figure D.17. Tornado plot of the dermal percent change for user defined variables in P_DER1a.

Continuous

There are three input parameters for the near-field, far-field option for product inhalation models in CEM. To determine the sensitivity of the model results to these three parameters, P_INH1 was run in the base scenario and was the near-field option. Then separate runs were performed where the near-field volume was increased by 10%, the far-field volume was increased by 10%, and then the air exchange rate was increased by 10%. Each run was then compared to the base model run. As seen in **Table D.10** and Figure D.16 there were notable changes in inhalation ADR and CADD. For inhalation, the air exchange rate and volume had negative elasticities but the air exchange rate had an elasticity near one while change in volume was -0.11. Increasing the air exchange rate would dilute the concentration in the near field, thus resulting in a lower exposure.

Table D.10. Elasticity of Near Field-Far Field variables.

Parameter Full Name	Parameter	Inhalation Elasticity CADD	Inhalation Elasticity ADR
NFFF Air Exchange Rate-A Near-field-Boundary	AER_nf_ff	-1.04997	-1.02616
NFFF Near-Field Volume	Vnf	-0.11407	-0.10447

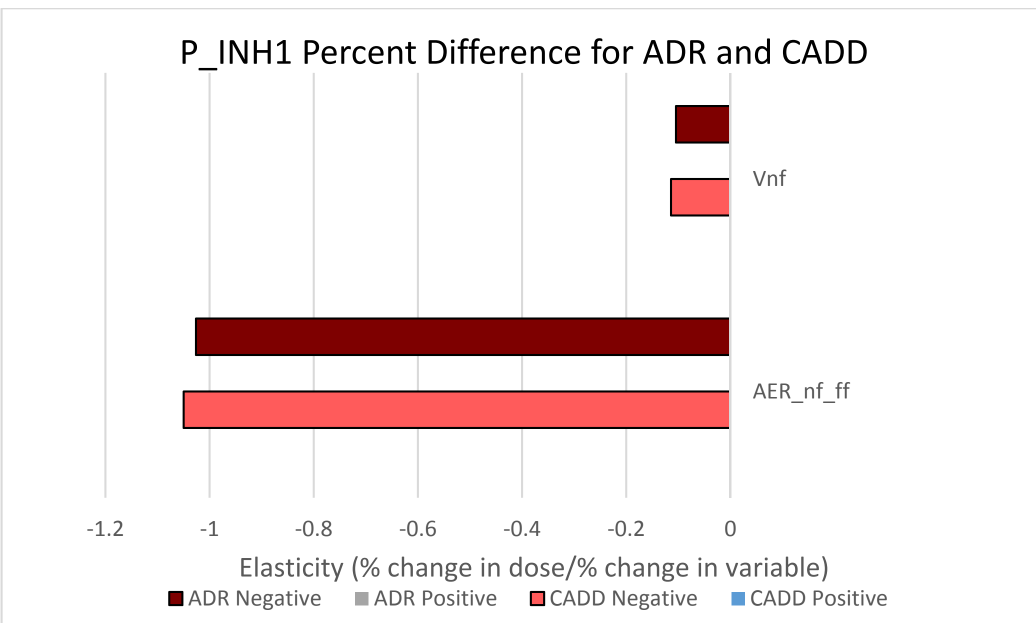

Figure D.16. Tornado plot of the elasticity for Near Field-Far Field variables.

Table D.11. Elasticity results for non-linear parameters in SVOC models. (Parameters with an absolute elasticity ≥ 0.05 are shaded).

Parameter Full Name	Model Name For Parameter	Gas Phase CADD	Gas Phase ADR	Particulate Phase CADD	Particulate Phase ADR	Ingestion After Inhalation CADD	Ingestion After Inhalation ADR	Incidental Dust Ingestion CADD	Incidental Dust Ingestion ADR	Skin Contact CADD	Skin Contact ADR	Vapor to Skin Chronic	Vapor to Skin Acute
RP Particle Deposition Rate Constant	kdep_TSP	-0.000625	0.000000	0.000000	0.000000	-0.000026	-0.000026	0.000000	0.000000	0.000000	0.000000	-0.000544	-0.000053
Abraded Article Particle Deposition Rate Constant	kdep_AbArt	0.000000	0.000000	-0.091148	-0.091063	-0.091090	-0.091090	-0.000011	0.000001	0.000000	0.000000	0.000018	0.000002
Abraded Article Particle Overall Gas-Phase Mass Transfer Coefficient	H_AbArt	0.000208	0.000000	1.000000	1.000000	-0.000153	-0.000153	-0.006257	-0.000363	0.000000	0.000000	0.000194	0.000021
Abraded Article Particle Resuspension Rate Constant	kres_AbArt	0.000000	0.000000	0.018315	0.016908	0.018476	0.018476	0.000109	0.000000	0.000000	0.000000	0.000018	0.000002
Area of Emitting Surface	As	0.000000	0.000000	0.000000	0.000000	0.000419	0.000419	0.000183	0.000069	1.000000	1.000000	0.999789	0.999978
Area of Internal Surfaces	A_Int	-0.093267	-0.093304	0.000000	0.000000	-0.000039	-0.000039	-0.000017	-0.000006	-0.100000	-0.100000	-0.093262	-0.093313
Cleaning Efficiency	Cl_Eff	0.000000	0.000000	-0.010316	-0.010204	-0.010161	-0.010161	0.002899	-0.000024	0.000000	0.000000	-0.000058	-0.000006
Cleaning Frequency	CL_Fr	-0.000318	-0.000632	-0.003720	-0.004599	-0.003276	-0.003276	0.000899	-0.000003	0.000000	0.000000	0.000462	0.000013
Concentration of RP in Ambient Air	AmbPartConc	0.000000	0.000000	0.000000	0.000000	0.000002	0.000002	0.000000	0.000000	0.000000	0.000000	-0.000058	-0.000006
Density of Dust Particle	rho_Dust	0.000000	0.000000	0.000000	0.000000	-0.000031	-0.000031	0.000000	0.000000	0.000000	0.000000	0.000030	0.000003
Density of Dust Particle, Modified	rho_Dust*	0.000000	0.000000	0.000000	0.000000	-0.000031	-0.000031	0.000000	0.000000	0.000000	0.000000	0.000030	0.000003
Density of RP Particle	rho_TSP	0.000000	0.000000	0.000000	0.000000	-0.000011	-0.000011	-0.000006	-0.000006	0.000000	0.000000	0.000313	0.000033
Density of RP Particle, Modified	rho_TSP*	0.000208	0.000000	0.000000	0.000000	-0.000011	-0.000011	-0.000006	-0.000006	0.000000	0.000000	0.000313	0.000033
Diffusion Coefficient	Diffusion_Coef	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Diffusion Coefficient, Modified	Diffusion_Coef*	-0.005420	-0.005182	0.000000	0.000000	-0.000002	-0.000002	-0.000001	0.000000	0.000000	0.000000	-0.005287	-0.005308
Dust Deposition Rate Constant	kdep_Dust	0.000000	0.000000	0.000000	0.000000	-0.111111	-0.111111	-0.111111	-0.111111	0.000000	0.000000	-0.000015	-0.000001
Dust Overall Mass Transfer Coefficient	H_Dust	-0.000417	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	-0.000303	-0.000031
Dust Resuspension Rate Constant	kres_Dust	0.000000	0.000000	0.000000	0.000000	0.000178	0.000178	0.000000	0.000000	0.000000	0.000000	0.000007	0.000000
Environment of Use	Vol_Zone1	-0.000625	-0.000829	-0.091148	-0.091365	-0.091120	-0.091120	-0.000013	0.000000	0.000000	0.000000	-0.000563	-0.000051
Fraction of Organic Matter Dust	Fom_DUST	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Parameter Full Name	Model Name For Parameter	Gas Phase CADD	Gas Phase ADR	Particulate Phase CADD	Particulate Phase ADR	Ingestion After Inhalation CADD	Ingestion After Inhalation ADR	Incidental Dust Ingestion CADD	Incidental Dust Ingestion ADR	Skin Contact CADD	Skin Contact ADR	Vapor to Skin Chronic	Vapor to Skin Acute
Fraction of Organic Matter TSP	Fom_TSP	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Fraction of Organic Matter Abraded Article	Fom_AbArt	0.000000	0.000000	1.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Henry's Law Constant	H_law	0.000000	0.000000	0.000000	0.000000	0.000002	0.000002	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Henry's Law Constant, Modified	H_law*	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	-0.087201	-0.087201
HVAC Air Filter Penetration Efficiency	Fil_Pen	-0.000208	0.000000	0.000000	0.000000	0.000002	0.000002	0.000000	0.000000	0.000000	0.000000	-0.000058	-0.000006
Ingestion Fraction Abraded Article	IF_Abr	0.000000	0.000000	0.000000	0.000000	0.999584	0.999584	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Ingestion Fraction Dust	IF_DUST	0.000000	0.000000	0.000000	0.000000	0.000307	0.000307	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Ingestion Fraction RP	IF_TSP	0.000000	0.000000	0.000000	0.000000	0.000109	0.000109	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Initial Concentration of SVOC in Article	C0_art	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	0.000000	0.000000	1.000000	1.000000
Interior Surfaces Overall Mass Transfer Coefficient	H_Int	-0.093162	-0.093201	0.000000	0.000000	-0.000039	-0.000039	-0.000017	-0.000006	0.000000	0.000000	-0.093147	-0.093214
Interzone Ventialtion Rate	Q_z12	-0.087763	-0.087687	-0.090720	-0.090821	-0.090694	-0.090694	-0.000003	-0.000009	0.000000	0.000000	-0.087680	-0.087737
Log KOA	LogKoa	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Log KOA, Modified	LogKoa*	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Log Kow	LogKow	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Log Kow, Modified	LogKow*	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.075542	0.075542
Mass Generation Rate of Abraded Article Particles	g_AbArt	0.000000	0.000000	1.000000	1.000000	0.999584	0.999584	0.000000	0.000001	0.000000	0.000000	0.000018	0.000002
Mass Generation Rate of Dust into Indoor Air	g_ADust	-0.000208	0.000000	0.000000	0.000000	0.000227	0.000227	0.000000	0.000000	0.000000	0.000000	-0.000224	-0.000023
Mass Generation Rate of Dust onto Indoor Floor	g_FDust	0.000000	0.000000	0.000000	0.000000	0.000194	0.000194	0.000000	0.000000	0.000000	0.000000	0.000005	0.000000
Mass Generation Rate of RP Particle onto Indoor Floor	g_FTSP	-0.000208	0.000000	0.000000	0.000000	0.000003	0.000003	0.000000	0.000000	0.000000	0.000000	-0.000098	-0.000010
Mass Generation Rate of RP Particle into Indoor Air	g_ATSP	-0.002918	-0.000207	0.000000	0.000000	0.000102	0.000102	-0.000001	0.000000	0.000000	0.000000	-0.002919	-0.000313
Molecular Weight	MW	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Parameter Full Name	Model Name For Parameter	Gas Phase CADD	Gas Phase ADR	Particulate Phase CADD	Particulate Phase ADR	Ingestion After Inhalation CADD	Ingestion After Inhalation ADR	Incidental Dust Ingestion CADD	Incidental Dust Ingestion ADR	Skin Contact CADD	Skin Contact ADR	Vapor to Skin Chronic	Vapor to Skin Acute
Molecular Weight, Modified	MW*	-0.146341	-0.145522	0.000000	0.000000	0.001132	0.001132	0.003109	0.000088	0.000000	0.000000	-0.988648	-0.988665
Radius of Dust Particle	r_DUST	0.000000	0.000000	0.000000	0.000000	-0.000031	-0.000031	0.000000	0.000000	0.000000	0.000000	0.000030	0.000003
Radius of Dust particle, Modified	r_DUST*	0.000000	0.000000	0.000000	0.000000	-0.000031	-0.000031	0.000000	0.000000	0.000000	0.000000	0.000030	0.000003
Radius of RP Particle	r_TSP	0.000208	0.000000	0.000000	0.000000	-0.000011	-0.000011	-0.000006	-0.000006	0.000000	0.000000	0.000313	0.000033
Radius of RP Particle, Modified	r_TSP*	0.000208	0.000000	0.000000	0.000000	-0.000011	-0.000011	-0.000006	-0.000006	0.000000	0.000000	0.000313	0.000033
Radius of Abraded Article Particles	r_AbArt	0.000000	0.000000	0.000000	0.000000	0.000016	0.000016	0.000669	0.000036	0.000000	0.000000	-0.000021	-0.000002
Radius of Abraded Article Particles Modified	r_AbArt*	0.000000	0.000000	0.000000	0.000000	0.000016	0.000016	0.000669	0.000036	0.000000	0.000000	-0.000021	-0.000002
RP Particle Overall Mass Transfer Coefficient	H_TSP	-0.003127	-0.000207	0.000000	0.000000	0.000105	0.000105	0.000055	0.000060	0.000000	0.000000	-0.003031	-0.000326
RP Particle Resuspension Rate Constant	kres_TSP	0.000000	0.000000	0.000000	0.000000	0.000060	0.000060	0.000000	0.000000	0.000000	0.000000	0.000018	0.000000
Saturation Concentration	CSATA	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SVOC Article-Air Partition Coefficient	K_art	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SVOC Dust Air Partition Coefficient	K_DUST	0.000000	0.000000	0.000000	0.000000	0.000306	0.000306	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SVOC Gas Phase Mass Transfer Coefficient	h	0.958307	0.000000	-0.004274	0.000000	-0.003683	-0.003683	-0.003612	0.000050	0.000000	0.000000	0.958871	0.999639
SVOC Gas Phase Mass Transfer Coefficient, Modified	h*	0.180738	0.191542	-0.003663	0.000604	-0.003063	-0.003063	-0.009453	-0.000191	0.000000	0.000000	0.179950	0.191580
SVOC Interior Surface Air Partition Coefficient	K_Solid	-0.099979	-0.100000	0.000000	0.000000	0.000395	0.000395	0.001054	0.000032	0.000000	0.000000	-0.099962	-0.100000
SVOC Interior Surface Air Partition Coefficient, Modified	K_Solid*	-0.097895	-0.100518	0.000000	0.000000	0.000394	0.000394	0.001054	0.000032	0.000000	0.000000	-0.100493	-0.100531
SVOC RP-Air Partition Coefficient	K_TSP	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Thickness of Article Surface Layer	Source_Thick	0.000417	0.000000	0.000000	0.000000	0.000420	0.000420	0.000389	0.000002	0.000000	0.000000	0.000421	0.000003
Thickness of Emitting Surface	Int_Thick	-0.000208	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	-0.000045	0.000000

Parameter Full Name	Model Name For Parameter	Gas Phase CADD	Gas Phase ADR	Particulate Phase CADD	Particulate Phase ADR	Ingestion After Inhalation CADD	Ingestion After Inhalation ADR	Incidental Dust Ingestion CADD	Incidental Dust Ingestion ADR	Skin Contact CADD	Skin Contact ADR	Vapor to Skin Chronic	Vapor to Skin Acute
Transdermal Permeability Coefficient	Kp_g	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	1.000000	1.000000
Vapor Pressure	VP	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Vapor Pressure, Modified	VP*	0.697728	0.716003	-0.002442	0.000000	-0.002134	-0.002134	-0.005674	-0.000170	0.000000	0.000000	0.698265	0.715184

APPENDIX D: Model Corroboration

Introduction

In order to critically evaluate the CEM models, corroboration exercise was performed to compare the results of CEM with other model results and measured data. A literature search was conducted to identify data sources that could potentially be used for corroboration. The most appropriate and complete paper for each model was selected for comparison.

There were very few studies that reported internal doses, therefore CEM media concentrations were compared with measured media concentrations and model results. There were five CEM models for which we could not identify a suitable corroboration source (A_DER2, P_ING1, P_ING2, A_ING2, A_ING3). For each paper, the available data were reviewed and used to build a scenario in CEM. CEM defaults were used for any input parameters that were not reported.

One issue which complicated the corroboration was the lack of internal dose measurements reported and comparable parameters used in CEM models. CEM defaults were used and assumptions were made for papers that did not fully report required inputs. This could have led to an unfaithful comparison of concentrations between the published experiments and CEM results. This includes comparing media concentrations instead of internal doses. Another issue was the lack of comparison studies for five CEM models. These models could be corrobroated as suitable data become available. Overall CEM performed well for the models that were compared.

Product models

Emission models

For E1, E2, E3, E4, and E5 the media concentration measured in the study was compared to the concentrations estimated in Zone 1. For all models, the difference between the models was calculated by dividing the models estimation by the modeled or empirical data from the study. The near field-far field (NF/FF) option was switched to off for all runs except for the corroboration scenario comparing the NF/FF option. The model inputs that were assumed and held constant across all corroboration scenarios for product models are shown in Table 11. The selected user was an adult with a Stay-At-Home activity pattern since it was assumed the experiments enrolled adult users and a Stay-At-Home activity pattern maximized the exposure similar to the corroboration studies. The value for background concentration was the concentration in the air for both Zone 1 and 2.

Table 11. Model inputs held constant across corroboration exercise.

Variable	Input
Emission Rate	CEM estimated
Frequency of Use	1 per day, 365 days/year
User	Adult
Activity Pattern	Stay-At-Home
Building Volume (m^3)	492
Air Exchange Rate from Zone 2 (per hour)	0.45

Dilution Fraction	1
Background Concentration (mg/m^3)	0

E1

The van Veen et al. 2002 reference was selected for comparison with the E1 Emission from Product Applied to a Surface Indoors Incremental Source Model. In this study, 400 grams of paint stripper was weighed out and participants were instructed to spread the paint thinner on a table top in an equal layer. After application, participants were asked to move around the room for an hour then scrape off the remaining paint stripper into a receptacle. The study was conducted in a single room and focused on measuring dichloromethane. The concentration was measured at a height of 1.5 cm above the surface of the table. There were three experiments and each had two runs, A and B. Runs A and B from experiment one were selected to compare against E1 results since they were the two runs that were closest to each other in terms of environmental conditions.

This paper was selected to corroborate model E1 because there was not a paint layer for the stripper to penetrate. Thus this could approximate a first order decay. The product type selected was all-purpose liquid cleaner/polish (neat) as this type of product uses the E1 model. Although paint stripper is a product option, it assumes that the stripper is applied to something to remove a layer of paint, which was not the case in this study. Table 1 shows the variables that were extracted from the paper and used in the CEM model. The "Mass of Product Used Acute" is less than 400 because the actual amount of paint stripper that was used by the study participant was less than the total amount provided in the original experimental design.

Table 12. Model inputs from Van veen 2012 for E1.

Variable	Input
Air Exchange Rate, Zone 1 (per hour)	0.2844
Chemical of Interest	Dichloromethane
Duration of Use Acute (min/use)	13
Duration of Use Chronic (min/use)	13
Mass of Product Used Acute (g/use)	350
Molecular Weight (g/mol)	84.9
Use Environment Volume (m^3)	47.65
Vapor Pressure (torr)	352.529
Weight Fraction (-)	0.659

Since there was no similar room in CEM to the experimental set up in the paper, the living room was chosen; since the size of the room was changed based on the experimental data, this only affected the interzone ventilation rate. The interzone ventilation rate is fixed with the room choice and was not changed. Since the room was flushed between each experiment there should not have been any background concentration, and the CEM estimates did not include a background concentration.

Table 13. Estimated and assumed defaults for E1.

Variable	Input	Note
Saturation in Air Concentration (mg/m^3)	1.6 x10^7	Estimated
Environment of Use	Living Room	Assumed
Interzone Ventilation rate (m^3/hr)	108.978	Assumed
Body Weight (kg)	80	Assumed
SA-BW Ratio (cm^2/kg)	122.94	Assumed

This paper did not report internal dose concentrations, therefore the CEM estimated concentrations at set time points were compared to the concentrations reported in the paper, Figure 2(a) from van Veen et al. 2002 (Figure 3). The article reported that the experiment started measurements after the application was completed at 13 minutes, therefore T_0 was set to 13 minutes in CEM. However, CEM measures air concentrations when the product is applied.

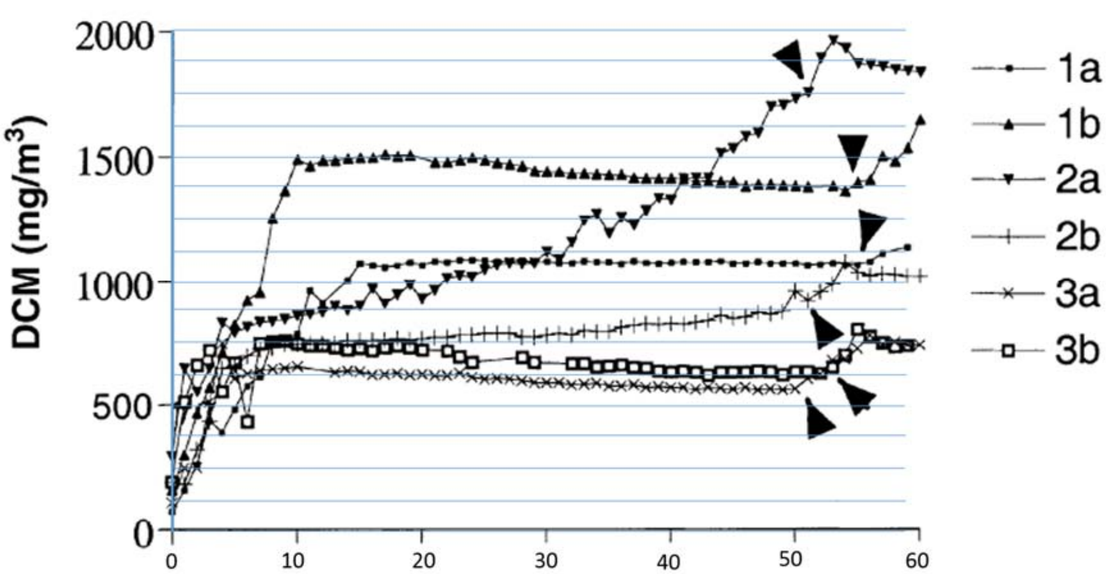

Figure 3. Time series from van Veen et al. 2002**.**

Each symbol on Figure 1 is a minute interval. To be comparable with the experimental set up, lines were added to **Error! Reference source not found.** to estimate the minute concentration levels based on the graph. These concentrations were compared to the time points generated in the CEM model. Since CEM measures every ½ minute, the empirical value for the minute was repeated for the half minute time step.

The data points from experiment 1, Run A and B, (shown in black circles and the triangles, respectively) were used to compare against CEM results. The larger black triangles represent when the paint stripper was scrapped off the table. Since the E1 model assumes the source is still present, the comparison ended at 54 minutes when the paint was scrapper off. The concentration in zone 1 from CEM averaged to be 1.80x 10^3 mg/m^3; E1 on average overestimated the measured concentration by 1.65 times the experimental concentrations.

The difference could be due to the interaction of other chemicals within the stripper formula. According to Raoult's law (Eq 1) the partial pressure of a compound is less than the vapor pressure of the compound in pure solution. Since E1 models the emission of a pure chemical, the rate that dichloromethane vaporized was higher than the rate of dichloromethane in the paint stripper formula which may have resulted in CEM estimating a higher emission concentration.

$$P_i = P_i^* \times x_i \qquad [1]$$

Where,

P_i = Partial pressure of compound *i*

P_i^* = Vapor pressure of compound *i* in pure solution

x_i = Mole fraction of compound *i* in the mixture

E2

The E2 Emission from Product Applied to a Surface Indoors Double Exponential Model has been extensively compared to chamber data and air concentrations from a test house, which has been documented in the user's guide of EPA's Wall Paint Exposure Model (GEOMET Technologies, Inc, 2001). In particular, Appendix E documents model inputs for scenarios that were compared with measurements in different rooms of the test house. There was generally a high degree of correspondence between modeled and measured values, although there was variation across chemical and paint-product scenarios.

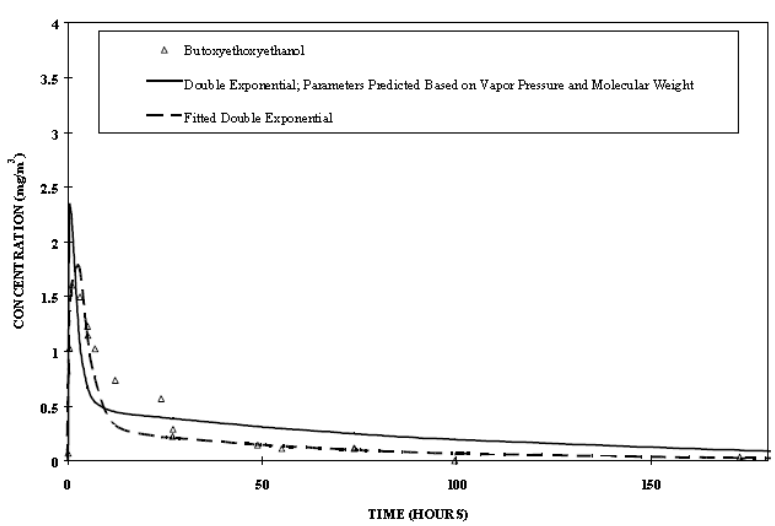

Figure 2. Time series from Wall Paint Exposure Model Guide

E3

Bartzis et al. 2015 was selected as a comparison study for E3, Emission from Product Sprayed Model. The paper measured the emission rate of different products in three different labs. The particular set of experiments that was compared to E3 was perfume spraying and the chemical limonene. The perfume was sprayed onto a piece of cloth in a test chamber. The concentration of the limonene was measured at set time intervals and it was assumed that the experiment was over after all the perfume evaporated. The paper reported the total amount emitted of limonene.

This paper was selected to compare to E3 because the perfume was sprayed, thus some of it was aerosolized. The chamber volume was used as the environment of use volume, shown in Table 4. It was assumed that the weight fraction of limonene was equal to the amount emitted over the course of the experiment. The amount of product being aerosolized was set to the default amount since the amount aerosolized was not measured (Table 5). The paper reported that it was vaporized so this value was appropriate. There was no indication of the amount of time that it took to spray the perfume but it was assumed to be a short period of time, 3 minutes. This may have been an underestimation but the small amount, 0.2 grams, was assumed to be sprayed over a short period of time.

Table 4. Model inputs from Bartzis et al. 2015 for E3.

Variable	Input
Air Exchange Rate, Zone 1 (per hour)	0.5
Chemical of Interest	Limonene
Interzone Ventilation rate (m^3/hr)	0
Mass of Product Used Acute (g/use)	0.2
Use Environment Volume (m^3)	20.24
Weight Fraction (-)	0. 000611

Table 5. Estimated and assumed defaults for E3.

Variable	Input	Note
Saturation in Air Concentration (mg/m^3)	9.5×10^3	Estimated
Aerosol Fraction	0.06	Assumed
Duration of Use Acute(min/use)	3	Assumed
Body Weight (kg)	80	Assumed
SA-BW Ratio (cm^2/kg)	122.94	Assumed
Vapor Pressure (torr)	1.3	ScienceLab.com, 2005
Molecular Weight (g/mol)	136.23	ScienceLab.com, 2005

The total amount emitted after 306 minutes reported in the paper was compared to the E3 output. To calculate the total amount that would be emitted by CEM, the emission rate was used to determine the total amount that would have been emitted after 306 minutes. CEM calculates the emission rate every half minute in mg/hr. To calculate the amount emitted, each half minute emission rate was multiplied by 120 (the number of half minutes in an hour). This was then summed over the duration of 612 half minute emission amounts. The sum of this (which equals total amount emitted up to that point) was compared to the total amount emitted in the paper.

CEM estimated the total amount emitted to be 2.03×10^{-3} mg; this corresponds to the model estimating 0.02 as much would have been emitted compared to the actual measured amount. Differences between the model results and the paper could be attributed to the actual concentration in the perfume being much higher than what was estimated by the amount emitted. It was assumed that the cut off time in the lab corresponded to all of the material evaporating, however this could be an underestimation of the true concentration. If the initial amount was higher, then more would be able to evaporate at once.

E3 NFFF

Nicas 2016 was selected to compare against E3 using the near field-far field (NFFF) option. The paper modeled exposure to benzene concentrations reported in Williams et al., 2007. In Williams et al. 2007, a participant took a formulated 10 ml of liquid wrench and applied it to a few objects in a garage. The person did this for 15 minutes then moved to a zone away from the application area for 15 minutes. After that, the person went back and applied the product again for 15 minutes and then retreated for 15 minutes. Personal exposure was recorded during the application period. There were two runs for each of the 11 exposure scenarios, for a total of 22 experimental runs. The values from the first and second application period were averaged from both runs to produce an average 15 minute time-weighted average exposure in the near field.

The Nicas paper used a series of differential equations to estimate what the inhalation exposure was using this scenario. The Nicas model estimated that the exposure for the second application would be the sum of an application by itself plus the residual decay of the benzene already present if it was modeled by itself. The same methodology was applied in the E3 NFFF CEM model.

The fifth experimental run was selected to compare to E3 NFFF results since the specific gravity was available to estimate the mass of liquid wrench used. Nicas and the CEM simulation assumed that the 10 ml was applied over the 15 minute period. The paper stated the benzene concentration between experimental runs was lower than the level of detection. Therefore, the background concentration was set to zero in the CEM simulation, as shown in Table 6.

To derive the percent mass of liquid wrench used, the specific gravity of liquid wrench was assumed to be compared to water with a density of one. The amount of benzene that was added to spike the concentration was assumed to not change the density (although it would, the initial concentration was not reported). The specific gravity was multiplied by the volume (10 mL) to obtain the amount of liquid wrench used (Table 7). Other required input values that were not provided in the paper were assumed and estimated (Table 7). Equation 2 was used to obtain the percent mass.

$$M_{\%} = \rho \times \frac{V_{\%}}{M_{sol}} \quad [2]$$

Where,

$M_{\%}$ = Percent mass

ρ = density of benzene at 25°C (g/cm^3)

$V_{\%}$ = Percent volume by solution

M_{sol}= Mass of solution (g)

Table 6. Model inputs from Nicas 2016 for E3 NF/FF.

Variable	Input
Air Exchange Rate, Zone 1 (per hour)	6.8
Background Concentration (mg/m^3)	0
Chemical of Interest	Benzene
Duration of Use Acute(min/use)	15
Duration of Use Chronic(min/use)	15
Environment of Use	Garage
Use Environment Volume (m^3)	140

Table 7. Estimated or assumed defaults for E3 NF/FF.

Variable	Input	Note
Saturation in Air Concentration (mg/m^3)	3.1 x 10^5	Estimated
Aerosol Fraction	0.01	Assumed
Air Exchange rate between NF/FF (per hour)	402	Assumed
Far Field Volume (m^3)	139.00	Assumed
Interzone Ventilation rate (m^3/hr)	108.978	Assumed
Mass of Product Used Acute (g/use)	8.5	Assumed
Mass of Product Used Chronic (g/use)	8.5	Assumed
Near Field Volume (m^3)	1	Assumed
Weight Fraction (-)	0.028784	Assumed
Body Weight (kg)	80	Assumed
SA-BW Ratio (cm^2/kg)	122.94	Assumed
Molecular Weight (g/mol)	78.1	NIOSH 2003
Vapor Pressure (torr)	75.00	NIOSH 2003
Density (g/cm^3)	0.87383[a]	DDBST, 2017

[a] Density at 298 K

The empirical data from Experiment 5 in Williams et al. 2007 and the model predicted values from Nicas 2016 were used for comparison with concentration estimates from the near-field model. In addition, the previously described additive assumption for the second dose was utilized. The average dose between all the time steps (even the initial concentration of zero at time zero) were used to derive the average 15 minute concentration in the near field zone.

The results from CEM were 2.71 mg/cm^3 for zone 1 near field; this is 3.81 times higher than the modeled data from Nicas and 3.01 times more than the empirical data from Williams et al. 2007. This is because the Nicas model underestimated the empirical data. A large portion of this deviance, although it is very close to the real value, could be explained by the near-field zone size. Since the paper did not describe whether the product was sprayed over a large area, nor how much of the benzene would have mixed, this volume is likely to be smaller than what was used. If the high estimate volume for near field zone (5 m^3) was used instead then the average concentration be lower and would be closer to both the model and the empirical data.

E4 & P_DER1b

In this experiment by Webster et al. 2016, the authors created a physiologically based pharmacokinetic (PBPK) model for exposure to chloroform from showering. The authors compared the modeled results to actual measured exposure. This paper was used as a comparison for E4 Emission from Product Added to Water and for P_DER1b Dermal Dose from Product Applied to Skin, Permeability Model. The person was an average man who took a 10 minute shower that contained 0.021 mg/L of chloroform (Table 8). After that, the person dried off and an air sample was taken from the person exhaling. To obtain the difference between dermal and inhalation, the initial experiment had people bathe in such a way that they did not have dermal exposure, and then repeated the experiment with dermal exposure. Webster et al., 2016 did not explain how the original study was able to replicate bathing without dermal exposure. The modeled values were then compared to the actual measured values with all values being within an order of magnitude.

For this scenario in CEM, it was assumed that water was not draining. This had to be assumed for the model corroboration because CEM does not allow for the product to disappear unless by evaporation. The mass of the amount used was calculated from the assumption that 87 liters were used and that a liter of water was 1000 g. This resulted in a used mass of 8700 grams. The weight fraction was calculated by dividing the concentration of chloroform in water (0.021 mg/L) by the mass of a liter of water as shown in Table 9. The SA-BW was calculated by the amount of skin exposed used in the model (1.9 m^2) and a body weight of 73 kg, as shown in Table 9.

Table 8. Model inputs from Webster et al., 2016 for E4 and P_DER01b.

Variable	Input
Air Exchange Rate, Zone 1 (per hour)	0.52
Body Weight (kg)	73
Chemical of Interest	Chloroform
Duration of Use Acute(min/use)	10
Environment of Use	Bathroom
Interzone Ventilation rate	125
Log Octanol-water Coefficient	2
Molecular Weight (g/mol)	119
SA/BW	260.27
Skin Permeability Coefficient (cm/hr)	0.1
Use Environment Volume (m^3)	50

Vapor Pressure (torr)	196.51616

Table 9. Estimated and assumed defaults for E4 and P_DER01b.

Variable	Input	Note
Saturation in Air Concentration (mg/m^3)	1.2 x 10^6	Estimated
Density of water (g/cm^3)	1	Assumed
Product Dilution Factor	1	Assumed
Weight Fraction of Chemical in Product	2.1 x 10^{-8}	Assumed

The mass of chloroform in various compartments of the body was calculated based on concentrations in each compartment estimated by the PBPK model and the respective volumes, shown in Table 10. This was done by multiplying the compartment concentration by the compartment volume. Then the exposure dose for the body was calculated using Equation 3. The approximate dose per day was calculated for each exposure route using Equation 4 (with the assumption that a person only takes one shower a day).

Table 10. Body compartments values from PBPK model.

Body Compartment	Concentration (ng/m^3)	Volume (m^3)	Mass of chloroform in compartment (ng)
Arterial	285000	0.000954	271.89
Venous blood	208000	0.004346	903.968
Liver tissue	65405	0.0018	117.729
Skin	689000	0.003	2067
Slowly perfused tissue	179000	0.0402	7195.8
Richly perfused tissue	1740000	0.0045	7830
Fat tissue	103000	0.0182	1874.6
		Total chloroform	20261

$$Dose_{body} = \frac{\sum_i^j m_i}{m_{body} * 1 * 10^{-3}} \quad [3]$$

Where,

$Dose_{body}$ = Total body burden (µg/kg)

m_i= Mass of chloroform for compartment *i* (µg)

m_{body}= Mass of body, 73 kg

$$DD_{path} = Dose_{body} \times \frac{C_{path}}{C_{tot}} \times \frac{C_{report}}{C_{path}} \times CF_1 \quad [4]$$

Where

DD_{path}= Dose per day per pathway (mg/kg/day)

C_{report}= Reported concentration (μg/m^3)

CF_1= 1 x 10^{-3} (mg/μg)

C_{path}= PBPK model concentration for exposure pathway (μg/m^3)

C_{tot}= Total PBPK model concentration (μg/m^3)

The estimated daily dose per exposure pathway was then compared to the CEM values. Inhalation exposure was estimated using an intermediate value calculated by CEM for the adult user in Zone 1 at 15 minutes. For E4, CEM predicted almost the same actual inhalation dose as seen in Table 11, however the dermal dose from P_DER1b was 1.6 times larger as also seen in Table 11. The higher dose of chloroform entering the skin could be attributed to the fact that CEM did not include the amount of water that was removed when the person dried off and the amount of water that washed over the body but did not allow the chemical to penetrate the skin. CEM assumes that all of the chemical in the water would have had a chance to enter the skin which would lead to an over estimation.

Table 11. Comparison of Internal doses from CEM and Webster et al., 2016.

Parameter	CEM's Value	Value from Mitro et al., 2016
Inhalation dose (mg/kg/day)	2.62 * 10^{-5}	2.61* 10^{-5}
Dermal dose (mg/kg/day)	9.11*10^{-5}	5.67 *10^{-5}

E5

Singer et al. 2006 was selected for comparison against E5, Emission from Product Placed in Environment Model. The study tested various home products in a model room, which contained a wooden floor with a small portion with vinyl tiles, two gypsum walls, and a table. For one of the experiments, the initial weight of air freshener oil was measured and an air freshener was plugged in for three days. Air samples and the mass of the air freshener oil was measured at 2, 8, 21, 29, 51, and 73 hours after installation. The chemical benzyl acetate was selected for analysis because it was not reactive with ozone, which could have skewed the concentration measurements.

The product scenario from CEM was a continuous action air freshener. Other input values extracted from the paper are shown in Table 12. The interzonal rate between the two rooms was set to the default of 108.978 m^3/hr as shown in Table 13. Equation 5 was used to calculate the mass fraction of benzyl acetate.

$$M = \frac{C_{BA}}{\sum X_i / 0.65} \quad [5]$$

Where

X_i = individual components listed in Table 5 from Singer et al., 2006

M= Mass fraction of benzyl acetate

C_{BA}= Concentration of benzyl acetate, 136 mg/L

Table 12. Model inputs from Singer et al., 2006 for E5.

Variable	Input
Air Exchange Rate, Zone 1 (per hour)	0.54
Chemical of Interest	Benzyl acetate
Duration of Use Acute(min/use)	1440
Environment of Use	Living room
Mass of Product Used Acute (g/use)	1.5
Use Environment Volume (m^3)	50
Weight Fraction (-)	0.205

Table 13. Estimated and assumed default values for E5.

Variable	Input	Note
Saturation in Air Concentration (mg/m^3)	1.4×10^3	Estimated
Interzone Ventilation rate (m^3/hr)	108.978	Assumed
Body Weight (kg)	80	Assumed
SA-BW Ratio (cm^2/kg)	122.94	Assumed
Molecular Weight (g/mol)	150.2	ICSC 2012
Vapor Pressure (torr)	1.42512	ICSC 2012

Due to the way CEM is programed, use of a chemical cannot last beyond a 24 hour period. Therefore, the start time for the product use was set at midnight and the concentration of benzyl acetate was averaged over a 24 hour day. The average ambient concentration in compartment 1 from CEM was compared to the average concentration from Singer et al. 2006 study. It was found that CEM's average concentration was 0.104 mg/cm^3; this was 0.470 of the concentration measured in Singer et al. 2006.

While this is within an order of magnitude, sampling time and the amount used were quite different for CEM and Singer et al 2006. Singer et al. 2006 used more than three times the amount of product than what was used in the CEM model scenario, as the oil did not run out before the experiment ended. Even though the model used the actual amount used per day in terms of oil consumed, the experiment had a larger quantity of benzyl acetate to evaporate. This could lead to a larger amount of chemical released than what was predicted by the CEM model. Also, since CEM is a two zone model, the amount of chemical released would have migrated to the second room and would therefore lead to an overall lower concentration.

P_DER1a

In addition to the input values required to estimate exposure for all pathways, such the frequency and duration of product use, estimating dermal exposure from product use requires an understanding of the amount of product in contact with the skin (thickness of product layer and area of skin contact) and a value that describes absorption of the chemical through the skin, either in the form of a fraction absorbed or a permeability coefficient.

In CEM, values describing absorption can be either specified or estimated using equations built into CEM. Estimating the permeability coefficient requires the chemical's molecular weight and octanol-water partitioning coefficient. The fraction absorbed estimator requires these properties as well as the chemical's vapor pressure and solubility.

Publications that present experimentally determined thickness of product layer, fraction absorbed, or permeability coefficients along with the chemical name or appropriate physical-chemical properties were considered for corroboration. However, no papers that meet all of these criteria were identified.

Article Models

Two different papers were used to corroborate the CEM article models: Sukiene et al. 2016 and Mitro et al. 2016. The article models in CEM required a large number of parameters that were not reported in either paper. CEM defaults listed in Table 16 were used for the unreported input parameters in both papers. The only difference was that Sukiene et al. 2016 reported the environment of use (Living Room) while this was not reported in the Mitro et al. 2016 paper. Sukiene et al. 2016 was selected to compare the CEM results from E6, Emission from Article Placed in Environment Model and A_ING1 Ingestion after Inhalation Model. Mitro et al. 2016 was selected to compare against A_DER1, Dermal Dose from Direct Transfer from Vapor Phase to Skin Model.

Table 16. Model inputs held constant across corroboration exercise for SVOC article model.

Variable	Input
User	Adult
Activity Pattern	Stay-at-home
Building Volume (m^3)	492
Background Dust Concentration (µg/g)	0
Environment of Use	Living Room[a]
Thickness of Article Surface Layer (cm)	0
Interzone Ventilation Rate (m^3/hr)	108.987
Thickness of Interior Surface (m)	0.005
HVAC Filter Penetration	0.05%
Cleaning Efficiency	0.46%
Ambient RP Concentration (mg/m^3)	0.052
RP Deposition Rate (per hour)	1
RP Deposition Rate (per hour)	3.3
Abraded Particles Deposition Rate (per hour)	2.34

RP Resuspension Rate (per hour)	2.6×10^{-5}
Dust Resuspension Rate (per hour)	2.1×10^{-4}
Dust Resuspension Rate (per hour)	2.2×10^{-4}
RP Mass Generation Rate, Suspended (mg/hr)	14.7
Dust Mass Generation Rate, Suspended (mg/hr)	117.9
Abraded Particle Mass Generation Rate (mg/hr)	5.31×10^{-3}
RP Mass Generation Rate, Floor (mg/hr)	0.1
Dust Mass Generation Rate, Floor (mg/hr)	25.3
RP Radius of Particle (m)	5.0×10^{-6}
Dust Radius of Particle (m)	5.0×10^{-4}
Abraded Radius of Particle (m)	5.0×10^{-5}
RP Density of Particle (mg/m^3)	1.0×10^{9}
SA-BW Ratio (cm^2/kg)	122.94

[a] This was assumed in the Mitro et al. 2016, but was the actual room used in the Sukiene et al. 2016 study.

E6 and A_ING1

In Sukiene et al. 2016, four different objects were doped with different SVOCs in five different model apartments. The objects included a carpet, a counter top, a piece of vertical plastic, and another piece of vertical plastic that was under a heat lamp. None of the chemicals contained in one object were found in another. The carpet was placed near the front door of the apartment so as to increase the amount of abrasion due to heavy traffic. Every two weeks the room was cleaned and dust samples were collected off the floor. Every four weeks passive air samples were collected in which particles, such as dust, were captured. The air samples were divided into two fractions, where Fraction 1 contained particles >2mm and Fraction 2 contained particles < 2mm.

For the corroboration exercise, the rug was selected as the object of comparison and the CEM furniture cover scenario was used. The first apartment was selected and the chemical of interest was 1, 2-benzenedicarboxylic acid, dioctyl ester. The number of cleaning frequencies were calculated so that it was approximately once every 14 days, as shown in Table 17. The molecular weight and vapor pressure were obtained by looking up values in CEM's internal list of chemical properties. Based on the inputs and defaults, the article model estimated a number of parameters, shown in Table 18. The paper stated that the amount of organic carbon found in the dust was 0.7. Since the cutoff size for the dust fraction reported in the paper was much larger than the cutoff used by CEM, for all particles (dust, abraded, and TSP), the fraction of organic matter set to 0.7 as shown in Table 19. This was done since it could not be determined if the particles or dust had a larger or smaller composition. The chemical that was added to the rug had a purity of 100% so the weight fraction was set to 1.

Table 17. Model inputs from Sukiene et al., 2016, for E6 and A_ING1.

Variable	Input
Chemical of Interest	1, 2-benzenedicarboxylic acid, dioctyl ester
Cleaning Frequency (per hour)	0.003
Henry's Law Coefficient	2.57 E -06

Initial Concentration of SVOC in Article (mg/cm^3)	0.59
Log Kow	8.1
Log KOA	12.1
Molecular Weight (g/mol)	390.56
Surface Area of Article (m^2)	0.5016
Use Environment Volume (m^3)	88
Vapor Pressure (torr)	1 x -07
Weight Fraction (-)	1

Table 18. Variables estimated through CEM.

Variable	Input
Saturation in air concentration (mg/m^3)	2.1×10^{-3}
Solid-Phase Diffusion Coefficient (m^2/hr)	2.5×10^{-11}
Solid Air Partition Coefficient	2.2×10^{9}
SVOC Partition Coefficient, RP (m^3/mg)	8.8×10^{2}
SVOC Partition Coefficient, Dust (m^3/mg)	4.4×10^{2}
SVOC Partition Coefficient, Abraded Paricles (m^3/mg)	8.8×10^{2}
SVOC Gas Phase Transfer Coefficient (m/hr)	1.6
Overall Mass Transfer Coefficient, RP (m/hr)	1.6
Overall Mass Transfer Coefficient, Dust (m/hr)	1.6
Overall Mass Transfer Coefficient, Internal surface (m/hr)	1.5
Overall Mass Transfer Coefficient, Abraded Particle (m/hr)	1.6

Table 19. Assumed defaults for E6 and A_ING1.

Variable	Input
Dust, Fraction of Organic Matter	0.7
Abraded, Fraction of Organic Matter	0.7
RP, Fraction of Organic Matter	0.7
Density of Product/Article (g/cm^3)	1
Area of Interior Surface (m^2)	183.04

Since the paper did not measure internal dose, the concentration in the air and in the dust was compared. For CEM, the concentration in air was the sum of the chemical in the gaseous phase, the concentration in dust, TSP, and abraded particle times the respective mass of those particles in the air. The daily amounts were then averaged over a month to get the ambient concentration. Since the first two months were below the limit of detection, only the last month was compared. The concentration from CEM was 5.71×10^{-4} ug/m^3; this was 8.79 times than what was measured.

The concentration in the dust was calculated using Equation 6. The concentration of chemical at 2, 4, 6, 8, 10, and 12 weeks in the dust in CEM were compared against the concentration of Fraction 2 of the dust sample concentration from the paper per each week as seen in Table 20. The average of the differences between CEM values and the paper resulted in CEM predicting 2.24×10^{-4} times the value reported in Sukiene et al. 2016.

$$C_{dust} = \frac{\sum_i^j m_i \times C_i}{M_{tot}} \quad [6]$$

Where,

C_{dust}= Concentration of 1, 2-benzenedicarboxylic acid, dioctyl ester in the dust (µg/g)

m_i= Mass of component *i* (dust, TSP, and abraded particles) (g)

C_i= Relative concentration of 1, 2-benzenedicarboxylic acid, dioctyl ester in each component (µg/g)

M_{tot} = Total mass of dust, TSP, and abraded particles (g)

Table 20. Average concentration of 1, 2-benzenedicarboxylic acid, dioctyl ester in the dust (ug/g).

Week	CEM's Value (ug/g)	Value from Sukiene et al. 2016 (ug/g)
2	2.90×10^{-2}	130
4	2.93×10^{-2}	170
6	1.83×10^{-2}	110
8	2.08×10^{-2}	110
10	2.28×10^{-2}	82
12	2.45×10^{-2}	78

There are two possible reasons why the dust concentration values were different than the air concentrations. First, since the carpet was selected as the article modeled, there could have been a higher generation rate of abraded particles than what was estimated by CEM. Abraded particles have the highest concentration of the chemical with the smallest amount of mass. If the rate generation rate was underestimated, then the overall concentration in the estimated dust would be lower. The carpet may have captured dust and other particles such as abraded particles. This would lead to a higher concentration of particles that have a higher concentration of the chemical of interest to be in the carpet rather than in the air.

Second, having more particles captured in the carpet would lower the amount of dust that would be in the air. Since the average concentration of 1, 2-benzenedicarboxylic acid, dioctyl ester in the air is a concentration of the gaseous and all of the various particles, having a higher number of particles would not lower the concentration. This is unlike the dust, which is proportional to the amount of chemical over the amount of dust. Thus, if the rate that dust and the other particles being re-suspended from the article was overestimated, it would lead to a higher concentration in the air.

A_DER1

Mitro et al., 2016 was a meta-study that looked at the concentrations of 45 chemicals in 26 papers and one unpublished data set. All the samples came from workplaces and homes within the United States. They estimated the various intake from the range of dust concentrations using dose estimation equations. The chemical properties were estimated by using the EPA's EPI Suite program. Of the 45 chemicals reported, TDCIPP was selected for the comparison scenario.

The comparison was made between the equation in Mitro et al. 2016, and A_DER1 using a sofa as the article scenario since TDCIPP is used mainly as a flame retardant in furniture. The vapor pressure of the compound was obtained from the National Institute of Health as shown in Table 23 (National Library of Medicine HSDB Database 2013). As with the E6 and A_ING1, there were many parameters that had to be estimated in CEM since they were not reported in the paper, as shown in Table 22. To calculate an approximate concentration of TDCIPP in foam, a concentration of 3% was assumed (median value of what was reported in Stapleton et al., 2009) and multiplied it by the median value of foam density (0.04 g/cm^3 found in PFA, 1991) to obtain the value of 1.2 mg/cm^3 as shown in Table 23.

Table 21. Model inputs from Mitro et al., 2016, for A_DER1.

Variable	Input
Chemical of Interest	TDCIPP
Henry's Law Coefficient	2.61×10^{-9}
Log K_{ow}	3.65
Log K_{OA}	10.6
Molecular Weight (g/mol)	430.91
Vapor Pressure (torr)	2.90 E -07

Table 22. Variables estimated through CEM.

Variable	Input
Saturation in air concentration (mg/m^3)	671×10^{-3}
Solid-Phase Diffusion Coefficient (m^2/hr)	2.3×10^{-11}
Solid Air Partition Coefficient	9.6×10^{8}
SVOC Partition Coefficient, RP (m^3/mg)	1.7 x 10
SVOC Partition Coefficient, Dust (m^3/mg)	4.2
SVOC Partition Coefficient, Abraded Paricles (m^3/mg)	1.1×10^{-1}
SVOC Gas Phase Transfer Coefficient (m/hr)	1.5
Overall Mass Transfer Coefficient, RP (m/hr)	1.5
Overall Mass Transfer Coefficient, Dust (m/hr)	1.5
Overall Mass Transfer Coefficient, Internal surface (m/hr)	1.3
Overall Mass Transfer Coefficient, Abraded Particle (m/hr)	1.5
Transdermal Permeability Coefficient (m/hr)	1.25

Table 23. Assumed defaults for A_DER1.

Variable	Input	
Area of Interior Surface (m^2)	104	Assumed
Chemical Migration Rate ($mg/cm^2/hr$)	0.06	Assumed
Cleaning Frequency (per hour)	0.006	Assumed
Density of Article	0.04	Assumed
Film Thickness on Skin	0.1	Assumed
Surface Area of Article	3	Assumed
Thickness of Contact Layer (cm)	0.1	Assumed
Use Environment Volume (m^3)	50	Assumed
Weight Fraction	1	Assumed

Initial Concentration of SVOC in Article (mg/cm^3)	1.2	Calculated using Stapleton et al. 2009 and Polyurethane Foam Association 1991
Vapor Pressure (torr)	2.90 x 10^{-7}	National Library of Medicine HSDB Database 2013
Body Weight (kg)	80	Body Weight (kg)

To calculate the dose by adsorption out of the air that would have been predicted by Mitro et al., 2016, the geometric mean of the TDCIPP in residential dust samples were used. The equations found in the Supplemental Information portion of the paper were also used. The dust to gaseous air concentrations was calculated using Equations 7-13.

$$C_{Gas} = C_{dust} \times \frac{\rho}{x_{org} \times \log(K_{OA})} \times CF_1 \times CF_2 \quad [7]$$

Where,

C_{dust}= Dust concentration (µg/g)

ρ= density of dust (mg/m^3)

x_{org}= Fraction of organic material in dust (unitless)

K_{OA}= Octanol-air partition coefficient (unitless)

C_{gas} = Gaseous concentration (ng/m^3)

CF_1= Conversion factor (1 x 10^{-6} g/µg)

CF_2= Conversion factor (1 x 10^3 ng/µg)

Then using the following equations,

$$D_{dermal} = \frac{C_{gas} \times K_p \times SA \times Dur}{BW \times CF_1} \quad [8]$$

Where,

C_{gas}= Gaseous air concentration (ng/m^3)

K_p= Indoor air transdermal permeability (cm/hr)

SA= Body surface area (m^2)

Dur= Exposure time (hr)

BW= Body weight (kg)

CF_1 = Conversion factor (1 m/ 100 cm)

D_{dermal} = Dermal dose of TDCIPP (ng/kg/day)

Where,

$$K_p = \frac{1}{\left(\frac{1}{v_d}\right)+\left(\frac{1}{K_{p\_b}}\right)} \quad [9]$$

Where,
v_d = 600 cm/hr

K_{p_b} = 2.1 x 10^5 cm/hr

$$K_{p\_cw} = \left(10^{(0.07\times\log K_{ow}-0.0722\times MW^{2/3})} - 5.252\right) \times 3600 \quad [10]$$

Where,

K_{p_cw} = 5.5 x 10^{-4}

$\log K_{ow}$ = 10.6

MW = Molecular weight (g/mol)

$$B = \frac{K_{p\_cw}\times MW^{1/2}}{2.6} \quad [11]$$

Where,
B = 4.4 x 10^{-3}

$$K_{p\_w} = \frac{K_{p\_cw}}{(1+B)} \quad [12]$$

Where,

K_{p_cw} = 5.5 x 10^{-4}

$$K_{p\_b} = K_{p\_w} \times 10^{|\log K_{aw}|} \quad [13]$$

Where,

K_{p_w} = 2.1 x 10^5

K_{aw} = -8.58

The exposure was set to 24 hours and the exposure from Equation 8 was converted to mg/kg-day. Based on the outcome, the CEM model's estimated dose was 7.22×10^{-6} mg/kg/day (as seen in Table 24) to have be 3.24×10^{2} times more than was estimated using Equations 7-13 from Mitro et al., 2016. To investigate the discrepancy, the average concentration of TDCIPP in dust was calculated the same way as for E6 and A_ING1, using Equation 6. The total amount of TDICPP estimated in CEM was compared against the reported average concentration of TDCIPP found in residential homes in Mitro et al. 2016. The amount estimated by CEM was 0.413 of what was reported. This would indicate that the starting material and subsequent concentration a comparable estimate of possible emission of TDCIPP.

Table 24. Comparison Mitro et al. 2016 and CEM's values.

Parameter	CEM's Value	Value from Mitro et al., 2016
Average concentration of chemical in the dust (ug/g)	0.994	2.41
Average gas Phase concentration (ng/m^3)	23.3	0.57
Internal Dose (mg/kg/day)	7.22×10^{-6}	2.23×10^{-8}

The concentration of TDCIPP in the gaseous phase was also compared. In both the A_DER1 model and the model in Mitro et al. 2016 it is the concentration in the gaseous phase that sorbs onto the skin and then permeates into the body. For the concentration in the gaseous phase, CEM estimated 40.6 times more than what was estimated by the Mitro et al. 2016 equation. Since the concentration in dust was about half the actual amount, CEM estimates more moving into the gas phase. If the results from the E6 and A_ING1 comparison is an accurate representation of CEM's predictive ability, then Mitro et al. 2016's simplified equation underestimates the amount that moves into the gaseous phase. This could stem from the fact that only dust was used as a source in Mitro et al., 2016 compared to the CEM model where off-gasing from the article itself occurs. This only partially explains the difference in dose. The rest may occur from the indoor air transdermal permeability variable since CEM also incorporates body mass, an exposure duration of 24 hours, and the concentration of the chemical in the air.

Conclusions

Most corroborations were within one order of magnitude; one was within two orders of magnitude of the actual concentrations reported in the comparison studies. The inhalation models more accurately predicted concentrations than the dermal and ingestion models. The exception for this was P_DER1b, for which the comparison paper had actually measured internal doses which could be compared to CEM internal doses.

One issue which complicated the corroboration was the lack of internal dose measurements reported and comparable parameters used in CEM models. CEM defaults were used and assumptions were made for papers that did not fully report required inputs. This could have led to an unfaithful comparison of concentrations between the published experiments and CEM results. This includes comparing media concentrations instead of internal doses. Another issue was the lack of comparison studies for five CEM models. These models could be corroborated as suitable data become available. Overall CEM performed well for the models that were compared.

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