Toward an Understanding of Children's Exposure to Semi-Volatile Organic Compounds in the Indoor Environment

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A thesis
submitted in partial fulfillment of the
requirements for the degree of

Master of Science

University of Washington
2012

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Program Authorized to Offer Degree:
School of Public Health and Community Medicine-
Environmental & Occupational Health Sciences

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Acknowledgements

I am most appreciative of the time, effort and dry wit of Dr. John Kissel in this process. Our weekly meetings were invaluable in my work. My perspective of environmental health is significantly shaped by my time with him.

Jeff Shirai provided the support both in technical terms and in personal communications that allowed me to maintain some semblance of sanity. I am forever grateful for his kindness, his knowledge and his mad excel skills.

For Keith, my friends and family, thank you for giving me the opportunity to make a go at this, and for your support, even when it was hard. I hope that I can repay my debt of gratitude.

Introduction

The prevalence of smoking has declined significantly from the middle of the last century in most developed nations. Since the mid-1990s however, the rates of decline have slowed and prevalence of smoking among young women is projected to rise in some countries (World Health Organization, 2011; Centers for Disease Control and Prevention, 2011). Most U.S. states and many countries have restricted the smoking of cigarettes in public places, which has made the home the major site for exposure for non-smokers. These patterns of tobacco use place more infants and children at risk for involuntary exposure to tobacco smoke. While many smokers recognize the potential harm of secondhand smoke, and change their behavior to mitigate direct exposure to people around them, the extent to which constituents of tobacco smoke, termed thirdhand smoke (THS), persist in the indoor environment and contribute to exposure is poorly understood by the public (Winickoff et al., 2009). Rehan et al. (2011) described THS as a “stealth toxin” due to its presence in places and on surfaces that are used by unsuspecting and vulnerable populations, and because most people, both smokers and non-smokers do not recognize any danger associated with THS.

The risk posed by THS may be even greater than newly emitted secondhand smoke (SHS) due to reactions with ambient nitrous acids to form Tobacco Specific Nitrosamines (TSNAs) (Sleiman et al., 2010). Schick and Glantz (2005) examined tobacco industry documents, and reported that the sidestream condensate of cigarettes is approximately two to six times more tumorigenic per gram than that of mainstream smoke, when they were applied dermally. The two main TSNAs that have been identified as products of aging tobacco smoke, 1-(*N*-methyl-*N*-nitrosamino)-1-(3-pyridinyl)-4-butanal (NNA) and 4-(methylnitrosamino)-1-(3-pyridinyl)-1-butanone (NNK), are known human carcinogens.

Tobacco smoke is comprised of myriad different chemicals, about 400 of which have been measured in both mainstream and sidestream smoke (Daisey, 1999). Many residual tobacco smoke pollutants in dust and on surfaces have been identified as potential sources of exposure to harmful tobacco-related chemicals for non-smokers. Nicotine is a useful tracer for environmental tobacco smoke (ETS), and may be representative of exposure to other ETS constituents. Matt et al. (2004) measured surface and dust concentrations of nicotine in the homes of smokers in which smokers avoided active smoking in the home and compared the results to homes in which no such restrictions were placed. Matt et al. (2011a) also measured surfaces and dust in homes where smokers had previously lived, but were currently occupied by non-smokers. Increased environmental levels of nicotine were found in both the homes of smokers who practiced home smoking bans, and in the former homes of smokers. These findings are consistent with research by Singer et al. (2002, 2003) which found that a number of compounds from smoke, especially nicotine, adsorb to indoor surfaces and can then be reemitted into the indoor environment, and then be readsorbed and may persist for a long time. Human exposure to chemicals can occur through inhalation and dietary ingestion, but children are at increased risk for exposure from contaminated surfaces through ingestion of dust and contact with surfaces (US Dept. of Health and Human Services, 2006). As nicotine has been measured on surfaces indoors, this presents a potential pathway of exposure for children. Nicotine in smokers' homes is a continually recharging system with limited flushing due to nicotine's physical properties and numerous potential sink materials in homes. Prediction of exposures to children via indoor surface residues is the focus of the current study, although other exposure pathways are included in the model.

This work builds on the finding by Diamond and co-workers (2000) that organic films are reservoirs for semi-volatile organic compounds (SVOCs) in indoor environments, Bennett and Furtaw's (2004) application of the fugacity approach to the indoor environment, and Weschler and Nazaroff's (2008) review of SVOC partitioning from air. The estimation of concentrations of multiple contaminants in tissues and biomarkers resulting from exposures to environmental chemicals in a mechanistic physiologically based pharmacokinetic model based on partitioning is described by Cahill et al.

(2003). Singer et al. (2002, 2003) demonstrated that chemicals associated with tobacco smoke are continually redistributed in the indoor environment and can therefore be presumed to contribute to chronic whole body exposures.

The model used here was originally developed as a general tool to assess the pathways that contribute to indoor exposure to SVOCs. Initial implementation of the model evaluated the exposure of children to a plasticizer common in vinyl flooring (Greenhall et al., 2011). The model links a fugacity-based multi-compartment indoor environment component to a physiologically-based pharmacokinetic component, and can be used to estimate exposures to a number of potential environmental contaminants of concern. This work presents additional use of the model in the consideration of children's aggregate exposure to nicotine at levels commensurate with those found in experimental studies (Tables 1 & 2). Traditional models of the skin have been described as continually stirred-tank reactors (CSTRs) because they have treated internal concentrations in each compartment as uniform (Norman et al., 2008). The novelty of the approach in this work is that it includes skin as a multi-compartment membrane with concentrations varying by position, rather than a one or two-compartment CSTR skin model. Dermal contact with surface films containing environmental tobacco smoke has the potential for being an important pathway of exposure, especially for children. Use of this particular model will allow an in-depth evaluation of aggregate exposures for environmental tobacco smoke, including from surfaces. The work presented here aims to predict the total aggregate exposure of a child to nicotine from environmental sources, and to determine the relative contribution of each route of exposure.

Table 1. Measured Nicotine Concentrations and Loads in Air, Surface Wipe, and Vacuum Dust from Smokers' Homes and Cotinine

Study	**Air Concentration [µg/m^3]**		**Surface Wipe [µg/m^2]**		**Dust Concentration [µg/g]**		**Dust Load [µg/m^2]**		**Urinary Cotinine**			
									[ng/ml]		**[µg/g Cr]**	
	mct [a]	mov [b]	mct	mov	mct	mov	mct	mov	mct	mov	mct	mov
Matt *et al* (2004)	2.57[c] (gm)[h]	1.61-3.89 [d]	51.3 (gm)	19.2-32.2 [d]			6.85 (gm)		15.5 (gm)	10.1-23.4 [d]		
Willers *et al* (2004)					212 (med)	28-393 [e]			13 (med)	0.6-50 [e]		
Matt *et al* (2006)	1.72 (gm)	0.83 [f]							11.4 (gm)	0.37[f]		
Gehring *et al* (2006)	1.37 (med)[h]	0.08-14.3 [d]									5.8 (med)	< LOD-74.6 [e,g]
Matt *et al* (2011a)	1.86 (am)	1.38-2.44 [d]	98.7 (am)[h]	61.2-169 [d]	39.6 (am)	30.0-52.2 [d]	58.8 (am)	40.9-84.3 [d]	5.42	3.88-7.46 [d]		
Torrey *et al* (2011)	1.14 (gm)	0.01-6.65[e]			86 (gm)	0.63-360[e]			26 (gm)	0.56-142		

[a] measure of central tendency (reported); [b] measure of variability (reported); [c] mean from living room air; [d] 95% confidence interval on mct; [e] min-max range; [f] coefficient of variation; [g] LOD = 0.2 [h] gm = geometric mean; am = arithmetic mean; med = median

Table 2. Demographic characteristics from comparison studies

Study	Home Size (m^2)	Median Age of Child (yr)	No. Residents in Home	Study Location
Matt *et al* (2004)	61.4	0.6	4	US
Willers *et al* (2004)		7.8		EU
Matt *et al* (2006)		1.8		US
Gehring *et al* (2006)		5.7		EU
Matt *et al* (2011a)	58.4	3.5	2	US
Torrey *et al* (2011)		9.0		US

Methods

The environment is modeled as a single-room residence with air, walls and ceiling, floors finished with carpet and backing, vinyl or hard surface, furnishings (fabric covered foam), dust and suspended particles. The source of the nicotine is estimated based on Benowitz (1994, 1996 & 2009) and Hukkanen (2005) and assumes 71% of 1.0 mg nicotine emitted per cigarette is available in sidestream smoke. Henderson et al. (1989) reported a mean nicotine concentration in air of 3.74 $\mu g/m^3$ and a Health Canada survey reported that in households where smoking occurred, 47% reported consumption of 1-10 cigarettes, 28% 11-20 and 25% 21 or more cigarettes (Health Canada 2000). This model assumed that 8 cigarettes are consumed in the environment per day. The approximately 4 year-old child in the model is adjusted for 24 hours per day in the one-room home. Organic film layers are added to all of the environmental surfaces as well as to the personal fabric (which includes both clothing and bedding). Losses from the home are from cleaning, laundering, bathing, handwashing, air flow and excretion from the child. The model (shown schematically in Figures 1 and 2) includes both environmental compartments described above and physiological compartments.

In Figure 1, the relationship between the environment and the human is represented with the arrows illustrating movement of the chemical (nicotine) between compartments. The organic film layers on walls, hardwood and vinyl floors, carpet, windows, personal fabric and fabric are not shown individually, but are represented as “film on surface” in Figure 1, and are included in the model. Figure 2 more explicitly defines the relationships between physiological compartments and the arrows represent movement of blood within or excreta from the person. The model contains information pertaining to the pathways of exposure, how the chemical is distributed in the body, and how it is excreted. Pathways include inhalation of both vapors and particles, ingestion of dust and dermal absorption. Air to blood is modeled as a diffusion process across the boundary layer between the lung and blood. This mechanism is assumed to be similar for ingested dust, but from the gut wall to blood. Dermal exposure occurs between the surface film layer on the skin and both vapors and environmental surface films, and dermal absorption takes place across the layers of the stratum corneum and viable epidermis as compartments in series.

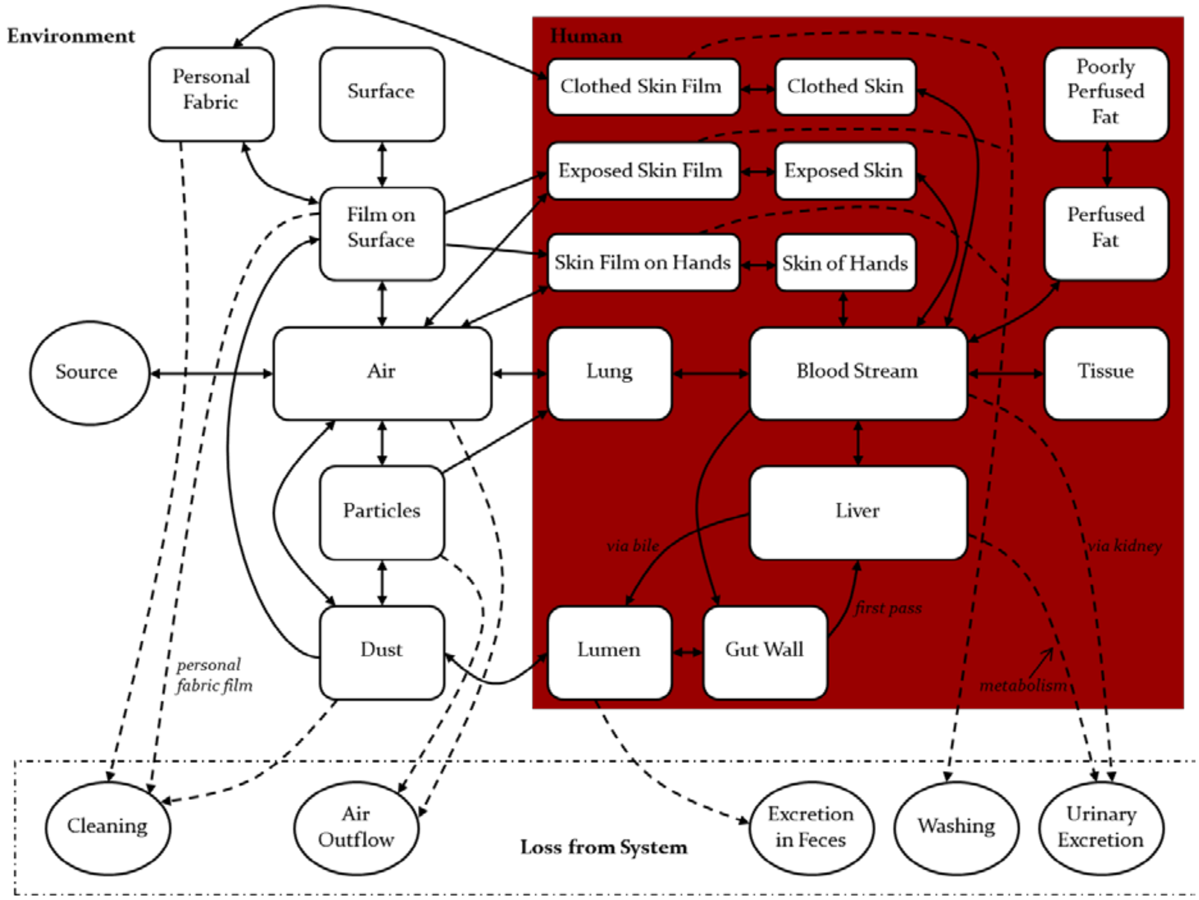

Figure 1. Schematic of Fugacity-based Indoor Environment and PBPK Human Model

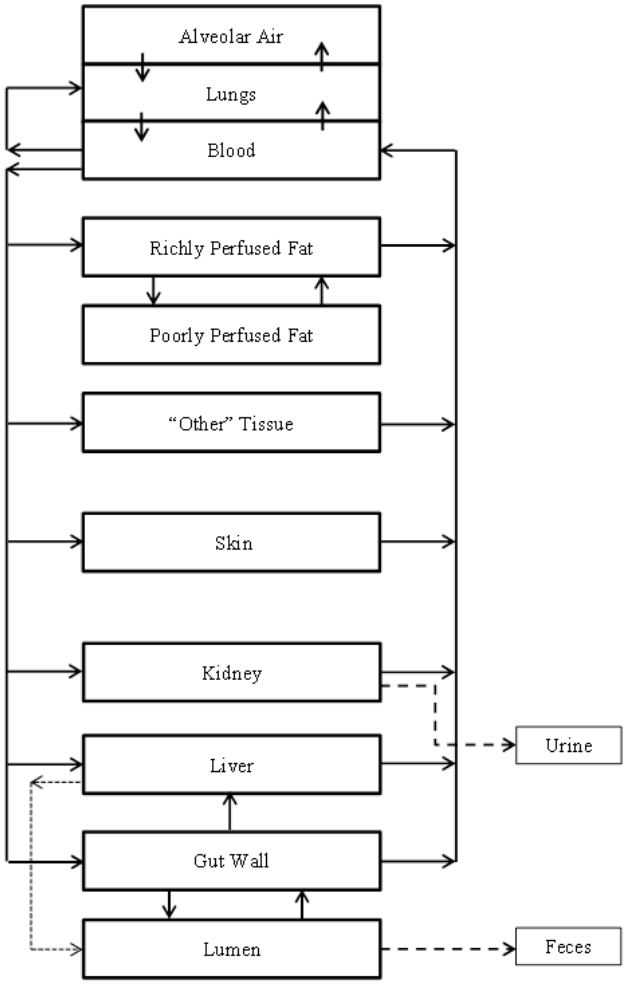

Figure 2. Schematic Diagram of PBPK Model Transport Processes.

The physiologically-based pharmacokinetic (PBPK) portion of the model includes a membrane representation of skin (hands, other non-hand exposed and clothed skin are modeled separately) comprised of 15 layers of stratum corneum and 30 layers of viable epidermis. Mass balance checks are built into the code. The model consists of a system of differential equations implemented in

MATLAB®2011b (The Mathworks, Natick, MA) using ode15s, a stiff solver that utilizes Runge-Kutta methods and variable time steps.

The fugacity approach, (Mackay, 2001), was utilized as the framework for both the environmental and physiological components of the model used in this study. In this method, a chemical concentration in a medium equals the fugacity of a chemical (f) multiplied by the fugacity capacity (Z) of the medium for that chemical. Fugacity can be considered the escaping tendency of a chemical and fugacity capacity can be thought of as the affinity of a medium for a chemical. The fugacity capacity for many chemicals in the gas phase is equivalent to the reciprocal of the gas constant (8.314 Pa·m^3/mol·K) and the environmental temperature (K). In other phases, the fugacity capacity can be related to dimensionless partition coefficients like octanol-water or air-water. Reactions and transport of chemicals are described using mass transfer coefficients (D values) or by other fugacity rate coefficients. Simply stated, a chemical will tend to move from media with high fugacity to media with low fugacity depending on mass transfer conditions and on the gradient between media.

The model utilizes the fugacity approach in which

$$M_i = Z_i \cdot V_i \cdot f_i$$

where M is mass (mol), Z is fugacity capacity (mol Pa^{-1} m^{-3}), V is volume (m^3) and f is fugacity (Pa) for compartment i. For constant Z and V, mass balances expressed as differential equations can be rewritten in terms of fugacity. Generic mass balances on environmental compartments take the following form:

$$\frac{df_i}{dt} = \left[\frac{1}{Z_i \cdot V_i}\right] \cdot \left(Q_i \cdot Z_i \cdot (f_{ext} - f_i) + \sum_{n=1}^{n_{adj}} \left[D_{adj,i} \cdot \left(f_{adj} - f_i \right) \right] + \sum_{j=1}^{n_{loss}} k_{loss} \cdot f_i \right)$$

where Q is an advective flow rate in $m^3\ hr^{-1}$, $D_{adj,i}$ is a mass transfer coefficient, expressed in mol Pa^{-1} hr^{-1}, describing non-advective exchange between compartment i and an adjacent compartment and k_{loss} is a first-order rate constant describing some loss process (if any) with units of hr^{-1}. Loss terms include dust removal by cleaning, laundering of personal fabric (clothing and bedding), hand-washing and bathing.

Generic mass balances on non-skin human compartments take the form:

$$\frac{df_i}{dt} = \left[\frac{1}{Z_i \cdot V_i}\right] \cdot \left[Q_{bld,i} \cdot Z_{bld} \cdot \left(f_{bld} - f_i\right) - k_{met} \cdot f_i\right]$$

where $Q_{bld,i}$ is blood flow ($m^3\ day^{-1}$) to compartment i and $k_{met,i}$ is the first order metabolic activity constant (if any) in compartment i (hr^{-1}).

Skin is modeled as a membrane. A generic mass balance in the interior of the skin takes the form:

$$\frac{df_i}{dt} = \left[\frac{1}{Z_i \cdot V_i}\right] \cdot \left[D_{prev,i} \cdot \left(f_{prev} - f_i\right) + D_{next,i} \cdot \left(f_{next} - f_i\right)\right]$$

At the exterior surface of the stratum corneum, the preceding compartment is a film (sebum) layer on the surface of the skin. At the interior of the viable epidermis transport is balanced by removal by the blood. Stratum corneum and viable epidermis differ in depth and transport characteristics.

Tables 3-5 contain a partial list of model parameters including physic-chemical and physiologic properties, and some of the partition coefficients and fugacity capacities used in the model (complete list can be found in Appendix A). A copy of the Matlab code, including parameters, can be found in Appendix B

Table 3. Key physiologic parameters

Model Parameter (units)	**Value**	**Source/Notes**
Body weight (kg)	17	Estimated using US EPA CSEFH (2008)
Cotinine in urine excretion ratio (-)	0.13	Benowitz et al. (1994)
Dust ingestion absorption efficiency (-)	0.5	Best judgement
Fractional absorption of inhaled particles (-)	0.5	Best judgement
Fractional absorption of inhaled vapor (-)	1	Best judgement
Inhalation rate (m^3/hr)	7.4	Brochu et al. (2011)
Dust ingestion rate (g/day)	0.007	Ozkaynak et al. (2011)
Urine production (L/day)	0.38	Miller & Stapleton (1989)
Surface area of child (m^2)	0.68	Estimated using US EPA CSEFH (2008)
Fraction of total surface area that is exposed skin (minus hands) (-)	0.2	Best judgement
Fraction of total surface area that is exposed skin of hands (-)	0.05	Best judgement
Fraction of total surface area that is clothed skin (-)	0.75	Best judgement
Stratum corneum depth (m)	1.50E-05	McCarley and Bunge (2001)
Viable epidermis depth (m)	0.1E-03	EPA RAGS E
Elimination half-life of nicotine (h^{-1})	0.33	Benowitz et al. (2009)
Degradation rate in liver (day^{-1})	-log(0.5)/((half-life)*24)	
Elimination rate (feces) (day^{-1})	1	Best judgement
Volume-blood (L)	1.26	7.4% BW Cahill et al.(2003)
Volume-gut (L)	0.24	1.4% BW Cahill et al. (2003)
Volume-liver (L)	0.44	2.6% BW Cahill et al.(2003)
Volume-lung (L)	0.12	0.7% BW Reference Man (Snyder 1975)
Volume-richly perfused fat (L)	1	5.9% BW Richly perfused fat Cahill et al.(2003)
Volume-poorly perfused fat (L)	2.89	17% BW Poorly perfused fat Cahill et al.(2003)
Volume-tissue (L)	11.05	65% BW (all tissues not described above)
Blood perfusion of fat	0.052	Norman et al. (2008) % cardiac output
Blood perfusion of liver	0.227	Norman et al. (2008)
Blood perfusion of gut	0.013	Norman et al. (2008)
Blood perfusion of last layer skin	0.039	Rowell (1974)
Perfusion rate to gut (ml/min/g)	0.84	Kissel & Robarge (1988)
Cardiac output (L/min)	3	Alverson (1982)

Table 4. Key environmental and chemical parameters

Model Parameter (units)	**Value**	**Source/Notes**
H (Pa m3/mol)	3.04E-04	
R (m3 Pa/mol/K)	8.314472	
Vapor Pressure (Pa)	5.07	EpiSuite
logKow (-)	1.17	EpiSuite
Molecular weight nicotine (g/mol)	162.26	EpiSuite
MW Cotinine (g/mol)	176.22	EpiSuite
Fraction of organic carbon in films	0.57	Diamond et al. (2000)
Fraction organic carbon in dust	0.19	Bennett & Furtaw (2004)
Fraction organic carbon in particles	0.55	Naumova et al. (2003)
Soil tracked in (g/day)	0.1	Layton (2009)
Loss from sweeping (day^{-1})	0.0053	Layton (2009)
Loss from clothes laundering (day^{-1})	0.07	Best judgement
Loss from hand washing (day^{-1})	3	assumes 3 hand washes per day
Loss from bathing (day^{-1})	0.3	assumes 2 baths per week
Rate of re-suspension (h^{-1})	1.00E-06	Liu (2010)
Deposition velocity (m/h)	0.2	
Nicotine emission (g/day)	0.0057	cigarette nicotine estimate based on Benowitz (1996) 1.0mg nicotine/cigarette *71% nicotine dose in sidestream*8cigarettes/day
Room height (m)	2.4	Layton (2009)
Room length (m)	10	
Room width (m)	10	
Surface area of fabric (m^2)	0.19 * total volume of room	Hodgson et al. (2005)
Surface area of foam (m^2)	0.26 * total volume of room	Hodgson et al. (2005)
Fraction floor area carpeted (-)	0.40	Best judgement
Fraction floor area vinyl (-)	0.20	Best judgement
Fraction floor area hard surface (-)	0.40	Hard surfaces other than vinyl
Fiber factor (-)	50	greater surface area due to fibers- Morrison & Nazaroff (2002)
Mass loading of dust (kg/m^2)	0.001	Bennett & Furtaw (2004)
Thickness of organic film (m)	20 *1E-09	Diamond et al. (2000)
Thickness of film on human (m)	1.3*1E-06	Weschler & Nazaroff (2012)

Table 5. Partition coefficients (K values) and fugacity capacities (Z values)

Model Parameter (units)	**Value**	**Source/Notes**
K(octanol/air)	Kow*R*T/H	Bennett & Furtaw (2004)
K(particles/air)	$10^{-0.860*\log10(VP)-4.67}$	
K(dust/air)	(K(octanol/air))+log10(fraction(orgCarboninDust)/0.74)-11.91	Bennett & Furtaw(2004)
K(vinyl/air)	$10^{(5.20-0.68*\log10(VP))}$	Bennett & Furtaw (2004), VP in Pa, Eq. 18
K(wall/air)	$10^{(2.93-0.31*\log10(VP))}$	Bennett & Furtaw (2004), VP in Pa, Eq. 17
K(carpet/air)	$10^{(3.82-0.62*\log10(VP))}$	Bennett & Furtaw (2004), VP in Pa, Eq. 20
K(fabric/air)	4,500	Piade et al. (1999)
K(clothing/air)	44,000	Piade et al. (1999)
K(stratum corneum/water) (L/kg)	$Kow^{0.74}$	Norman et al. (2008)
K(viable epidermis/water)	1	Assume epidermis behaves as water pA-33 RAGS-E
K(stratum corneum/air) (L/kg)	K(stratum corneum/water)/K(air/water)	
Z(nicotine) (mol/Pa/m3)	(1/molecular volume)/VP	
Z(water)	1/H	
Z(air)	1/(R*T)	
Z(particles)	K(particles/air)*density(particles)* 10^9/(R*T)	Bennett & Furtaw (2004)
Z(film)	0.48*K(octanol/water)*fraction(orgCarbonInFilm)*density(organicFilm)/H/1000	Bennett & Furtaw (2004)
Z(vinyl)	K(wall/air)/(R*T)	
Z(wall)	K(wall/air)/(R*T)	Bennett & Furtaw (2004)
Z(dust)	K(dust/air)*density(dust)*10^9/(R*T)	
Z(carpet)	k(carpet/air)/(R*T)	
Z(fabric)	k(fabric/air)/(R*T)	
Z(clothing)	k(clothing/air)/(R*T)	
Z([backing, foam])	Z(fabric)	Best judgement
Z(hard floor)	Z(wall)	Best judgement
Z(blood)	0.01 * K(octanol/water) / H	assume 1% lipids
Z(gut)	0.01* K(octanol/water) / H	
Z(lumen)	0.1* K(octanol/water) / H +0.9*Z(water)	Cahill et al. (2003)
Z(liver)	0.0667* K(octanol/water) / H	assume 0.067% lipids - Reference Man
Z(lung)	0.01* K(octanol/water) / H	assume blood
Z(fat)	1.0* K(octanol/water) / H	assume 100% lipids
Z(tissue)	0.01* K(octanol/water)/ H	
Z(stratum corneum)	Z(water) * K(stratum corneum/water)	
Z(viable epidermis)	Z(water) * K(viable epidermis/water)	
Z(bile)	0.1* K(octanol/water)/ H	Cahill et al. (2003)

Results

Modeled Environmental Conditions

Model predicted environmental concentrations and urine cotinine concentrations are shown in Table 6. Ratios of urine cotinine to measured air and dust concentrations of nicotine are illustrated in Figures 6 and 7, and are within the range of reported values. The ratio for the modeled values is 9,584, and the range for measured values is 2,914-22,807, for urine cotinine to nicotine air concentrations. For urine cotinine to dust concentrations the modeled ratio is 0.25 g/l, with a range for measured values of 0.06-0.30 g/l.

Table 6. Model predicted environmental nicotine concentrations and loads and urine cotinine

Air Concentration (μg/m^3)	**Surface Load**[a] (μg/m^2)	**Dust Concentration** (μg/g)	**Dust Load** (μg/m^2)	**Urinary Cotinine** [b] (μg/l)
3.85	15.99	145	72.5	36.9

[a] Surface load is from organic surface films only and does not include dust. [b] The model assumes a daily exposure of 24 hours and physiological parameters of a 4 year-old.

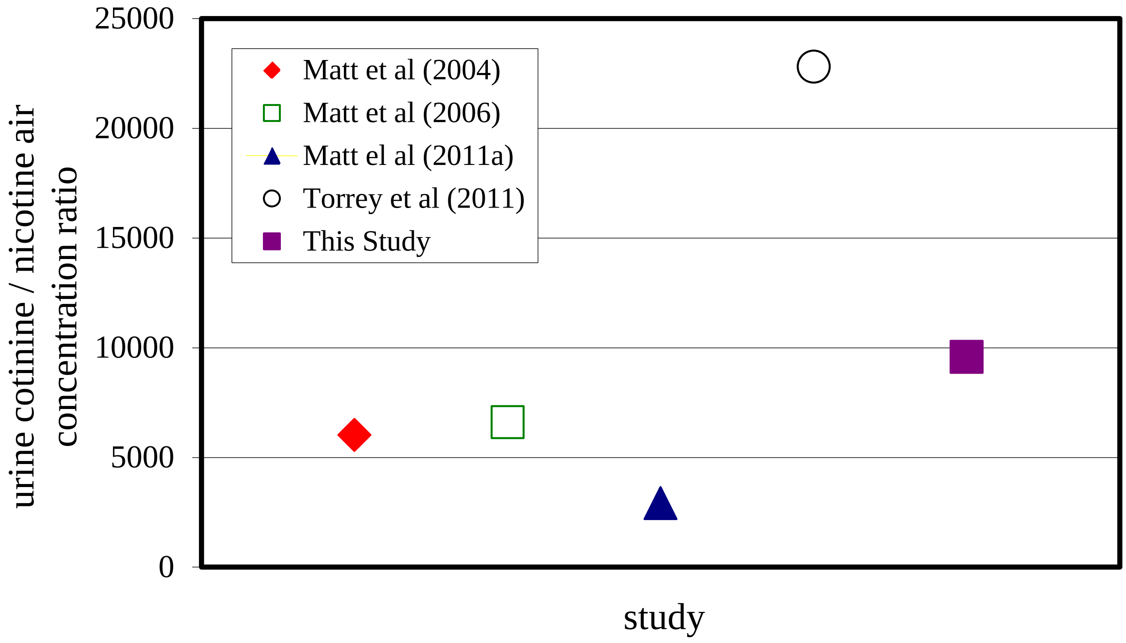

Figure 3. Urine cotinine to nicotine air concentration ratios from different studies. Ratios for Matt et al (2004, 2006) and Torrey et al (2011) are of two geometric mean values, while that of Matt et al (2011a) is of two arithmetic mean values. The ratio for the current study is of model-generated point estimate predictions. The model assumed a daily exposure duration of 24 hours and physiological parameters of a 4 year-old.

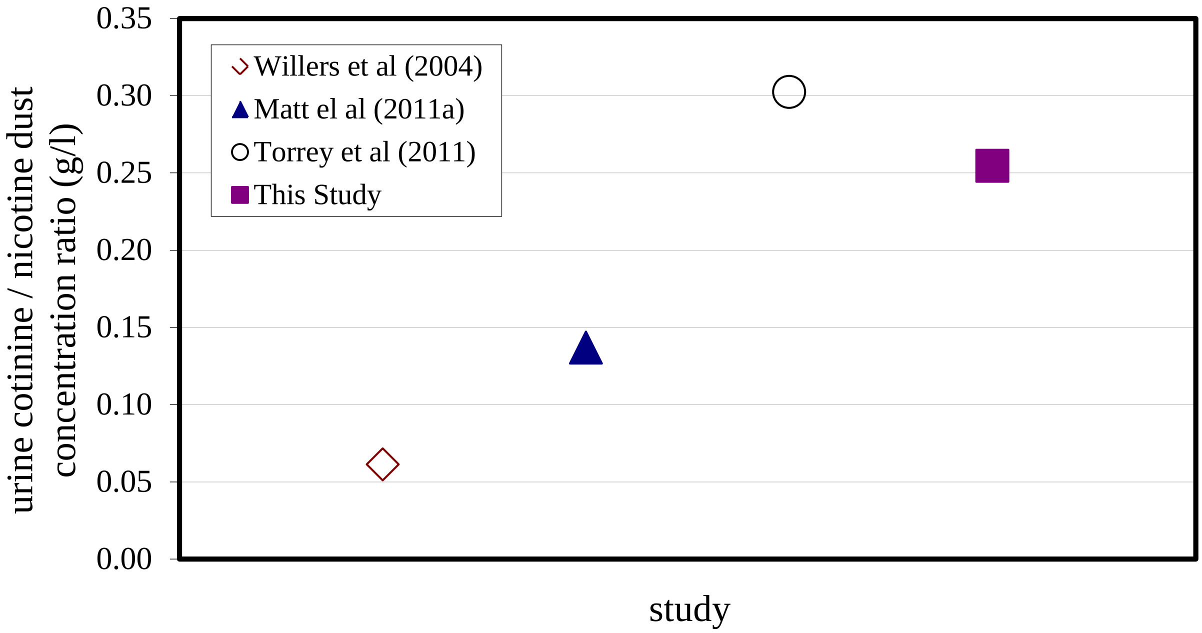

Figure 4. Urine cotinine to nicotine dust concentration ratios from different studies. Ratios for Willers et al (2004), Torrey et al (2011), Matt et al (2011a) are of two median values, two geometric mean values, and two arithmetic mean values respectively. Ratio for the current study is of model-generated point estimate predictions. The model assumed a daily exposure duration of 24 hours and physiological parameters of a 4 year-old.

At the end of the simulation time, the distribution of nicotine in the different compartments indicates that the bulk of the mass in the system is in the plush materials, such as carpet, fabric and foam. In the human, the bulk of the mass is in the adipose tissue (Table 7 & Figure 5). However, the concentration of nicotine in films is many orders of magnitude more than the concentration in air due to the relatively small volumes of films (Figure 6).

Table 7. Modeled distribution of nicotine in select compartments at end of one year simulation

Compartment	**Mass(mg)**
Air	0.93
Films	7.0[a]
Particles	$9.8\text{x}10^{-5}$
Dust	3.0
Hard Surfaces	6.8[b]
Carpet	186
Fat	0.27
Exposed Skin (no hands)	$1.4\text{x}10^{-3}$
Clothed Skin	$7.9\text{x}10^{-3}$
Skin on Hands	$2.2\text{x}10^{-4}$
Body	0.28[c]

[a] Total of all films from vinyl, hard floors, walls, fabric, clothing and carpet; [b] hard surfaces includes vinyl and hard floors, and walls; [c] body includes lung, liver, lumen, gut, fat, tissue, and blood

Fugacities for most of the environmental compartments reach steady state at about the same value after approximately 200 simulation days. Environmental compartment fugacities reach steady state values in the range of $6 \text{ x } 10^{-5}$ Pa (Figure 5). The skin compartments reach steady state fugacities on the order of 10^{-7} Pa (Figures 8-10). Environmental compartments closest to the skin, clothing and clothing film, have fugacities close to $4 \text{ x } 10^{-5}$ Pa (Figure 5).

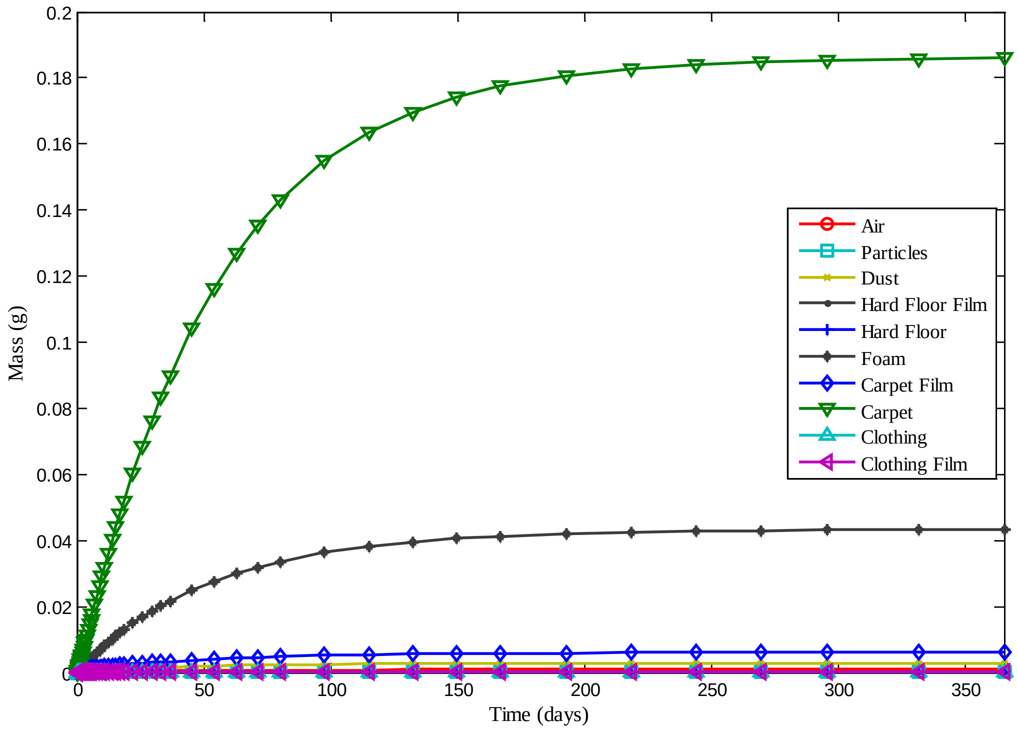

Figure 5. Mass of nicotine in select environmental compartments

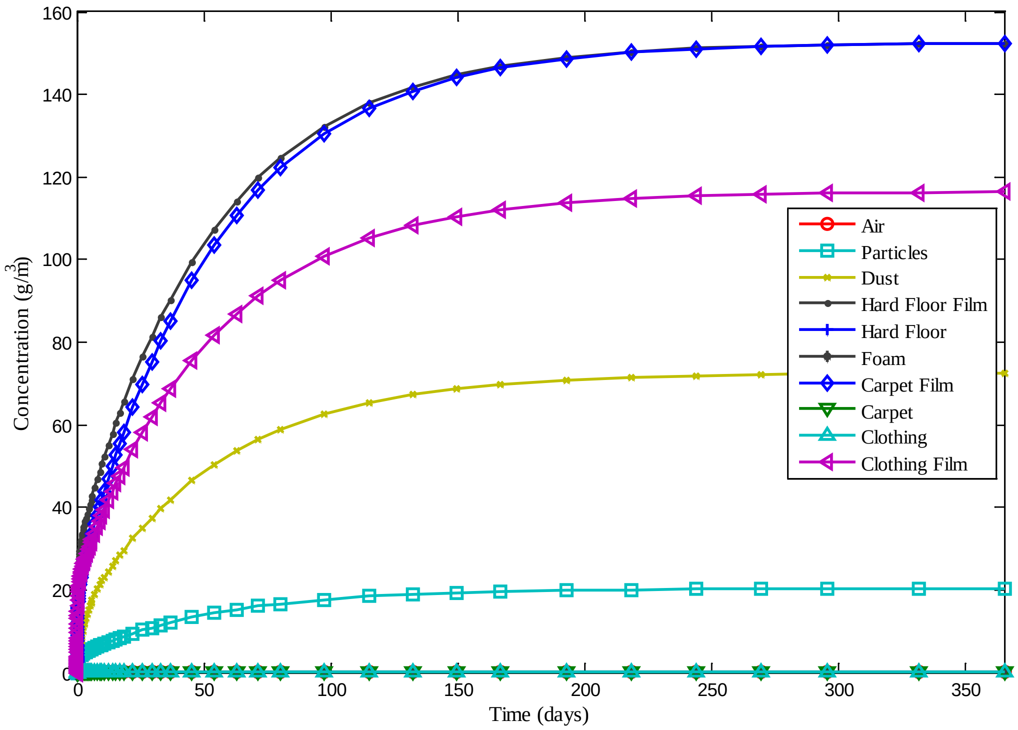

Figure 6. Concentration of nicotine in select environmental compartments

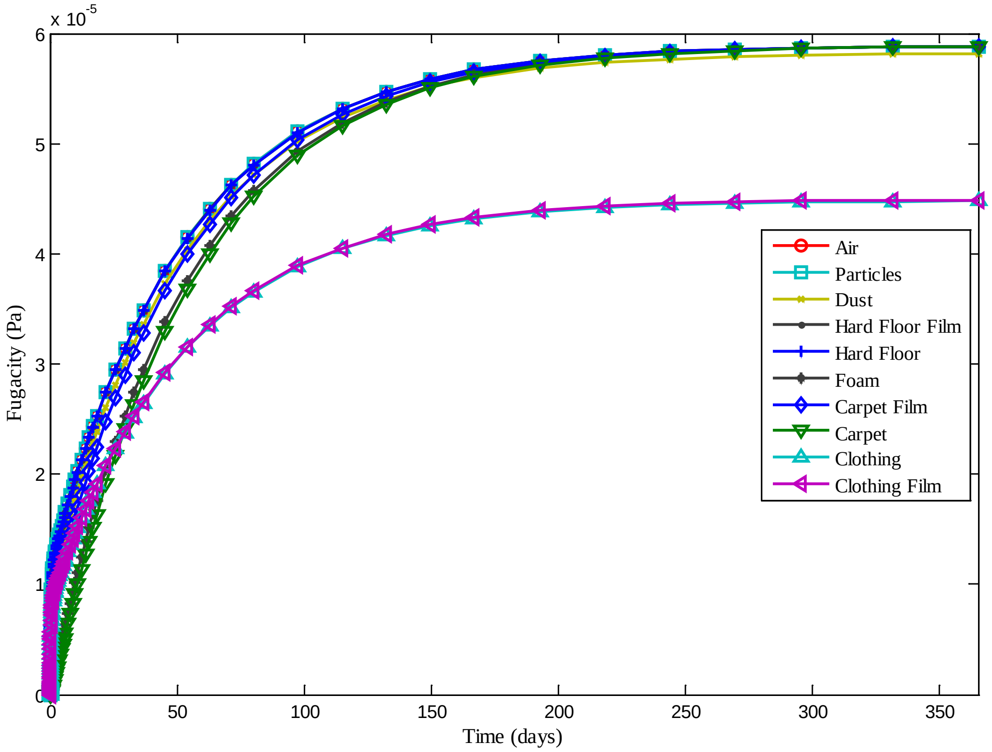

Figure 7. Fugacity of nicotine in select environmental compartments

Fugacity Gradient and Flux through the Skin

Figures 8-10 show fugacity gradients of nicotine through skin from the outermost layer of stratum corneum through to the innermost layer of viable epidermis. For each type of skin, exposed not hands, hands and clothed skin, the fugacity at the outermost layer begins at near equilibrium with the fugacity at the skin surface and decreases as nicotine moves through the stratum corneum. The inflection point is the transition between the last layer of stratum corneum and the first layer of viable epidermis.

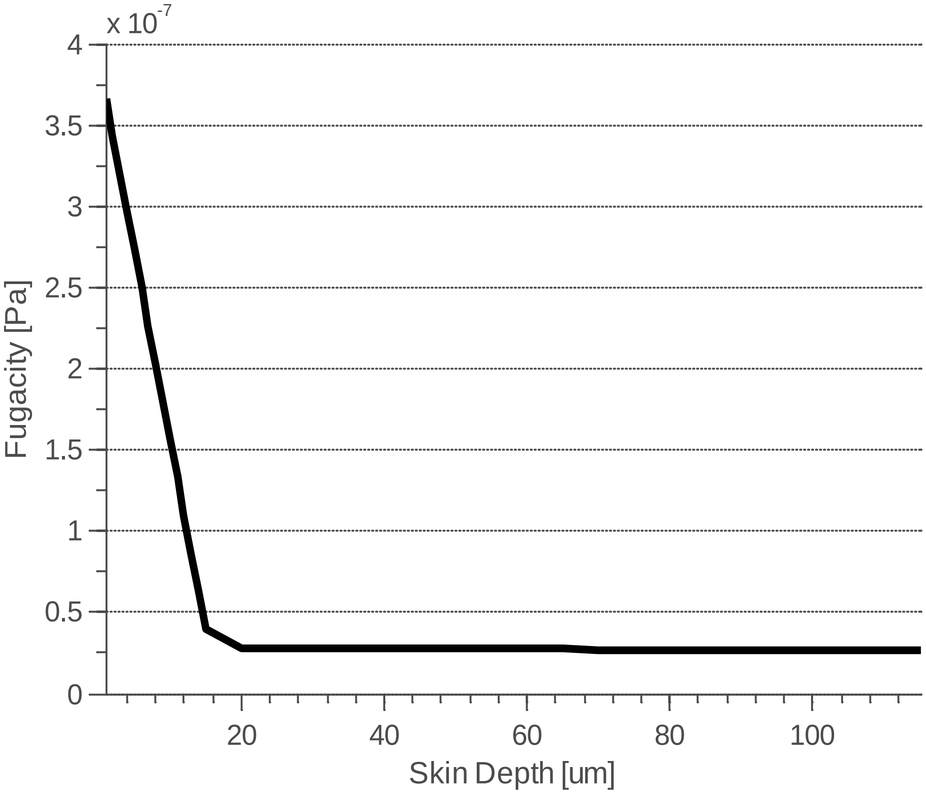

Figure 8. Fugacity gradient in the exposed skin not including hands

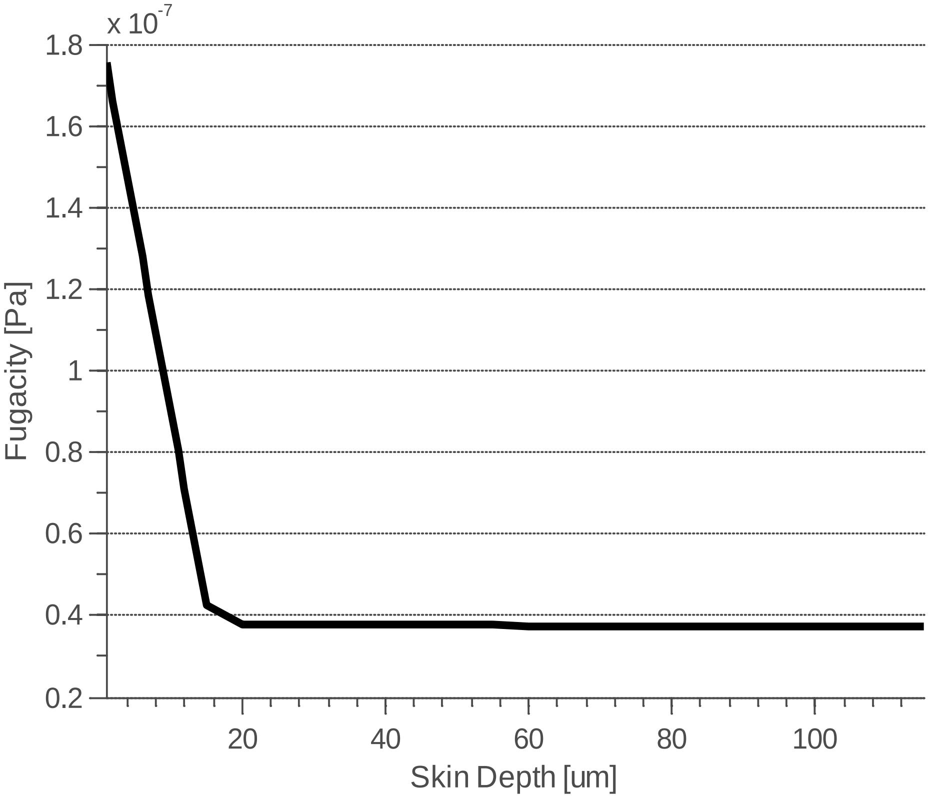

Figure 9. Fugacity gradient in the skin of hands

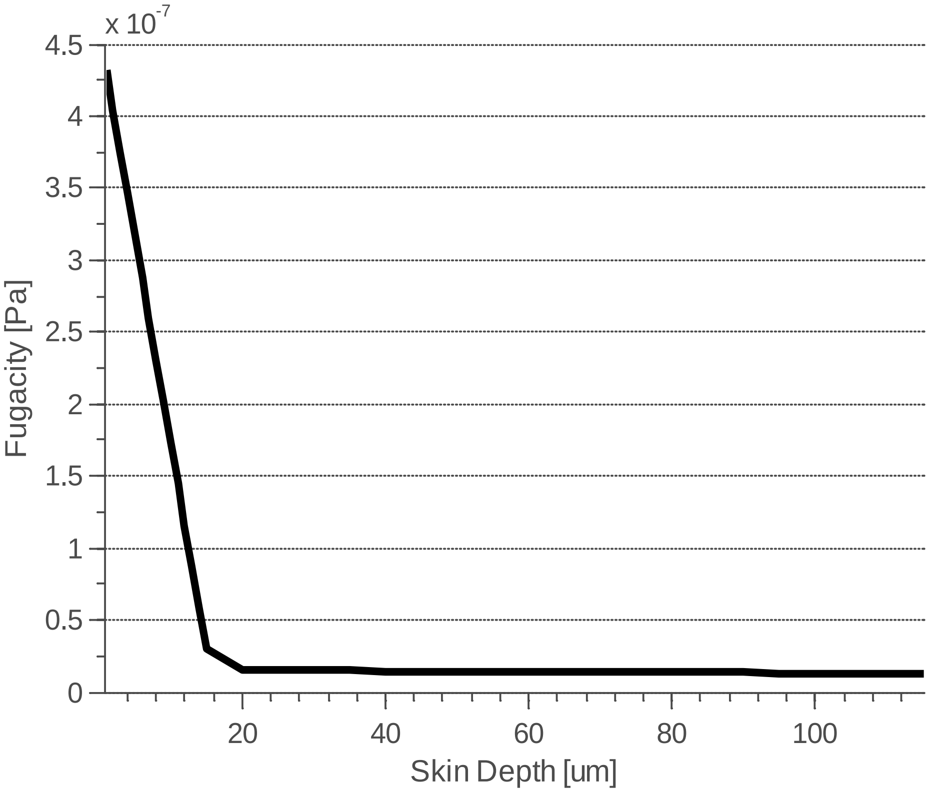

Figure 10. Fugacity gradient in the clothed skin

Available experimentally derived fluxes through skin are typically many orders of magnitude greater than the flux through skin predicted in the model (Table 8). However, the modeled skin loading is many orders of magnitude smaller than what is typically applied in *in vitro* or *in vivo* skin studies (Zorin et al., 1999). Assuming that the experimental loads are of fully saturated solutions, the vapor pressure of nicotine (5.07 Pa) can be used to describe fugacity. The modeled fugacity at the outermost layer of stratum corneum in all skin types is approximately 4.00E-07 Pa. The model therefore, is in relatively strong linear agreement with measured flux through skin (Figure 11).

Table 8. Modeled fugacity at first layer of stratum corneum, predicted flux of nicotine from skin to blood and relative dose through the three modeled skin types

Source	**Fugacity (Pa)**	**Flux (µg/cm^2/hr)**	**Dose (µg/kg/day)**
Skin Exposed (not hands)	4.55x10^{-7}	9.5x10^{-4}	1.83
Skin of Hands	4.25x10^{-7}	1.5x10^{-3}	0.74
Skin Unexposed	1.94x10^{-7}	3.1x10^{-4}	2.25

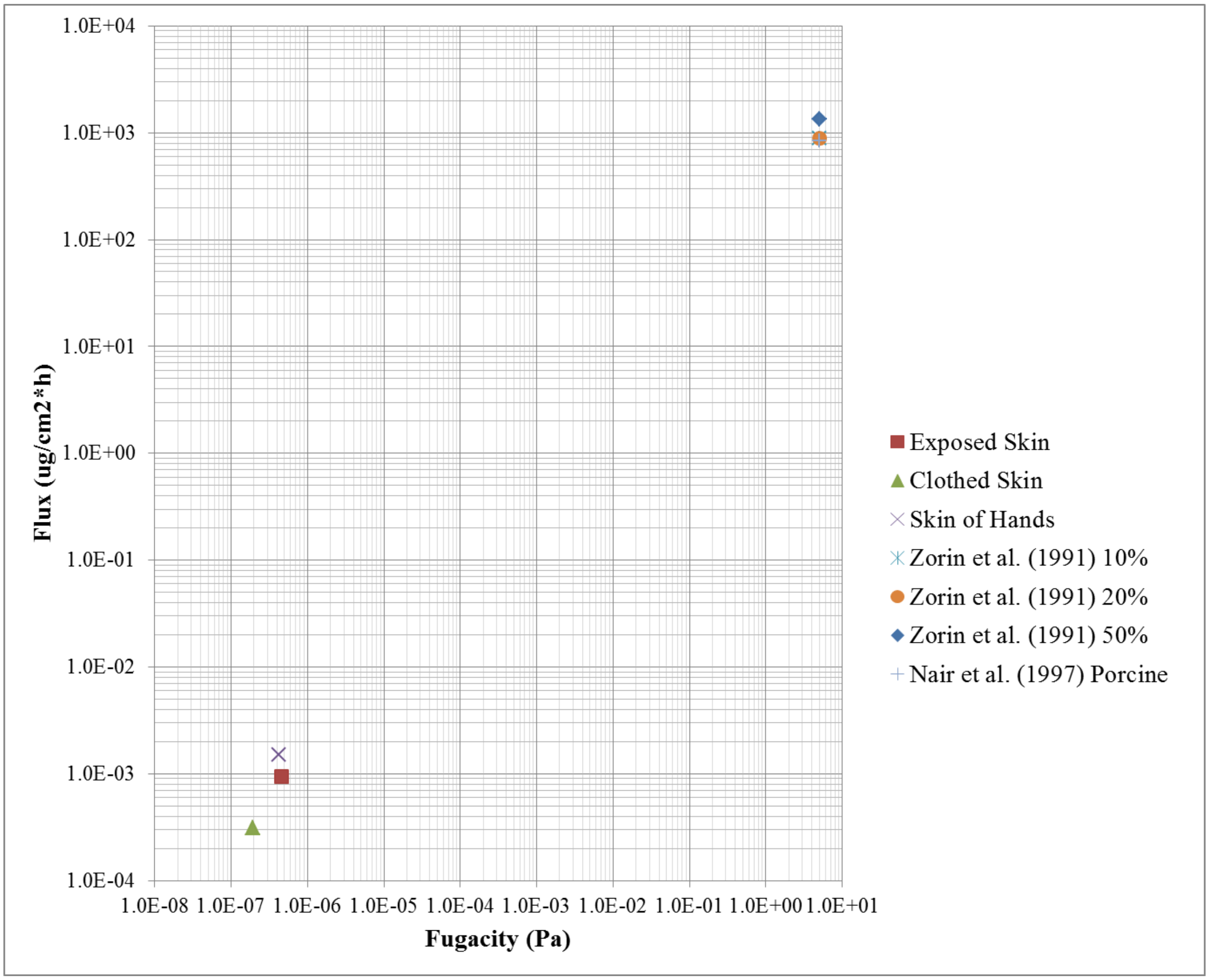

Figure 11. Modeled flux compared to experimental flux through skin. Zorin et al. (1991) utilized human cadaver skin and nicotine solutions (% w/w) in water. Nair et al. (1997) used porcine skin and nicotine in phosphate buffer solution. Experimental fugacity is assumed to be equal to vapor pressure of nicotine (5.07 Pa)

Exposure Pathways

Dermal absorption is predicted to be the dominant pathway of exposure to nicotine from THS. More than three-quarters of the dose is expected to come from dermal absorption with most of the remaining dose being attributed to inhalation of vapors (Table 9).

Table 9. Modeled total dose and relative contributions of routes of exposure

Measure	Oral(dust)	Inhalation(vapor)	Inhalation(particles)	Dermal	Total
Dose(µg/kg/day)	0.06	1.46	$1.3\text{x}10^{-4}$	4.82	6.34
% of Total	0.95	23.0	$2.7\text{x}10^{-5}$	76.0	100

The predicted intake of nicotine was based on inhalation rates from US EPA Child Specific Exposure Factor Handbook (CSEFH) and on dust ingestion estimates from Ozkaynak et al. (2010).

Discussion

There has been a call for a better understanding of the acute and chronic exposure to THS in non-smokers (Matt et al., 2011b). The "three r' definition of thirdhand smoke, that pollutants *remain* on surfaces and in dust, are *re-emitted* in the gas phase and *react* with other compounds in the environment (ASH Scotland, 2011), may be inadequate to describe all potential exposure pathways. That is, nicotine and other tobacco smoke constituents do persist in the environment in dust and on surfaces, but re-emission back into gas phase is not required for exposure. In fact, according to Rehan et al. (2011), many of the components of THS have vapor pressures that make it unlikely that significant levels of those compounds will be available for exposure through direct inhalation. These results support a growing body of evidence that the surface residue contribution of THS to the total dose of nicotine and tobacco specific nitrosamines (TSNAs) for non-smokers, especially children, is non-negligible.

Exposure to secondhand smoke has been recognized as having no safe level, and as a result public smoking bans and changes in smoking behaviors have been occurring over the past couple of decades. It is therefore not inconceivable that similar changes in behavior could occur if the risks associated with thirdhand smoke were better understood and better communicated to the public. Along with an understanding of the pathways of exposure, a better grasp on the environmental chemistry, toxicology and health effects is critical to creating a complete picture of the risks associated with THS exposure.

This study sheds more light on the potential pathways of exposure to nicotine in indoor environments other than by passive smoking. Previous studies have failed to fully account for observed urinary excretion of cotinine in children solely through direct inhalation or dust ingestion. Based on reported environmental measurements from Matt et al., 2004 & 2011a, and Torrey et al., 2011, and published exposure factors, we estimate shortfalls of as much as 90% between reported urinary cotinine and predicted nicotine intake (Table 10). The observed discrepancies between the predicted exposure to nicotine via inhalation and ingestion of dust and observed urinary cotinine excretion can potentially be explained by dermal absorption from vapor phase and/or interaction with organic surface films. These findings contribute to the understanding of the role of surface residues in the exposure to third-hand smoke in the indoor environment, and are especially relevant in consideration of children's exposure to THS, due to their increased contact with surfaces and larger relative body surface area.

Table 10. Predicted versus observed urinary cotinine levels due to inhalation of vapors and ingestion of dust with relative shortfalls

Study	**Predicted intake from Air**[a] (µg/day)	**Predicted intake from Dust**[b] (µg/day)	**Predicted total intake** (µg/day)	**Predicted urine cotinine**[c] (µg/l)	**Reported urine cotinine** (µg/l)	**% Shortfall**
Matt et al. (2004)	9.18	0.37	9.55	6.54	15.47	57.7
Matt et al. (2011a)	13.76	1.07	14.83	5.13	5.42	5.4
Torrey et al. (2011)	10.49	2.32	12.81	2.8	26	89.2

[a] estimated using US EPA CSEFH (2008) inhalation rate of 5.4 m^3/day for <1 year-old, and 7.4 m^3/day for 4 year-old and 9.2 m^3/day for a 9 year-old; [b] 27 mg dust ingestion/day from Ozkaynak et al. (2010); [c] urine production estimated from US EPA CSEFH (2008) 190 ml/day for <1 year-old, 380 ml/day for 4 year-old and 620 ml/day for a 9 year-old and nicotine dose excreted in urine as cotinine 13% (Benowitz et al., 1994)

As has been demonstrated previously, surface films provide a reservoir for exposure to chemicals in the indoor environment (Greenhall et al., 2011). Nicotine provides a good case study for the contribution of the dermal pathway to total exposure because it is unequivocally recognized to be absorbed dermally, and because it remains a common indoor contaminant. The extent~~s~~ to which the levels of exposure from THS pose a health risk~~,~~ is not yet well described. However, given the potential development of known human carcinogens due to chemical reactions in the environment, the behaviors and physiology of children, and the relatively large fugacity capacity for the surface films, further research is warranted.

The limitations of this study include the inadequacies of the available data, which reflect changing trends in analytical methods, small sample sizes, disparate environmental conditions and various age groups, as well as secular trends in indoor smoking behavior. The current work only describes physiologically relevant parameters for an approximately four year-old child. The model can be adjusted to estimate exposures to children of other ages or adults. Additionally, these findings are based on a simplified box-model system. The one room building of 100 m^2 (approx. 1,076 ft^2) with varying types of flooring materials and furnishings probably does not adequately represent a typical home. The U.S. Census Bureau's (2010) published median area for single-family residences was 2,169 ft^2. The studies used for reference values in this study, however, reported median house sizes of approximately 650 ft^2 (Matt et al., 2004, 2011).

An additional limitation of the study is the difficulty in parameterizing the complex processes describing the transport of chemical between compartments that leads to dermal exposure. A conceptual model of the processes leading to dermal absorption, but not including it, from multiple compartments including air, surface contaminant layer, outer and inner clothing contaminant layer and a skin contaminant layer, was proposed, but not implemented, by Schneider et al. (1999, 2000). The model presented here attempts to parameterize the dermal exposure processes earlier described by Schneider et al.

Intake fraction (*iF*) is a tool for expressing the source-to-intake relationship, and is the fraction of the emitted mass of a pollutant in the environment that passes into the population through ingestion, inhalation or dermal absorption (Bennett et al., 2002). An estimation of *iF* can be derived using this model, which in combination with information about emission factors and the likelihood of adverse effects, can be used to determine the risk associated with exposure. Intake fraction can be expressed in the aggregate for whole populations over multiple pathways, or it can be disaggregated, for example within a population or for specific routes of exposure. Nazaroff (2008) examined *iF* associated with the episodic release of indoor pollutants, but the only exposure pathway considered was inhalation. Bennett et al. (2002) employed intake fraction for multimedia pollutants for multiple pathways. A strength of the model presented here is the relative contributions to intake fraction by exposure route (inhalation, ingestion and dermal) can be estimated, and the effects of differing environmental scenarios (eg. building characteristics, loss terms and emission rates) can be explored. Future work could extend to other semi-volatile compounds such as pesticides, flame retardents, methamphetamine and plasticizers.

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Appendix A. Parameters Table

Model Parameter	**Value**	**Source/Notes**
Physical Properties		
VP (mmHg)	0.038	EPI SUITE
H (Pa*m^3/mol)	3.04E-04	EPI SUITE
logKow	1.17	EPI SUITE
Nicotine CAS No.	54-11-5	
MW-NIC (g/mol)	162.26	EPI SUITE
MW-cotinine (g/mol)	176.22	
excrRatio(cotinine)	0.13	Benowitz (1994)
BW (kg)	17	4 year-old, US EPA Child Specific EFH (2008)
soiltrackin (g/day)	0.1	Layton (2009)
sweepLoss (/day)	0.0053	Layton (2009)
launderLoss (/day)	0.07	Best judgement
handwashLoss	3	assumes 3 hand washes per day
bathLoss	0.3	assumes 2 baths per week
Unitless Fractions		
fraction(GIabsDust)	0.5	Dust Ingestion absorption efficiency (assumption)
fraction(absorbPart)	0.5	Fractional Absorption of Inhaled Particles (assumption)
fraction(inhVap)	0.75	Fract. Abs. of inhaled in vapor Iwase et al. (1991)
fraction(orgCarbonInFilm)	0.57	Diamond(2000)
fraction(orgCarbonInDust)	0.19	Bennett (2004)
fraction(orgCarbonParticles)	0.55	Naumova (2003)
Rates		
rate-inhalation (m^3/hr)	6.3	Brochu (2010)
rate dust ing (g/day)	0.007	Ozkaynak (2010)
rate urineProduction (L/day)	0.38	urine production for 3 year 22.4ml/kg day (Miller & Stapleton 1989)
rate-resuspension (/h)	1.00E-06	Liu (2010)
deposVel (m/h)	0.2	
Nicotine (g/day)	0.0057	cigarette nicotine estimate based on Benowitz (1996) 1.0mg nicotine/cigarette *71% nicotine dose in sidestream*8cigarettes/day
Room Dimensions		
rmheight (m)	2.4	Layton (2009)
rmlength (m)	10	
rmwidth (m)	10	

Surface Areas		
surfaceAreaAllFloor	rmlength*rmwidth	
SAWallsandWindows	rmlength*rmheight + rmwidth*rmheight	
surfaceArea (wall,wallFilm)	percentageWall* SAWallsandWindows	
surfaceArea(windowFilm)	percentageWindow* SAWallsandWindows	
surfaceArea(vinyl, dustOnVinyl, vinylFilm)	percentageVinyl * surfaceAreaAllFloor	20% Vinyl
surfaceArea (hardFloor, hardFloorFilm,dust)	percentageHardFloor* surfaceAreaAllFloor	40% hardfloors (not vinyl)
crinkleFactor	50	greater surface area due to fibers- Morrison & Nazaroff (2002)
surfaceArea (carpet, carpetFilm)	percentageCarpet*surfaceAreaAllFloor*crinkleFactor	40% carpeted
surfaceArea(backing)	percentageCarpet*surfaceAreaAllFloor	
surfaceArea(fabric, fabricFilm)	0.19 * totalVolume	Hodgson (2005)
surfaceArea(foam)	0.26 * totalVolume	Hodgson(2005)
surfaceAreaKid	0.68	US EPA CSEFH (2008) Avg of 0.65 3-4, 0.715 4-5 (m^2)
fsaske	0.2	fraction of total surface area that is exposed skin (minus hands)
fsaskh	0.05	fraction of total surface area that is exposed skin of hands
fsaskc	1- fsaske-fsaskh	fraction of total surface area that is clothed skin
surfaceAreaFilm	431.6	sum of all surface areas of films
Mass Loadings (kg/m^2)		
massLoading-dust, hardfloor	0.5*1E-3	0.25-0.3 g/m2 from Layton (2009), up to 1.5 g/m2 Coronado
massLoading-vinylFilm,vinyl	0.001	Bennett (2004)
massLoading-wallFilm,wall	0.001	Bennett (2004)
massLoading-windowFilm,windowFilm	0.001	Bennett (2004)
massLoading-hardFloorFilm,hardFloor	0.001	Bennett (2004)
Density (kg/m^3)		
density-air	1.3	
density-particles	1000	
density-vinyl	1500	Cox (2001)
density-wall	1650	
density-dustOnVinyl,dust	500	

density-fat,fat2,liver,kidney,gut,tissue	1000	
density-film,organicFilm	1200	Diamond (2000)
Thicknesses (m)		
thickness-organicFilm	20 *1E-09	(10-100nm) Diamond (2000)
thickness-vinyl	0.0005	Bennett (2004)
thickness-wall	0.005	thickness of wallboard Bennett (2004)
thickness-boundaryLayer	0.03	Bennett (2004)
depthStratum Corneum(SC)	1.50E-05	McCarley and Bunge (2001)
depth Viable Epidermis(VE)	0.1*1E-3	100um EPA RAGS E page A-33
thickness-vinylFilm	massLoading(vinylFilm,vinyl)/density(vinylFilm)	
thickness-dustOnVinyl	massLoading(dustOnVinyl,vinyl)/ density(dustOnVinyl)	Layton estimated .28 um
thickness-dust	massLoading(dust,hardFloor)/density(dust)	
thickness-hardFloor	thickness(wall)	
thickness-hardFloorFilm	massLoading(hardFloorFilm,hardFloor)/density (hardFloorFilm)	
thickness-windowFilm	massLoading(windowFilm,windowFilm)/density (windowFilm)	
thickness-carpet	0.01	1 cm (Bennett 2004 and VanLoy 2001)
thickness-backing	0.0024	.24cm from VanLoy 2001)
thickness-fabric	0.9*1E-3	non-clothing fabric (assume 2x avg. sampled clothing fabric from Chien 2011)
thickness-persfabric	0.45*1E-3	clothing (Chien 2011- avg. of sampled fabrics)
thickness-foam	0.04	4 cm (assumption for apholstered items)
thickness-film	thickness(organicFilm)	
thickness-bothLayersSkin	depthSC+depthVE	
thickness-skinSC	depthSC/nSkinSC	
thickness-skinVE	depthVE/nSkinVE	
Volumes		
Volume-blood (L)	1.26	7.4% BW Cahill (2003)
Volume-gut (L)	0.24	1.4% BW Cahill (2003)
Volume-liver (L)	0.44	2.6% BW Cahill (2003)
Volume-lung (L)	0.12	0.7% BW Reference Man (Snyder 1975)
Volume-fat (L)	1	5.9% BW Richly perfused fat Cahill

		(2003)
Volume-fat2 (L)	2.89	17% BW Poorly perfused fat Cahill (2003)
Volume-tissue	11.05	65% BW (all tissues not described above)
Volume-kidFilm (m^3)	thickness(kidFilm)*surfaceArea(kidFilm)	
Volume-skin (m^3)	surfaceAreaKid * thickness(skin)	
Volume-bothLayersSkin (m^3)	sum(V(skin))	
Volume-air (m^3)	rmlength * rmwidth * rmheight	
Volume-particles (m^3)	TSP * V(air) /density(particles)	TSP = Total Suspended Particles
Degradation Rate Constants k		
halfLife(blood)	0.33	h, Benowitz (2009)
degradationRate(liver) /day	log(0.5)/(halfLife(blood (1)) / 24)	
eliminationRate(lumen) /day	1	
Partition Coefficients K		
K(octanol,water)	10^(logKow)	
K(octanol,air)	K(octanol, water) * R*T/H	Bennett (2004)
K(air,water)	K(octanol,water)/ K(octanol,air)	L water/L air
logKp	-0.860*log10(pL)-4.67	Naumova (2003)
Kp	10^(logKp)	m^3/ug
K(particles,air)	Kp	m^3/ug
logK(dustOnVinyl,air)	log10(K(octanol,air))+log10(fraction(orgCarbonInDust)/0.74)-11.91	
K(dustOnVinyl,air)	10^(logK(dustOnVinyl, air))	BF(2004)
K(dust,air)	K(dustOnVinyl,air)	
K(vinyl,air)	10^(5.20-0.68*log10(VP))	Bennett (2004), VP in Pa, Eq. 18
K(wall,air)	10^(2.93-0.31*log10(VP))	Bennett (2004), VP in Pa, Eq. 17
k(carpet,air)	10^(3.82-0.62*log10(VP))	Bennett (2004), VP in Pa, Eq. 20
k(fabric, air)	4500	Piade (1999)
k(persfab,air)	45000	Piade (1999)
K(skinSC,water)	K(octanol,water)^0.74	(L/kg) Norman (2008)
K(skinVE,water)	1	Assume epidermis behaves as water pA-33 RAGS-E
K(skinSC,air)	K(skinSC,water)/ K(air,water)	L air/ kg sc
Z Fugacity Capacities [mol/(m^3*Pa)]		

sgNIC	1.01	
molecVol	1/(1E6*sgNIC/mw(NIC))	m^3/mole molecular volume
Z(Nicotine)	(1/molecVol)/VP	moles/Pa/m3
Z(water)	1/H	
Z(air)	1/(R*T)	
Z(particles)	K(particles,air)*density (particles)*10^9/(R*T)	Bennett (2004)
Z(film)	0.48*K(octanol,water)* fraction(orgCarbonInFilm) *density(organicFilm)/ H/1000	Bennett (2004)
Z(vinyl)	K(wall,air)/(R*T)	
Z(wall)	K(wall,air)/(R*T)	Bennett (2004)
Z(dustOnVinyl)	K(dustOnVinyl,air)*density(dustOnVinyl)*10^9/ (R*T)	
Z(dust)	K(dust,air)*density(dust)* 10^9/(R*T)	
Z(carpet)	k(carpet,air)/(R*T)	
Z(fabric)	k(fabric,air)/(R*T)	
Z(persfab)	k(persfab,air)/(R*T)	
Z([backing, foam])	Z(fabric)	
Z(hardFloor)	Z(wall)	
Z values Human		
Z(blood)	0.01 * K(octanol,water) / H	(assume 1% lipids)
Z(gut)	0.01* K(octanol,water) / H	
Z(lumen)	0.1* K(octanol,water) / H +0.9*Z(water)	cahill est 10% lipid content
Z(liver)	0.0667* K(octanol,water) / H	assume 0.067% lipids - Reference Man
Z(lung)	0.01* K(octanol,water) / H	assume blood
Z(fat)	1.0* K(octanol,water) / H	assume 100% lipids
Z(fat2)	Z(fat)	
Z(tissue)	0.01* K(octanol,water)/ H	
Z(skinSC)	Z(water) * K(skinSC,water)	
Z(skinVE)	Z(water) * K(skinVE,water)	
Z(bile)	0.1* K(octanol,water)/ H	cahill 10% lipid
Z(octanol)	1.0* K(octanol,water) / H	
Perfusion of Blood		
perfusion(fat)	0.09	
perfusion(liver)	0.24	
perfusion(gut)	0.49	

perfusion(lastLayerSkin)	0.058	Rowell 1974 Roddie 1983 via Stumbaugh 2008 thesis pg 13
perfusion(tissue)	1-(perfusion(fat)+ perfusion(liver)+perfusion (gut)+ perfusion(lastLayerSkin)	
Flow Q [m3/day or g/day]		
Q(air)	V(air)*AEout	flow rate from outside [m^3/day]
Q(partFlowIn)	TSPout * 1E3 * Q(air)	g/day (TSP in kg/m3, Q(air) m3/day)
Q(partFlowOut)	TSP * 1E3 * Q(air)	g/day or ... Q(air)*(TSP/density(particles))
Q(soilTrackIn)	0.1	g/day Layton p S-20
Q(cleaningLoss)	cleanLoss* massLoading(dust,hardFloor)*1E3* surfaceAreaAllFloor	g/day
Q(resuspension)	rate(resuspension) * 24 * massLoading(dust,hardFloor) *1E3* surfaceAreaAllFloor	g/day
Q(deposition)	deposVel *24 * TSP * 1E3* surfaceAreaAllFloor	g/day
Q(particleProduction)	(Q(deposition)+Q(partFlowOut))-(Q(resuspension)+Q(partFlowIn))	g/day
Q(dustProduction)	(Q(resuspension)+Q(cleaningLoss))-(Q(deposition)+Q(soilTrackIn))	g/day
G Values: Flow of blood m3/day		
Q(lung)	264 *24/1000	(264 L/hr) m3/day Brochu (2011)
G(blood,lung)	180 *24/1000	Cardiac Ouput 3L/min Alverson (1982)
G(blood,skin)	G(blood,lung)*perfusion (lastLayerSkin)	m3/day (22.27 L/hr) compare to cutaneous flow rates 0.5 - 1.7 cm3/h/cm2 \McCarley (2001)
G(blood,fat)	G(blood,lung)*perfusion (fat)	
G(blood,tissue)	G(blood,lung)*perfusion (tissue)	
G(blood,gut)	0.302	0.84 ml/min/g gut; kissel (1988)
G(gut,liver)	G(blood,gut)	

G(blood,liver)	G(blood,lung)*perfusion (liver)	
G(liver,blood)	G(blood,liver)+ G(blood,gut)	
G(bile,gut)	0.25/1000	adult range 0.25-1L/day use lower value
Skin Permeability		
logPcw	-2.80 + 0.66*logKow-0.0056*mw(NIC)	Potts-Guy
Pcw	10^(logPcw)	
B	Pcw * sqrt(mw(NIC))/2.6	Ratio of stratum corneum permeability to viable epidermis permeability (Bunge 1995)
Pew	Pcw/B	
Diffusivity [m^2 / hr]		
diffusivity(air)	0.012	calc from Wilke & Lee Method, Lyman Ch 17
diffusivity(skinSC)	permeability(skinSC(1))* depthSC/K(skinSC(1),water)	
diffusivity(skinVE)	permeability(skinVE(1))* depthVE/K(skinVE(1),water)	
diffusivity(water)	2.20E-06	calc from Hayduk & Laudie Method, Lyman Ch 17
diffusivity(dustOnVinyl)	(diffusivity(air)*Z(air)/((0.38+0.12)*Z(dustOnVinyl))) *(0.5^(4/3))	
diffusivity(dust)	(diffusivity(air)*Z(air)/((0.38+0.12)*Z(dust))) *(0.5^(4/3))	kissel 1989
diffusivity(wall)	(diffusivity(air)*Z(air)/(0.2*Z(wall)))*(0.2^(4/3))	
k Related Media-specific MT Coefficients [m/hr]		
k(air)	3	Weschler and Nazaroff (for flat surfaces)
k(airParticle)	diffusivity(air)/thickness(boundaryLayer)	
k(dustOnVinyl)	diffusivity(dustOnVinyl)/thickness(dustOnVinyl)	
k(dust)	diffusivity(dust)/thickness(dust)	
k(particles)	diffusivity(air)/(particleDiameter/2)	

k(film)	(diffusivity(water)/30)/(thickness(organicFilm)*0.5)	
k(skin)	diffusivity(skin)/(thickness(skin)*0.5)	
Interfacial Mass Transfer Coefficients MT [mol/m2-hr-Pa]		
for i = [film]		
MT(air,i)	1/(1/(k(air)*Z(air))+1/(k(i)*Z(i)))	
for i = [dustOnVinyl dust]		
MT(air,i)	1/(1/(k(airParticle)*Z(air))+1/(k(i)*Z(i)))	
MT(air,particles)	1/(1/(k(particles)*Z(air))+ 1/(k(particles)*Z(particles)))	
MT(dustOnVinyl,vinylFilm)	1/(1/(k(dustOnVinyl)*Z(dustOnVinyl))+1/(k(vinylFilm)*Z(vinylFilm)))	
MT(vinyl,vinylFilm)	k(vinylFilm)*Z(vinylFilm)	assume no resist vinyl side
MT(wall,wallFilm)	1/(1/(k(wall)*Z(wall))+1/(k(wallFilm)*Z(wallFilm)))	
MT(hardFloorFilm,hardFloor)	1/(1/(k(hardFloorFilm)*Z(hardFloorFilm))+1/(k(hardFloor)*Z(hardFloor)))	
D Mackay-type Transport Coefficients [mol/(Pa*day)]		
D(vinyl,vinylFilm)	MT(vinyl,vinylFilm)*24*interfaceArea(vinyl,vinylFilm)	
for i = [film dustOnVinyl dust particles]		
D(air,i)	MT(air,i)*24*interfaceArea(i,air)	
D(dustOnVinyl,vinylFilm)	MT(dustOnVinyl,vinylFilm)*24*interfaceArea(dustOnVinyl,vinylFilm)	
D(wall,wallFilm)	MT(wall,wallFilm)*24*interfaceArea(wall,wallFilm)	
D(hardFloorFilm,hardFloor)	MT(hardFloorFilm,hardFloor)*24*interfaceArea(hardFloorFilm,hardFloor)	
D(air,carpetFilm)	D(air,wallFilm)	
D(carpetFilm,air)	D(air,carpetFilm)	
D(carpetFilm,carpet)	D(wallFilm,wall)	
D(carpet,carpetFilm)	D(carpetFilm,carpet)	

D(carpet,backing)	0.25 * D(carpetFilm,carpet)	
D(backing,carpet)	D(carpet,backing)	
D(air,fabricFilm)	D(air,wallFilm)	
D(fabricFilm,air)	D(air,fabricFilm)	
D(fabricFilm,fabric)	D(wallFilm,wall)	
D(fabric,fabricFilm)	D(fabricFilm,fabric)	
D(fabric,foam)	0.25 * D(fabricFilm,fabric)	
D(foam,fabric)	D(fabric,foam)	
D(particles,flowOut)	Q(partFlowOut)/(density(particles)*1E3)*Z(particles)	
D(air,flowOut)	Q(air)*Z(air)	
D(blood,gut)	G(blood,gut)*Z(blood)	
D(gut,blood)	G(blood,gut)*Z(blood)	
D(blood,liver)	G(blood,liver)*Z(blood)	
D(liver,blood)	G(blood,liver)*Z(blood)	
D(blood,fat)	G(blood,fat)*Z(blood)	
D(fat,blood)	G(blood,fat)*Z(blood)	
D(blood,tissue)	G(blood,tissue)*Z(blood)	
D(tissue,blood)	G(blood,tissue)*Z(blood)	
D(gut,liver)	G(gut,liver)*Z(blood)	
D(air,lung)	rate(inhalation)*Z(air)	
D(lung,air)	rate(inhalation)*Z(air)	
D(blood,lung)	G(blood,lung)*Z(blood)	
D(lung,blood)	G(blood,lung)*Z(blood)	
Aqueous Diffusion Transport term		
Bq	(T*R)/(6*pi*avogadro*molecRad*viscosityWater)	m^2/h
interfaceArea(lumen,gut)	10	m^2 Cahill (ref 8)
diffusPathLength	3.50E-04	m (cahill est in range 0.01-1 mm)
Dq	Bq*interfaceArea(lumen,gut)*Z(water)/ diffusPathLength	
Bc	(T*R)/(6*pi*avogadro*molecRad*viscosityOctanol)	Micelle Mediated Diffusion Transport Term
micelleFractionOfLumen	0.05	
Ac	interfaceArea(lumen,gut) * micelleFractionOfLumen	
Kcw	10^(-0.123 * (log(K(octanol,water)))^2 + 2.521 * log(K(octanol,water)) - 5.375)	partitioning micelle water Cahill from Dulfer, pg S-19
Zc	Kcw*Z(water)	

Dc	Bc*Ac*Zc/diffusPathLength	
Be	(T*R)/(6*pi*avogadro*molecRad*viscosityOctanol)	
Au	interfaceArea(lumen,gut)	
thicknessCellMembr	1.00E-08	m (10 nm) from Cahill ref 12 - Dulfer
De	Be*Au*Z(octanol)/thicknessCellMembr	
D(lumen,gut)	1/(1/(Dq+Dc) +1/De)* 24	
D(gut,lumen)	1/(1/Dq + 1/De)*24	
D(dust,lumen)	rate(ingDust)/(density(dust)*1E3)*fraction(GIabsDust)*percentageHardFloor*Z(dust)	
D(dustOnVinyl,lumen)	rate(ingDust)/(density(dustOnVinyl)*1E3)*fraction(GIabsDust)*percentageVinyl* Z(dustOnVinyl)	
D(gut,liver)	G(blood,liver)*Z(blood)	gut to liver
D(gut,blood)	G(blood,gut)*Z(blood)	blood from gut
D(blood,liver)	G(blood,liver)*Z(blood)	blood to liver
D(liver,blood)	G(liver,blood)*Z(blood)	
D(blood,fat)	G(blood,fat)*Z(blood)	blood to fat
D(fat,blood)	G(blood,fat)*Z(blood)	
D(fat,fat2)	D(blood,fat)*0.25	Transport from richly perfused fat to deep adipose
D(fat2,fat)	D(fat,fat2)	
D(blood,tissue)	G(blood,tissue)*Z(blood)	Transport blood to tissue
D(tissue,blood)	G(blood,tissue)*Z(blood)	
D(dustOnVinyl,particles)	Q(resuspension)*percentageVinyl/ (density(dustOnVinyl)*1E3) * Z(dustOnVinyl)	resuspension of dust to particles:
D(dust,particles)	Q(resuspension)*percentageHardFloor/(density(dust)*1E3) * Z(dust)	
D(particles,dustOnVinyl)	Q(deposition)/(density(particles)*1E3) *percentageVinyl *Z(particles)	deposition of particles into dust
D(particles,dust)	Q(deposition)/(density(particles)*1E3)*percentageHardFloor*Z(particles)	
D(dust,clean)	Q(cleaningLoss)*percentageHardFloor /(density(dust)*1E3)*Z(dust)	loss of dust to cleaning

D(dustOnVinyl,clean)	Q(cleaningLoss)*percentageVinyl/ (density(dustOnVinyl)*1E3)*Z(dustOnVinyl)	
D(bile,gut)	G(bile,gut)*Z(bile)	transport in bile from liver to gut
Ff	0.2	glomerular filtration rate
Fe	0.05	glomerular filtrate excr ratio-Benowitz
aqFrac	0.9	Cahill
G(blood,kidney)	0.82	m^3/day, 19% of cardiac output
D(blood,excrUrine)	G(blood,kidney)*Ff * Fe * Z(blood)*aqFrac	
D Skin		
MT(kidFilm,skin(1))	1/(1/(k(skinSC(1))*Z(skinSC(1)))+1/(k(kidFilm)*Z(kidFilm)))	mol/(m2-hr-Pa)
D(kidFilm,skin(1))	MT(kidFilm,skin(1))*24*interfaceArea(kidFilm,skin(1))	
D(skin(1),kidFilm)	D(kidFilm,skin(1))	
MT(skin(1),skin(2))	1/(1/(k(skin(1))*Z(skin(1)))+1/(k(skin(2))*Z(skin(2))))	First layer of skin to Second Layer
D(skin(1),skin(2))	MT(skin(1),skin(2))*24*interfaceArea(skin(end),blood)	
if nSkin >2		skin layers to adjoining skin layers
for i = skin(2):skin(end)-1		
prev = i-1; next = i+1;		
MT(i,prev)	1/(1/(k(i)*Z(i))+1/(k(prev)*Z(prev)))	
MT(i,next)	1/(1/(k(i)*Z(i))+1/(k(next)*Z(next)))	
D(i,prev)	MT(i,prev)*24*interfaceArea(skin(end),blood)	
D(i,next)	MT(i,next)*24*interfaceArea(skin(end),blood)	
MT(skin(end)-1,skin(end))	1/(1/(k(skin(end)) * Z(skin(end)))+1/(k(skin(end)-1) *Z(skin(end)-1)))	
D(skin(end)-1,skin(end))	MT(skin(end)-1,skin(end))*24*interfaceArea(skin(end),blood)	

D(skin(end),skin(end)-1)	D(skin(end)-1,skin(end))	
D(skin(end),blood)	G(blood,skin(end))*Z(blood)	(interfaceArea(skin(end),blood)*thickness(skin(end)))
D(blood,skin(end))	D(skin(end),blood)	
D(i,kidFilm)	(surfaceArea(i)/surfaceAreaFilm)*0.016* surfaceAreaKid/2.0	Rossbach mol/Pa-hr 2.0 to adjust for kid size

Appendix B. MATLAB Code

Parameters

```
function parameters_nicotine4()

%% _________  Fugacity, concentration, mass compartments
___________________
vinyl = 1;
vinylFilm = 2;
air = 3;
particles = 4;
dustOnVinyl = 5;
dust = 6;
hardFloorFilm = 7;
hardFloor = 8;
wallFilm = 9;
wall = 10;
windowFilm = 11;
fabric = 12;
fabricFilm = 13;
foam = 14;
carpetFilm = 15;
carpet = 16;
backing = 17;
persfab = 18;       % personal fabric
persfabFilm = 19;   % personal fabric film

nInanimateCompartments = 19;
    inanimates = 1:nInanimateCompartments;
%% _________  Body Compartments
startBodyComp = nInanimateCompartments + 1;
    kidFilme = startBodyComp;
    kidFilmc = startBodyComp + 1;
    kidFilmh = startBodyComp + 2;
    lung = startBodyComp + 3;
    liver = startBodyComp + 4;
    lumen = startBodyComp + 5;
    gut = startBodyComp + 6;
    fat = startBodyComp + 7;     % (richly) perfused fat
    fat2 = startBodyComp + 8;    % poorly perfused (or deep) fat
    tissue = startBodyComp + 9;
    blood = startBodyComp + 10;

    organs = [lung,liver,lumen,gut];
    bulk = [tissue,fat,fat2];

regularComp = startBodyComp + 10;
%% _________  Regular Compartment Legend

legendRegular = {'vinyl','vinyl film', 'air','particles',...
    'dust on vinyl','dust','hard floor film','hard floor',...
    'wall film','wall','window film','fabric','fabric film',...
    'foam','carpet film','carpet','backing','persfab','persfab film'...
```

```
    'kid film (e)','kid film (c)','kid film
(h)','lung','liver','lumen',...
    'gut','perfused fat','poorly perfused fat2','tissue','blood'};

nCompPlot=regularComp;  %#ok<*NASGU>
nMassExchangeComp = nInanimateCompartments;
%% _________  Special Mass Compartments [g] ______________________________

emitVinyl = regularComp + 1;
storageCompartments = regularComp + 2;
flowOut = regularComp + 3;
inhVap = regularComp + 4;
inhPart = regularComp + 5;
ingDust = regularComp + 6;
absDerme = regularComp + 7;
absDermc = regularComp + 8;
absDermh = regularComp + 9;
excrUrine = regularComp + 10;
excrFeces = regularComp + 11;
dose = regularComp + 12;
skinscTotal = regularComp + 13;
skinveTotal = regularComp + 14;
skinallTotal = regularComp + 15;
metabolites = regularComp + 16;
storageKid = regularComp + 17;
concUrine = regularComp + 18;    % SPECIAL UNITS: ug/L
sweep = regularComp + 19;
launder = regularComp + 20;
bathing = regularComp + 21;
handwash = regularComp + 22;
skinBloodFluxe = regularComp + 23;
skinBloodFluxc = regularComp + 24;
skinBloodFluxh = regularComp + 25;
massBalanceKid = regularComp + 26;
massBalance = regularComp + 27;
emitCig = regularComp + 28;

nSpecial = 28;
flowComps = [inhVap,inhPart,ingDust,excrUrine,excrFeces];
%% _________  Legend Strings
legendSpecial = {...
    'emitted vinyl', 'storage compartments' , 'outflow air',...
    'inhalation of vapor','inhalation of particles',...
    'ingestion of dust', 'dermal absorption (e)', 'dermal absorption
(c)',...
    'dermal absorption (h)','excretion in urine', 'excretion in feces',...
    'dose to kid','skin sc total','skin ve total','skin all total',...
    'metabolites','storage kid','conc in urine ug/L','sweep loss',...
    'launder loss','bathing loss','handwash loss','flux skin to blood
(e)',...
    'flux skin to blood (c)','flux skin to blood (h)','mass balance
kid',...
    'mass balance','emitCig'};
%% _________  Skin Compartments : Numbering
startTheSkin = regularComp+nSpecial;
```

```
nSkinSC = 15; nSkinVE = 20; % number of SC and VE layers
nSkin = 3*(nSkinSC+nSkinVE);
skin = startTheSkin+1:nSkin+startTheSkin;
skinSCe = skin(1:nSkinSC);
skinVEe = skin(nSkinSC+1:nSkin/3);
skinSCc = skin(nSkin/3+1:nSkin/3+nSkinSC);
skinVEc = skin(nSkin/3+nSkinSC+1:nSkin*(2/3));
skinSCh = skin(nSkin*(2/3)+1:nSkin*(2/3)+nSkinSC);
skinVEh = skin(nSkin*(2/3)+nSkinSC+1:nSkin);

skine = skin(1:nSkin/3);
skinc = skin(nSkin/3+1:nSkin*(2/3));
skinh = skin(nSkin*(2/3)+1:nSkin);

firstLayerSkine = skin(1);
lastLayerSkine = skin(nSkin/3);
firstLayerSkinc = skin(nSkin/3+1);
lastLayerSkinc = skin(nSkin*(2/3));
firstLayerSkinh = skin(nSkin*(2/3)+1);
lastLayerSkinh = skin(end);
%% _________  Lists
storageList = [storageCompartments,storageKid];
flowList =
[emitVinyl,flowOut,sweep,absDerme,absDermc,absDermh,inhVap,inhPart,ingDust
,excrUrine,excrFeces];
balanceList = [massBalanceKid,massBalance];
enviroList = 1:nInanimateCompartments;
bodyList =
[organs,bulk,kidFilme,kidFilmc,kidFilmh,skin(1),skin(nSkin/3),skin(nSkin/3
+nSkinSC),skin(nSkin*(2/3)),skin(nSkin*(2/3)+nSkinSC),skin(nSkin),blood];
totalBody = [organs,bulk,kidFilme,kidFilmc,kidFilmh,skin,blood];
%% _________  Legend Skin

legendSkin = cell(1,nSkin);
for i = 1:nSkin/3
           if i <= nSkinSC
               typeOfSkin = 'sc';
           else
               typeOfSkin = 've';
           end
    legendSkin{i} = sprintf('skin %i, %s',i,typeOfSkin);
end

for i = nSkin/3+1:nSkin*(2/3)
           if i <= nSkin/3+nSkinSC
               typeOfSkin = 'sc';
           else
               typeOfSkin = 've';
           end
    legendSkin{i} = sprintf('skin %i, %s',i,typeOfSkin);
end

for i = nSkin*(2/3)+1:nSkin
           if i <= nSkin*(2/3)+nSkinSC
               typeOfSkin = 'sc';
```

```
            else
                typeOfSkin = 've';
            end
    legendSkin{i} = sprintf('skin %i, %s',i,typeOfSkin);
end
%% _________  Define nComp
nComp = max(skin); % number of environmental and human compartments (minus
extra labels)

humanCompartments = [startBodyComp:regularComp,skin];
compartments = 1:regularComp;
% extracompartments =
specialCompartments = regularComp+1:regularComp+nSpecial;
plottingCompartments = [compartments, skin];
autoCalcCompartments = [compartments, skin];
%% _________  Extra labels:
organicFilm = nComp + 1;
boundaryLayer = nComp + 2;
bothLayersSkin = nComp + 3;
halfLife = zeros(nComp + 4);
urine = nComp + 5;
octanol = nComp + 6;
water = nComp + 7;
partFlowIn = nComp + 8;
partFlowOut = nComp + 9;
soilTrackIn = nComp + 10;
sweepingLoss = nComp + 11;
launderingLoss = nComp + 12;
bathingLosse = nComp + 13;
bathingLossc = nComp + 14;
bathingLossh = nComp + 15;
handwashingLoss = nComp + 16;
resuspension = nComp + 17;
deposition = nComp + 18;
particleProduction = nComp + 19;
dustProduction = nComp + 20;
bile = nComp + 21;
absorbPart = nComp + 22;
GIabsDust = nComp + 23;
orgCarbonInFilm = nComp + 24;
orgCarbonInDust = nComp + 25;
orgCarbonParticles = nComp + 26;
dehpInVinyl = nComp + 27;
timeIndoors = nComp + 28;
inhalation = nComp + 29;
urineProduction = nComp + 30;
dustDeposition = nComp + 31;
partVel = nComp + 32;
partSuspVel = nComp + 33;
resuspension = nComp + 34;
kidney = nComp + 35;
bloodTotal = nComp + 36;
airParticle = nComp + 37;
bothLayersSkine = nComp + 38;
bothLayersSkinc = nComp + 39;
```

```
bothLayersSkinh = nComp + 40;

nExtra = 40;
%% _________       Definition of Film
film = [kidFilme kidFilmc kidFilmh vinylFilm wallFilm hardFloorFilm ...
        windowFilm fabricFilm persfabFilm carpetFilm];

% envirofilm = [vinylFilm wallFilm hardFloorFilm windowFilm fabricFilm ...
%                persfabFilm carpetFilm];

% kidfilm = [kidFilme kidFilmc kidFilmh];

filmSubs = [vinylFilm wallFilm hardFloorFilm ...
            fabricFilm persfabFilm carpetFilm];

substrate = zeros(nComp+nExtra,1);
substrate(vinylFilm) = vinyl;
substrate(hardFloorFilm) = hardFloor;
substrate(wallFilm) = wall;
substrate(fabricFilm) = fabric;
substrate(persfabFilm) = persfab;
substrate(carpetFilm) = carpet;
%% _________  Full legend:
legendNames = [legendRegular legendSpecial legendSkin];
%% _________  NIC   ________________________________________
pL = 0.038 * 101325 / 760;    % Pa Subcooled Liquid VP (0.04 mmHg from EPI
Suite exp database, converted to pa)
VP = pL;
Ps = 1E-10;    % atm %W&N (currently unused)
H  = 3.04E-004;    % Pa*m^3/mol; Henry's law constant; EPI SUITE EST
R  = 8.314472;    % m^3*Pa/mol/K; gas constant
T  = 298;    % K; temperature
%% _________  LogKow
logKow = 1.17;    % log octanol/water partition coefficient
%% _________  MW and excretion Ratios
CASno = 'Nicotine CAS No. 54-11-5';
mw = zeros(5,1);
NIC = 1; cotinine = 2; Glucu = 3; NIC1Nox = 4; norNIC = 5;
mw(NIC) = 162.26;   % g/mol  mw(NIC)
mw(cotinine) = 176.22;   % g/mol  cotinine + 3-hydroxycotinine
% mw(Glucu) = 352.34;   % g/mol  of cotinine glucuronide +
% 3-hydroxycotinine
% mw(NIC1Nox) = 178.23;   % g/mol
% mw(norNIC) = 148.21;   % g/mol
mwRatio = ones(5,1);
mwRatio(cotinine) = mw(cotinine) / mw(NIC) ;
% mwRatio(Glucu) = mw(Glucu) / mw(NIC) ;
% mwRatio(NIC1Nox) = mw(NIC1Nox) / mw(NIC) ;
% mwRatio(norNIC) = mw(norNIC) / mw(NIC) ;
excrRatio = zeros(5,1);
excrRatio(cotinine) = 0.13;  % (%) \Benowitz 1996 free and conjugated
"total"
%excrRatio(Glucu) = 0.20; % (%) \Benowitz 1996 cotinine glucuronide
%excrRatio(NIC1Nox) = 0.044; % (%) \Benowitz 1996
% NHANESdata = zeros(5,2);
```

```
% GM = 1; percentile99=2;
% NHANESdata(cotinine,GM) = 36.9; %ug/L \cite{CDC2009}
% NHANESdata(cotinine,percentile99) = 318; %ug/L \cite{CDC2009}
% NHANESdata(metab5oxo,GM) = 25.1; %ug/L \cite{CDC2009}
% NHANESdata(metab5oxo,percentile99) = 197; %ug/L \cite{CDC2009}

%% _________  Body Weight ______________
BW = 17; %kg; Kids age 5-11, mean 27 kg, sd 7.3; lognormal distrib
    %Toddlers 0.5-4 years, mean 15kg, SD 3.8; \cite{Clark2003}
    %17 Child Specific EFH
%% _________  Conversions    _______________________________________
ng = mw(NIC) * 1E+9;
ug = mw(NIC) * 1E+6;
Lhr_m3d = 24 / 1000; % L/hr -> m3/day
cmhr_md = 24 / 100; % cm/hr -> m/day
%% _________  Other   __________________________________________
dtrackin = 0.001; % g/day; Soil track in
Csoil = 0; % g NIC / g outdoor soil
sweepLoss = 0.0053; % /day; dustOnVinyl 0.0053 \cite{Layton 2009}
launderLoss = 0.07; % /day (John estimate)
handwashLoss = 3; % assumes 3 handwashes per day
bathLoss = 0.3; % assumes about two baths per week
Cchemoa  = 0; % mol/m^3; concentration of chem in vapor in outside air
TSPoa = 0; % ug/m3; suspended particle concentration in outdoor air
Cchemsp1oa = 0; % g/g chemical concentration in suspended particles in
outdoor air
TSP = 20E-9; % THIS IS KG/M3 (20 ug/m3 x 1E-9) concentration of suspended
particles
             % in indoor air (Xu 2010)
TSPout = 24E-9; % THIS IS KG/M3
AEout = 6; % /day; air exchange with outside
%% _________  Unitless Fractions  _____________________________
fraction(GIabsDust) = 0.5; % Dust ingestion absorption efficiency
fraction(absorbPart) = 0.5; % Fractional absorption of inhaled particles
fraction(inhVap) = 1; % Fractional absorption of nicotine inhaled in vapor
fraction(orgCarbonInFilm) = 0.57; % Diamond(2000), used by BF
fraction(orgCarbonInDust) = 0.19; % Bennett & Furtaw p2144
fraction(orgCarbonParticles) = 0.55; % W&N p9035,indoor PM2.5 (via Naumova
2003)
%% _________  Rates      ____________________________
rate(inhalation) = 7.3; % 10.9 m3/day from CSEFH 2008 (3-6 yo); 7.3 m3/day
from
    % Brochu (2006) via CSEFH Table 6-5 (weighted ave); 8.3 m3/day from Xu
2010
    % supplement Table S6 (3-6 yo); 7.4 m3/day from Brochu 2011 alveolar
data
    % (5-7 yo); /cite{Clarke2003} age 5-11 rate 15 sd 3.2 m3/day and
toddler
    % 0.5-4 yo rate 9.3 sd 2.6 lognormal; lower rate chosen based on
Brochu
    % 2006 and 2011 being consistent (both were for "normal weight"
children;
    % their data shows for higher BW, the inhalation rate goes up; our
kids are
```

```
    % 17 kg, so the "normal weight" inhalation rate appears most
appropriate

rate(ingDust) = 0.027; % mean 7 mg/day object to mouth; mean 20 mg/day
hand-to-mouth
                       % Ozkaynak et al 2010
rate(urineProduction) = 380 * 1E-3; % L/day - urine production for 3 year
rate(resuspension) = 1E-6; % /h (from 1E-6 /h est from Liu 2010 table2)
deposVel = 0.2; % m/h
cig = 0.0057; % g/day cigarette nicotine estimate from Benowitz 1999 1.0
mg
              % nicotine/cigarette * 71 % nicotine dose in
sidestream*8cigarettes/day
%% _________  Dimensions [m] ___________________
rmheight = 2.4; % m; height of room (Layton & Beamer)
rmlength = 10; % m; length of room made up
rmwidth  = 10; % m; width of room made up
totalVolume = rmlength * rmwidth * rmheight;
surfaceAreaAllFloor = rmlength * rmwidth;
SAWallsandWindows = rmlength * rmwidth + 2*(rmlength*rmheight +
rmwidth*rmheight);
%% _________  Percentage of coverings
percentageWall = 0.95;
percentageWindow = 1 - percentageWall;
percentageVinyl = 0.20; %(Xu 2010: SA vinyl in main room = 19.2)
percentageCarpet = 0.40;
percentageHardFloor = 1 - (percentageVinyl + percentageCarpet);

%% _________  Surface Area [m2]
surfaceArea = zeros(nComp+nExtra,1);
surfaceArea([wall,wallFilm]) = percentageWall * SAWallsandWindows;
surfaceArea(windowFilm) = percentageWindow * SAWallsandWindows;
surfaceArea([vinyl, dustOnVinyl, vinylFilm]) = percentageVinyl * ...
                                               surfaceAreaAllFloor;
surfaceArea([hardFloor, hardFloorFilm, dust]) = percentageHardFloor * ...
                                                surfaceAreaAllFloor;
crinkleFactor = 50; % greater surface area due to fibers (Morrison and
Nazaroff,
                    % 2002)

surfaceArea([carpet, carpetFilm]) = percentageCarpet * surfaceAreaAllFloor
* ...
                                    crinkleFactor; % m2
surfaceArea(backing) = percentageCarpet * surfaceAreaAllFloor;
surfaceArea([fabric, fabricFilm]) = 0.19 * totalVolume; % hodgson
quantifying
                                                        % table 10
surfaceArea(foam)= 0.26 * totalVolume; % Hodgson table 10
surfaceAreaKid = 0.68; % CSEFH 0.65 3-4, 0.715 4-5/2 m^2  (6-11 years old)
=
                       % 8600 cm^2 Table S7 Xu

fsaske = 0.15; % fraction of surface area that is exposed skin (minus
hands) assumed
```

```
               % to have a range of 10% (night) to 20% (day), so 15% taken
as a
               % mean
fsaskh = 0.038; % fraction of hand surface area assumed to have a range of
2.5% (night)
                % to 5.0% (day), so 3.8% taken as a mean; assumed to be
exposed skin, so
                % total exposed skin % = 0.25)
fsaskc = 1 - fsaske - fsaskh; % fraction of total surface area that is
clothed skin

surfaceArea([kidFilme,skin(1)]) = surfaceAreaKid * fsaske;
surfaceArea([kidFilmc,skin(nSkin/3+1)]) = surfaceAreaKid * fsaskc;
surfaceArea([kidFilmh,skin(nSkin*(2/3)+1)]) = surfaceAreaKid * fsaskh;

surfaceArea(persfab) = fsaskc * surfaceAreaKid;
surfaceArea(persfabFilm) = fsaskc * surfaceAreaKid; % NEEDS TO BE CHECKED
surfaceAreaFilm = surfaceArea(wallFilm) + surfaceArea(windowFilm) + ...
                  surfaceArea(vinylFilm) + surfaceArea(hardFloorFilm) +
...
                  surfaceArea(carpetFilm) + surfaceArea(fabricFilm) + ...
                  surfaceArea(persfabFilm);

%% _________  Mass Loading [kg/m2]  ______________________________________
massLoading = zeros(nComp+nExtra,nComp+nExtra);
massLoading(dustOnVinyl,vinyl) = 0.5*1E-3;
massLoading(dust,hardFloor) = massLoading(dustOnVinyl,vinyl); %
References:
    % 0.25-0.3 g/m2 from Layton & Beamer, up to 1.5 g/m2 Coronado
massLoading(vinylFilm,vinyl) = 0.001; %
massLoading(wallFilm,wall) = 0.001; %
massLoading(windowFilm,windowFilm) = 0.001; %
massLoading(hardFloorFilm,hardFloor) = 0.001; %

massLoading = makeSymmetric(massLoading);
%% _________  Density [kg/m3]  ___________________________________________
density = zeros(nComp+nExtra,1);

density(air)= 1.3;
density(particles) = 1000; % however, Bennett & Furtaw used 1500
density(vinyl) = 1500; % 1.5 g/cm3 \cite{Cox2001}
density(wall) = 1650 ; % 1.62-1.66 g/cm3 \cite{Feldman1990}
density([dustOnVinyl,dust]) = 500; % 1000; (half density of water)
density(hardFloor) = density(wall);
density([fat,fat2,liver,kidney,gut,tissue]) = 1000; % 1000 kg/m3 = 1 kg/L
density([film,organicFilm]) = 1200; % \cite{Diamond2000}, used by BF
density([skin,blood,lung,lumen]) = 1000; % for calc tissue conc only
%% _________  Thickness [m]  ___________________________________________
thickness = zeros(nComp+nExtra,1);
thickness(organicFilm) = 20 * 1E-09; % m; for organic environmental films
(3-30 nm)
    % Weschler & Nazaroff (2012); 10-100 nm (Diamond 2000)
% thickness(envFilm)

thickness(vinyl) = 0.0005; % \cite{Bennett2004} BF
```

```
    % 2E-03 thickness of vinyl for Clausen experiments, used 17% (w/w)
DEHP
thickness(wall) = 0.005; % thickness of wallboard  BF (2004)
thickness(boundaryLayer) = 0.03; % 3 cm
depthSC = 15E-6; % m; 15 um
depthVE = 0.1*1E-3; % m; 100um EPA RAGS E page A-33
thickness(dustOnVinyl) =
massLoading(dustOnVinyl,vinyl)/density(dustOnVinyl);
    % Layton estimated .28 um
thickness(dust) = massLoading(dust,hardFloor)/density(dust);
thickness(hardFloor) = thickness(wall);
thickness(carpet) = 0.01; % 1 cm (changed per ELC, 2/21/2012)
thickness(backing) = 0.0024; % 0.24 cm  (changed per ELC, 2/21/2012)
thickness(fabric) = 0.9*1E-3; % 0.9 mm (changed per ELC, 2/21/2012)
thickness(persfab) = 0.45*1E-3; % 0.45 mm  (OK'd by ELC, 2/21/2012)
thickness(foam) = 0.04; % 4 cm

thickness(film) = thickness(organicFilm);

%thickness(vinylFilm) = thickness(organicFilm);
%thickness(wallFilm)= thickness(organicFilm);
%thickness(hardFloorFilm) = thickness(organicFilm);
%thickness(windowFilm) = thickness(organicFilm);
%thickness(fabricFilm) = thickness(organicFilm);
%thickness(persfabFilm) = thickness(organicFilm);
%thickness(carpetFilm) = thickness(organicFilm);

% thickness(skinFilm) = 1.3 * 1E-06; % m; Weschler & Nazaroff (2012)

%thickness(kidFilme) = thickness(organicFilm);
%thickness(kidFilmc) = thickness(organicFilm);
%thickness(kidFilmh) = thickness(organicFilm);

thickness(bothLayersSkin) = depthSC + depthVE;
thickness(skinSCe) = depthSC/nSkinSC;
thickness(skinVEe) = depthVE/nSkinVE;
thickness(skinSCc) = depthSC/nSkinSC;
thickness(skinVEc) = depthVE/nSkinVE;
thickness(skinSCh) = depthSC/nSkinSC;
thickness(skinVEh) = depthVE/nSkinVE;
%% _________  Volumes [m^3]  ______________________________
V = zeros(nComp+nExtra,1);
% Percent body mass (perbm) values are from Cahill (Table S-1) and were
calculated
% by dividing individual body part volumes by 70 L (assumes nominal organ
density
% of 1 kg/L); computed percent body mass this way vs using Table S-1's "%
of % body
% mass" values because the method described above incorporates individual
organ
% densities

bloodperbm = 7.4;
gutperbm = 1.4;
liverperbm = 2.6;
```

```
lungperbm = 0.7; % assumes that lung volume is made up of only the blood
in the
                 % lung; assumes blood volume is 10% of total blood volume
(based on
                 % Reference Man's lung blood volume of 0.5 L (~10% of 5.2
L of
                 % total blood in an adult));
fatperbm = 5.9;
fat2perbm = 17;
lumenperbm = 1.4;
tissueperbm = 100 - bloodperbm - gutperbm - liverperbm - lungperbm -
fatperbm ...
            - fat2perbm - lumenperbm;

V(blood) = BW * bloodperbm / 100;
V(gut)= BW * gutperbm / 100;
V(liver)= BW * liverperbm / 100;
V(lung)= BW * lungperbm / 100;
V(fat)= BW * fatperbm / 100;
V(fat2) = BW * fat2perbm / 100;
V(lumen) = BW * lumenperbm * 100;
V(tissue) = BW * tissueperbm / 100;

% Convert volumes to m3:
V = V/1000;

V(kidFilme) = thickness(kidFilme) * surfaceArea(kidFilme);
V(kidFilmc) = thickness(kidFilmc) * surfaceArea(kidFilmc);
V(kidFilmh) = thickness(kidFilmh) * surfaceArea(kidFilmh);

V(skinSCe) = surfaceAreaKid * fsaske * thickness(skinSCe);
V(skinVEe) = surfaceAreaKid * fsaske * thickness(skinVEe);
V(bothLayersSkine) = sum(V(skine));

V(skinSCc) = surfaceAreaKid * fsaskc * thickness(skinSCc);
V(skinVEc) = surfaceAreaKid * fsaskc * thickness(skinVEc);
V(bothLayersSkinc) = sum(V(skinc));

V(skinSCh) = surfaceAreaKid * fsaskh * thickness(skinSCh);
V(skinVEh) = surfaceAreaKid * fsaskh * thickness(skinVEh);
V(bothLayersSkinh) = sum(V(skinh));

%V(skin) = surfaceAreaKid * thickness(skin);
%V(bothLayersSkin) = sum(V(skin));

V(air) = rmlength * rmwidth * rmheight;
V(particles) = TSP * V(air) / density(particles);
for i = [dustOnVinyl dust vinyl hardFloor...
        carpet, wall, film, fabric, persfab, foam, carpet, backing]
    V(i) = thickness(i) * surfaceArea(i);
end

%% _________  Interface Areas [m^2]  _____________________________________
interfaceArea = zeros(nComp+nExtra,nComp+nExtra);
```

```
interfaceArea(air,vinylFilm) = surfaceArea(vinyl);
interfaceArea(vinyl,vinylFilm) = surfaceArea(vinyl);
interfaceArea(dustOnVinyl,vinylFilm) = 1E-5 * surfaceArea(vinyl);
interfaceArea(dustOnVinyl,air) = surfaceArea(vinyl);
interfaceArea(dust,air) = surfaceArea(hardFloor);
interfaceArea(dust,hardFloor) = surfaceArea(hardFloor);
    particleDiameter = 1E-6; % 1 um
interfaceArea(air,particles) = V(particles) / (particleDiameter/6);
interfaceArea(particles,kidFilme) = surfaceAreaKid * fsaske;
interfaceArea(air,kidFilme) = surfaceAreaKid * fsaske;
interfaceArea(particles,kidFilmh) = surfaceAreaKid * fsaskh;
interfaceArea(air,kidFilmh) = surfaceAreaKid * fsaskh;
interfaceArea(air,persfabFilm) = surfaceAreaKid * fsaskc;
interfaceArea(dustOnVinyl,kidFilme) = surfaceAreaKid * fsaske;
interfaceArea(dust,kidFilme) = surfaceAreaKid * fsaske;
interfaceArea(kidFilme,skinSCe(1)) = surfaceAreaKid * fsaske;
interfaceArea(kidFilmc,skinSCc(1)) = surfaceAreaKid * fsaskc;
interfaceArea(kidFilmh,skinSCh(1)) = surfaceAreaKid * fsaskh;
interfaceArea(skin,blood) = surfaceAreaKid;
interfaceArea(air,wallFilm) = surfaceArea(wall);
interfaceArea(wallFilm,wall) = surfaceArea(wall);
interfaceArea(air,windowFilm) = surfaceArea(windowFilm);
interfaceArea(air,hardFloorFilm) = surfaceArea(hardFloorFilm);
interfaceArea(hardFloorFilm,hardFloor) = surfaceArea(hardFloorFilm);

interfaceArea = makeSymmetric(interfaceArea);
%% _________  Degradation Rate Constants k
________________________________
% halfLife(urine) = 15; % h, benowitz
halfLife(blood) = 0.33; % h, benowitz
% halfLife(lumen) = 2; % h, est. based on blood from benowitz
degRate = zeros(nComp+nExtra); % /day
degRate(liver) = -log(0.5) / (halfLife(blood(1)) / 24); % /day

elimRate = zeros(nComp+nExtra); % /day
% elimRate(blood) = -log(0.5) / (halfLife(blood(1)) / 24); % /day
elimRate(lumen) = 1; % -log(0.5) / (halfLife(lumen) / 24); % /day

%% _________  Partition Coefficients K  ________________________
K = zeros(nComp+nExtra,nComp+nExtra);
K(octanol,water) = 10^(logKow);
K(octanol,air) = K(octanol,water) * R * T / H; % Eqn 10
\cite{Bennett2004a}
K(air,water) = K(octanol,water) / K(octanol,air); % L water/L air
logKp = -0.860 * log10(pL) - 4.67; % Xu estimate of Kp from Eq S3
(Naumova)
Kp = 10^(logKp); %  m^3/ug
K(particles,air) = Kp; % m^3/ug
logK(dustOnVinyl,air) = log10(K(octanol,air)) + ...
                      + log10(fraction(orgCarbonInDust)/0.74) - 11.91;
K(dustOnVinyl,air) = 10^(logK(dustOnVinyl,air)); % BF(2004) eq. 9 from
Harner
    % and Bidleman  (**old-19*(R*T/H))*1e-12; m^3/ug based on soil from
Lyman
    % (probably garbage--fraction(orgCarbonInDust)*K(octanol,air)/
```

```
    % density(dustOnVinyl))
K(dust,air) = K(dustOnVinyl,air);
K(vinyl,air) = 10^(5.20 - 0.68*log10(VP)); % B&F \cite{Bennett2004} Eq.
18, VP in Pa
K(wall,air) = 10^(2.93 - 0.31*log10(VP)); % B&F \cite{Bennett2004} Eq. 17,
VP in Pa
K(carpet,air) = 10^(3.82 - 0.62*log10(VP)); % B&F \cite{Bennett2004} Eq.
20, VP in
                                            % Pa
K(persfab,air) = 44000; % calculated based on information in Piade et al
(1999)
K(fabric,air) = 4500; % calculated based on information in Piade et al
(1999)
K(skinSCe,water) = K(octanol,water)^0.74; % L/kg Norman \cite{Norman2008a}
from
                                          % Vecchia & Bunge (1995)
K(skinVEe,water) = 1; % Assume epidermis behaves as water pA-33 RAGS-E
K(skinSCc,water) = K(octanol,water)^0.74; % copied K(skinSCe,water)
K(skinVEc,water) = 1; % copied K(skinVEe,water)
K(skinSCh,water) = K(octanol,water)^0.74; % copied K(skinSCe,water)
K(skinVEh,water) = 1; % copied K(skinVEe,water)
K(skinSCe,air) = K(skinSCe,water)/K(air,water); % L air/ kg sc
K(skinSCc,air) = K(skinSCc,water)/K(air,water); % L air/ kg sc; copied
                                                % K(skinSCe,air)
K(skinSCh,air) = K(skinSCh,water)/K(air,water); % L air/ kg sc; copied
                                                % K(skinSCe,air)

K = makeSymmetric(K);
%% _________  Z Fugacity Capacities [mol/(m^3*Pa)] _______________________
sgNIC = 1.01;
molecVol = 1 / (1E6 * sgNIC / mw(NIC)); % m^3/mole; molecular volume
ZNIC = (1 / molecVol) / VP; % moles/Pa/m3
Z = zeros(nComp+nExtra,1);
Z(water) = 1 / H;  % water
Z(air) = 1 / (R*T); % air
Z(particles) = K(particles,air) * density(particles) * 10^9 / (R*T); % B&F
(10)

Z(film) = 0.48 * K(octanol,water) * fraction(orgCarbonInFilm) ...
        * (density(organicFilm)/1000) / H; % film BF eq. 19; 1.0353e+006

%  Z(envirofilm) = 0.48 * K(octanol,water) * fraction(orgCarbonInFilm) ...
%        * (density(envFilm)/1000) / H; % film BF eq. 19; 1.0353e+006

% Z(kidfilm) = 0.48 * K(octanol,water) * fraction(orgCarbonInFilm)...
%             * (density(skinFilm)/1000) / H; % film BF eq. 19; 1.0353e+006

Z(vinyl) = K(vinyl,air) / (R*T);
Z(wall) = K(wall,air) / (R*T); % BF 2004
Z(dustOnVinyl) = K(dustOnVinyl,air) * density(dustOnVinyl) * 10^9 / (R*T);
Z(dust) = K(dust,air) * density(dust) * 10^9 / (R*T);
Z(carpet) = K(carpet,air) / (R*T);
Z(persfab) = K(persfab,air) / (R*T);
Z(fabric) = K(fabric,air) / (R*T);
Z(backing) = Z(fabric);
```

```
Z(foam) = Z(fabric);
Z(hardFloor) = Z(wall);

%% _________  Z values Human ________________
Z(blood) = 0.01 * K(octanol,water) / H; % assume 1% lipids
Z(gut) = 0.01 * K(octanol,water) / H;
Z(lumen) = 0.1 * K(octanol,water) / H + 0.9 * Z(water); % cahill est
10\%lipid
                                                         % content
Z(liver) = 0.0667 * K(octanol,water) / H; % assume 0.067% lipids - RMan
Z(lung) = 0.01 * K(octanol,water) / H; % assume blood)
Z(fat) = 1.0 * K(octanol,water) / H; % assume 100% lipids
Z(fat2) = Z(fat);
Z(tissue) = 0.01* K(octanol,water)/ H;
Z(skinSCe) = Z(water) * K(skinSCe,water);
Z(skinVEe) = Z(water) * K(skinVEe,water);
Z(skinSCc) = Z(water) * K(skinSCc,water); % copied Z(skinSCe)
Z(skinVEc) = Z(water) * K(skinVEc,water); % copied Z(skinVEe)
Z(skinSCh) = Z(water) * K(skinSCh,water); % copied Z(skinSCe)
Z(skinVEh) = Z(water) * K(skinVEh,water); % copied Z(skinVEe)
Z(bile) = 0.1 * K(octanol,water) / H; % cahill 10% lipid
Z(octanol) = 1.0 * K(octanol,water) / H;

%% _________  ZV
ZV = zeros(nComp+nExtra,1); ZV = Z(1:nComp+nExtra).*V(1:nComp+nExtra);
%% _________  Relative Film Surface Areas
listSurfaceFilms = [windowFilm, wallFilm, hardFloorFilm, carpetFilm, ...
                    fabricFilm, vinylFilm];
listSurfaceFilmsp = [windowFilm, wallFilm, hardFloorFilm, carpetFilm, ...
                     fabricFilm, vinylFilm, persfabFilm];
relFilmSA = zeros(nComp+nExtra,1);

%% _________  Perfusion of Blood   ____________________________________
% Perfusion Values from Norman et al (2008)
perfusion = zeros(nComp+nExtra,1);
perfusion(fat) = 0.052;
perfusion(liver) = 0.227;
perfusion(gut) = 0.013 ;
perfusion(lastLayerSkine) = 0.039 * fsaske; % Rowell 1974 Roddie 1983 via
Stumbaugh
                                            % 2008 thesis pg 13
perfusion(lastLayerSkinc) = 0.039 * fsaskc;
perfusion(lastLayerSkinh) = 0.039 * fsaskh;
perfusion(tissue) = 1 - (perfusion(fat) + perfusion(liver) +
perfusion(gut) + ...
                    perfusion(lastLayerSkine) + perfusion(lastLayerSkinc)
+ ...
                    perfusion(lastLayerSkinh)); % expanded
perfusion(lastLayerSkin)
                  % to perfusion(lastLayerSkine),
perfusion(lastLayerSkinc), and
                  % perfusion(lastLayerSkinh)

%% _________  Flow Q [m3/day or g/day]
_____________________________________
```

```
Q = zeros(nComp+nExtra,1);
Qunits = '$m^{3}/day$';
Q(air) = V(air) * AEout; % flow rate from outside [m^3/day]
Q(partFlowIn) = TSPout * 1E3 * Q(air); % g/day (TSP in kg/m3, Q(air)
m3/day)
Q(partFlowOut) = TSP * 1E3 * Q(air); % g/day or
Q(air)*(TSP/density(particles))?
Q(soilTrackIn) = 0.1; % g/day Layton p S-20
Q(sweepingLoss) = sweepLoss * massLoading(dust,hardFloor) * 1E3 * ...
                  surfaceAreaAllFloor; % g/day
Q(resuspension) = rate(resuspension) * 24 * massLoading(dust,hardFloor) *
1E3 * ...
                  surfaceAreaAllFloor; % g/day

Q(launderingLoss) = launderLoss * surfaceArea(persfabFilm) *
thickness(persfabFilm) * ...
                    density(persfabFilm) * 1E3; % g/day

Q(bathingLosse) = bathLoss * surfaceAreaKid * fsaske *
thickness(organicFilm) * ...
                  density(organicFilm) * 1E3; % g/day

Q(bathingLossc) = bathLoss * surfaceAreaKid * fsaskc *
thickness(organicFilm) * ...
                  density(organicFilm) * 1E3; % g/day

Q(bathingLossh) = bathLoss * surfaceAreaKid * fsaskh *
thickness(organicFilm) * ...
                  density(organicFilm) * 1E3; % g/day

Q(handwashingLoss) = handwashLoss * surfaceAreaKid * fsaskh *
thickness(organicFilm) * ...
                     density(organicFilm) * 1E3; % g/day

Q(deposition) = deposVel * 24 * TSP * 1E3 * surfaceAreaAllFloor; % g/day
Q(particleProduction) = (Q(deposition) + Q(partFlowOut)) -
(Q(resuspension) + ...
                         Q(partFlowIn)); % g/day
Q(dustProduction) = (Q(resuspension) + Q(sweepingLoss)) - (Q(deposition) +
...
                     Q(soilTrackIn)); % g/day

%% __________ G Values: Flow of blood  m3/day
___________________________________
G = zeros(nComp+nExtra,nComp+nExtra);
% Flow of air to lung
Q(lung) = 264 * 24 / 1000; % 264 L/hr alveolar ventilation rate changed
per ELC
                           % (2/21/2012)

%Flow of blood-total cardiac output:
G(blood,lung) = 180 * 24 / 1000; % child cardiac output of 3 L/min
(Alverson et al
```

```
    % (1982) (median 3.9 yrs, range 3 days - 17 yrs) and Calamandrei et al
(2008)
    % (median age 19 months, range 1 month - 17 yrs)); 5 L/min from Vinet
et al (2001)
    % (~11 year olds); used 3 L/min x 60 min/hr = 180 L/hr)

G(blood,skin(nSkin/3)) = G(blood,lung) * (perfusion(lastLayerSkine)); %
m3/day
G(blood,skin(nSkin*2/3)) = G(blood,lung) * (perfusion(lastLayerSkinc)); %
m3/day
G(blood,skin(nSkin)) = G(blood,lung) * (perfusion(lastLayerSkinh)); %
m3/day
% compare to cutaneous flow rates 0.8 - 1.7 cm3/h/cm2 \cite{McCarley2001}

G(blood,fat) = G(blood,lung) * perfusion(fat);
G(blood,tissue) = G(blood,lung) * perfusion(tissue);
G(blood,gut) = 0.302; % 0.84 ml/min/g -> 0.302 m3/day; Kissel 1988
(changed per ELC,
                      % 2/21/2012)
G(gut,liver) = G(blood,gut);
G(blood,liver) = G(blood,lung) * perfusion(liver);
G(liver,blood) = G(blood,liver) + G(blood,gut);
G(bile,gut) = 0.25 / 1000; % changed per ELC, 2/21/2012

%% _________  Skin Permeability  _________________________________________
% modified Potts Guy steady state SC permeability from water RAGS E pA-2
logPcw = -2.80 + 0.66*logKow - 0.0056*mw(NIC); % cm/h
Pcw = 10^(logPcw);
B = Pcw * sqrt(mw(NIC)) / 2.6;
% B = 0.79;% from Kretsos method @ log Kow 7.45
Pew = Pcw / B;
permeability = zeros(nComp+nExtra,1);
permeability(skinSCe) = Pcw / 100; % m/h (converted from cm/h)
permeability(skinVEe) = Pew / 100; % m/h (converted from cm/h)
permeability(skinSCc) = Pcw / 100; % m/h (converted from cm/h); copied
                                   % permeability(skinSCe)
permeability(skinVEc) = Pew / 100; % m/h (converted from cm/h); copied
                                   % permeability(skinVEe)
permeability(skinSCh) = Pcw / 100; % m/h (converted from cm/h); copied
                                   % permeability(skinSCe)
permeability(skinVEh) = Pew / 100; % m/h (converted from cm/h); copied
                                   % permeability(skinVEe)
%% _________ Diffusivity [m^2 / hr] and  _____
diffusivity = zeros(nComp+nExtra,1);
diffusivity(air) = 0.012; % calc from Wilke & Lee Method, Lyman Ch 17
diffusivity(skinSCe) = permeability(skinSCe(1)) * depthSC /
K(skinSCe(1),water);
diffusivity(skinVEe) = permeability(skinVEe(1)) * depthVE /
K(skinVEe(1),water);
diffusivity(skinSCc) = permeability(skinSCc(1)) * depthSC /
K(skinSCc(1),water);
diffusivity(skinVEc) = permeability(skinVEc(1)) * depthVE /
K(skinVEc(1),water);
diffusivity(skinSCh) = permeability(skinSCh(1)) * depthSC /
K(skinSCh(1),water);
```

```
diffusivity(skinVEh) = permeability(skinVEh(1)) * depthVE /
K(skinVEh(1),water);
diffusivity(water) = 2.2E-6; % calc from Hayduk & Laudie Method, Lyman Ch
17
diffusivity(dustOnVinyl) = (diffusivity(air) * Z(air) / ((0.38 + 0.12) *
...
                            Z(dustOnVinyl))) * (0.5^(4/3));
diffusivity(dust) = (diffusivity(air)*Z(air) / ((0.38 + 0.12) * Z(dust)))
* ...
                    (0.5^(4/3)); % kissel 1989
diffusivity(wall) = (diffusivity(air) * Z(air) / (0.2*Z(wall))) *
(0.2^(4/3));
for i = [carpet, backing, fabric, foam, hardFloor]
    diffusivity(i) = diffusivity(wall);
end

%% _________ k Related Media-specific MT Coefficients [m/hr] _____________
k=zeros(nComp+nExtra,1);
k(air) = 3; % Weschler and Nazaroff (for flat surfaces)
k(airParticle) = diffusivity(air) / thickness(boundaryLayer); % m/hr
k(dustOnVinyl) = diffusivity(dustOnVinyl) / thickness(dustOnVinyl); % m/hr
k(dust) = diffusivity(dust) / thickness(dust); % m/hr
k(particles) = diffusivity(air) / (particleDiameter/2); % m/hr

for i = [wall, carpet, backing, fabric, foam, hardFloor]
    k(i) = diffusivity(i)/thickness(i); % m/hr
end

k(film) = (diffusivity(water)/30) / (thickness(organicFilm)*0.5); % m/hr

% k(envirofilm) = (diffusivity(water)/30) / (thickness(envFilm)*0.5); %
m/hr

% k(kidfilm) = (diffusivity(water)/30)/(thickness(skinFilm)*0.5); % m/hr

for i = 1:nSkin
    k(skin(i))= diffusivity(skin(i)) / (thickness(skin(i))*0.5); % m/hr
CHECK:
                                                                  %
UNUSED??
end

%k(skinSCe) = diffusivity(skinSCe) / (thickness(skinSCe) * 0.5); % m/hr
CHECK:
                                                                  %
UNUSED??
%k(skinVEe) = diffusivity(skinVEe) / (thickness(skinVEe) * 0.5); % m/hr
CHECK:
                                                                  %
UNUSED??
%k(skinSCc) = diffusivity(skinSCc) / (thickness(skinSCc) * 0.5); % m/hr
CHECK:
                                                                  %
UNUSED??
```

```
%k(skinVEc) = diffusivity(skinVEc) / (thickness(skinVEc) * 0.5); % m/hr
CHECK:
                                                                 %
UNUSED??

%% _________  Interfacial Mass Transfer Coefficients MT [mol/m2-hr-Pa]
____
MT = zeros(nComp+nExtra,nComp+nExtra);
for i = (film)
    MT(air,i) = 1 / (1 / (k(air)*Z(air)) + 1 / (k(i)*Z(i)));
end

for i = [dustOnVinyl dust]
    MT(air,i) = 1 / (1 / (k(airParticle)*Z(air)) + 1 / (k(i)*Z(i)));
end

MT(air,particles) = 1 / (1 / (k(particles)*Z(air)) + 1 / (k(particles)*
...
                    Z(particles)));
MT(dustOnVinyl,vinylFilm) =  1 / (1 / (k(dustOnVinyl)*Z(dustOnVinyl)) ...
                          + 1 / (k(vinylFilm)*Z(vinylFilm))); % old =
0.005 m/hr;
MT(vinyl,vinylFilm) = k(vinylFilm) * Z(vinylFilm); % assumes no resist
vinyl side
MT(wall,wallFilm) = 1 / (1 / (k(wall)*Z(wall)) + 1 /
(k(wallFilm)*Z(wallFilm)));
MT(hardFloorFilm,hardFloor) = 1 / (1 / (k(hardFloorFilm)*Z(hardFloorFilm))
...
                            + 1 / (k(hardFloor)*Z(hardFloor)));

% MT = makeSymmetric(MT);
%% D    Mackay-type Transport Coefficients  [mol/(Pa*day)]_
transportCoeff = zeros(nComp+nExtra,nComp+nExtra);
D = zeros(nComp+nExtra,nComp+nExtra);
D(vinyl,vinylFilm) = MT(vinyl,vinylFilm) * 24 *
interfaceArea(vinyl,vinylFilm);

for i = [film dustOnVinyl dust particles] % film includes all kidFilms
    D(air,i) = MT(air,i) * 24 * interfaceArea(i,air);
end

D(dustOnVinyl,vinylFilm) = MT(dustOnVinyl,vinylFilm) * 24 * ...
                           interfaceArea(dustOnVinyl,vinylFilm);
D(wallFilm,wall) = MT(wall,wallFilm) * 24 * interfaceArea(wall,wallFilm);
D(hardFloorFilm,hardFloor) = MT(hardFloorFilm,hardFloor) * 24 * ...
                             interfaceArea(hardFloorFilm,hardFloor);

%D = makeSymmetric(D);
%% D values for carpet and fabric
D(air,carpetFilm) = D(air,wallFilm);
D(carpetFilm,air) = D(air,carpetFilm);
D(carpetFilm,carpet) = D(wallFilm,wall);
D(carpet,carpetFilm) = D(carpetFilm,carpet);
D(carpet,backing) = 0.25 * D(carpetFilm,carpet);
```

```
D(backing,carpet) = D(carpet,backing);
D(air,fabricFilm) = D(air,wallFilm);
D(fabricFilm,air) = D(air,fabricFilm);
D(fabricFilm,fabric) = D(wallFilm,wall);
D(fabric,foam) = 0.25 * D(fabricFilm,fabric);
D(foam,fabric) = D(fabric,foam);
D(persfab,persfabFilm) = D(wallFilm,wall);

%D = makeSymmetric(D);
%% D values
D(particles,flowOut) = (Q(partFlowOut) / (density(particles)*1E3)) *
Z(particles);

% Transport to lung
D(air,flowOut) = Q(air) * Z(air);

D(air,lung) = rate(inhalation) * Z(air) * fraction(inhVap);
D(lung,air) = rate(inhalation) * Z(air) * (1 - fraction(inhVap));
D(blood,lung) = G(blood,lung) * Z(blood);
D(lung,blood) = G(blood,lung) * Z(blood);

%**** Unused
% Bq = 6.2E-12;
% alveolarSA = 140; % m2 in cahill who cite Cassarett and Doull's
Toxicology,
                  % Modern Pharm cites range 50-100.
% diffusionDist = 3e-7; % um
% membraneResistance = Bq * alveolarSA * Z(blood) / diffusionDist;

D(air,blood) = 1 / (1 / (D(air,lung)) + 1 / (D(lung,blood)));
% membrane resistance as described in cahill:
% D(air,blood) = 1 / (1 / (D(air,lung)) +  1 / (D(lung,blood)) + 1 /
% membraneResistance);

D(blood,air) = D(air,blood);

D(particles,lung) = rate(inhalation) * fraction(absorbPart) * ...
                    (TSP/density(particles)) * Z(particles);

D(particles,lumen) = rate(inhalation) * (1-fraction(absorbPart)) * ...
                     (TSP/density(particles)) * Z(particles);

% Cahill Ingestion Parameterization
avogadro = 6.0221415e23;
molecVol = 157; % cm3/mol; from ChemSpider
molecRad = (molecVol*3 / (4*pi))^(1/3) / 100^3 ; % m
viscosityOctanol = 7.21 * 0.001 * 60^2; % Pa/h 7.21 centiPoise @ 25 C from
Viscosity
                     % of Liquids by Viswanath, Ghosh, Prasad, Dutt and
Rani
                     % (springer)
viscosityWater = 8.90E-4 * 60^2; % Pa/h @ 25 C

% AQUEOUS DIFFUSION TRANSPORT TERM
```

```
Bq = (T*R) / (6*pi*avogadro*molecRad*viscosityWater); % m2/h
interfaceArea(lumen,gut) = 10; % m2 (cahill ref 8)
diffusPathLength = 350E-6; % m (cahill est in range 0.01-1 mm)
Dq = Bq * interfaceArea(lumen,gut) * Z(water) / diffusPathLength;

% MICELLE MEDIATED DIFFUSION TRANSPORT TERM
Bc = (T*R) / (6*pi*avogadro*molecRad*viscosityOctanol);
micelleFractionOfLumen = 0.05;
Ac = interfaceArea(lumen,gut) * micelleFractionOfLumen;
Kcw = 10 ^ (-0.123 * (log(K(octanol,water)))^2 + 2.521 *
log(K(octanol,water)) ...
    - 5.375); % partitioning micelle water Cahill from Dulfer, pg S-19

Zc = Kcw * Z(water);
Dc = Bc * Ac * Zc / diffusPathLength;

% MEMBRANE DIFFUSION
Be = (T*R) / (6*pi*avogadro*molecRad*viscosityOctanol);
Au = interfaceArea(lumen,gut);
thicknessCellMembr = 10E-9; % m (10 nm) from Cahill ref 12 - Dulfer

De = Be * Au * Z(octanol) / thicknessCellMembr;

D(lumen,gut) = 1 / (1 / (Dq+Dc) + 1/De) * 24 ;
D(gut,lumen) = 1 / (1 / Dq + 1/De) * 24;

D(dust,lumen) = rate(ingDust) / (density(dust)*1E3) ...
              * fraction(GIabsDust) * percentageHardFloor * Z(dust);
D(dustOnVinyl,lumen) = rate(ingDust) / (density(dustOnVinyl)*1E3) ...
                     * fraction(GIabsDust) * percentageVinyl *
Z(dustOnVinyl);

% D(lumen,gut) = 7.75E+01 * 60;
% D(gut,lumen) = 2.58E-03 * 60;

% Gut to Liver
D(gut,liver) = G(gut,liver) * Z(blood);

% Transport to blood from gut
D(blood,gut) = G(blood,gut) * Z(blood);
D(gut,blood) = G(blood,gut) * Z(blood);

% Transport blood to liver
D(blood,liver) = G(blood,liver) * Z(blood);
D(liver,blood) = G(liver,blood) * Z(blood);

% Transport blood to fat
D(blood,fat) = G(blood,fat) * Z(blood);
D(fat,blood) = G(blood,fat) * Z(blood);

% Transport from richly perfused fat (fat) to poorly perfused (deep) fat
(fat2)
D(fat,fat2) = D(blood,fat) * 0.25;
D(fat2,fat) = D(fat,fat2);
```

```
% Transport blood to tissue
D(blood,tissue) = G(blood,tissue) * Z(blood);
D(tissue,blood) = G(blood,tissue) * Z(blood);

% Resuspension of dust to particles:
D(dustOnVinyl,particles) = Q(resuspension) * percentageVinyl ...
                         / (density(dustOnVinyl)*1E3) * Z(dustOnVinyl);
D(dust,particles) = Q(resuspension) * percentageHardFloor ...
                  / (density(dust)*1E3) * Z(dust);

% Deposition of particles into dust:
D(particles,dustOnVinyl) = Q(deposition) / (density(particles)*1E3) * ...
                           percentageVinyl * Z(particles);
D(particles,dust) = Q(deposition) / (density(particles)*1E3) * ...
                    percentageHardFloor * Z(particles);

% Loss of dust to sweeping
D(dust,sweep) = Q(sweepingLoss) * percentageHardFloor / ...
                (density(dust)*1E3) * Z(dust);
D(dustOnVinyl,sweep) = Q(sweepingLoss) * percentageVinyl / ...
                       (density(dustOnVinyl)*1E3) * Z(dustOnVinyl);

% Loss of NIC to laundering
% D(persfab,launder) = Q(launderingLoss) / (density(persfab)*1E3) *
Z(persfab);
D(persfabFilm,launder) = Q(launderingLoss) / (density(persfabFilm)*1E3) *
Z(persfabFilm);

% Loss of NIC to bathing
D(kidFilme,bathing) = Q(bathingLosse) / (density(kidFilme)*1E3) *
Z(kidFilme);
D(kidFilmc,bathing) = Q(bathingLossc) / (density(kidFilmc)*1E3) *
Z(kidFilmc);
D(kidFilmh,bathing) = Q(bathingLossh) / (density(kidFilmh)*1E3) *
Z(kidFilmh);

% Loss of NIC to handwashing
D(kidFilmh,handwash) = Q(handwashingLoss) / (density(kidFilmh)*1E3) *
Z(kidFilmh);

% Transport in bile from liver to gut
D(bile,gut) = G(bile,gut) * Z(bile);

% Filtration (excretion) via kidneys from blood
Ff = 0.2; % glomerular filtration rate (20% aqueous blood fraction from
Cahill)
Fe = 0.05; % glomerular filtrate excr ratio (5% from Benowitz (2009))
aqFrac = 0.9; % Cahill
G(blood,kidney) = 0.82; % m3/d; child cardiac output of 3 L/min (Alverson
et al
    % (1982) (median 3.9 yrs, range 3 days - 17 yrs) and Calamandrei et al
(2008)
```

```
    % (median age 19 months, range 1 month - 17 yrs)); 5 L/min from Vinet
et al
    % (2001) (~11 year olds); used 3 L/min x 60 min/hr x 24 hrs/day x 0.19
(% Gbk
    % from Cahill Table S-2) / 1000 L/m3 = 180 L/hr); 5 L/min child
cardiac output
    % from Vinet et al (2001)

D(blood,excrUrine) = G(blood,kidney) * Ff * Fe * Z(blood) * aqFrac;

%%  D Skin
MT(kidFilme,skin(1)) = 1 / (1 / (k(skinSCe(1))*Z(skinSCe(1))) + ...
                       1 / (k(kidFilme)*Z(kidFilme))); % mol/(m2-hr-Pa)
D(kidFilme,skin(1)) = MT(kidFilme,skin(1)) * 24 *
interfaceArea(kidFilme,skin(1));

MT(kidFilmc,skin(nSkin/3+1)) = 1 / (1 / (k(skinSCc(1))*Z(skinSCc(1))) +
...
                               1 / (k(kidFilmc)*Z(kidFilmc))); % mol/(m2-
hr-Pa)
D(kidFilmc,skin(nSkin/3+1)) = MT(kidFilmc,skin(nSkin/3+1)) * 24 * ...
                              interfaceArea(kidFilmc,skin(nSkin/3+1));

MT(kidFilmh,skin((nSkin*(2/3))+1)) = 1 / (1 /
(k(skinSCh(1))*Z(skinSCh(1))) + ...
                                  1 / (k(kidFilmh)*Z(kidFilmh))); %
mol/(m2-hr-Pa)
D(kidFilmh,skin((nSkin*(2/3))+1)) = MT(kidFilmh,skin((nSkin*(2/3))+1)) *
24 * ...

interfaceArea(kidFilmh,skin((nSkin*(2/3))+1));

D(skin(1),kidFilme) = D(kidFilme,skin(1));
D(skin(nSkin/3+1),kidFilmc) = D(kidFilmc,skin(nSkin/3+1));
D(skin((nSkin*(2/3))+1),kidFilmh) = D(kidFilmh,skin((nSkin*(2/3))+1));

% First layer of skin to second layer
MT(skin(1),skin(2)) = 1 / (1 / (k(skin(1))*Z(skin(1))) + ...
                      1 / (k(skin(2))*Z(skin(2))));
D(skin(1),skin(2)) = MT(skin(1),skin(2)) * 24 *
interfaceArea(skin(nSkin/3),blood);

MT(skin(nSkin/3+1),skin(nSkin/3+2)) = 1 / (1 / (k(skin(nSkin/3+1))* ...
                Z(skin(nSkin/3+1))) + 1 /
(k(skin(nSkin/3+2))*Z(skin(nSkin/3+2))));
D(skin(nSkin/3+1),skin(nSkin/3+2)) = MT(skin(nSkin/3+1),skin(nSkin/3+2)) *
24 ...
                                   *
interfaceArea(skin((nSkin*2/3)),blood);

MT(skin((nSkin*(2/3))+1),skin((nSkin*(2/3))+2)) = 1 / (1 /
(k(skin((nSkin*(2/3)) ...
                 +1))*Z(skin((nSkin*(2/3))+1))) + 1 /
(k(skin((nSkin*(2/3))+2))* ...
```

```
                 Z(skin((nSkin*(2/3))+2))));
D(skin((nSkin*(2/3))+1),skin((nSkin*(2/3))+2)) = MT(skin((nSkin*(2/3))+1),
...
                skin((nSkin*(2/3))+2)) * 24 *
interfaceArea(skin(nSkin),blood);

% Skin layers to adjoining skin layers
  if nSkin > 2
    for i = skin(2):skin(nSkin/3)-1
        prev = i-1; next = i+1;
        MT(i,prev) = 1 / (1 / (k(i)*Z(i)) + 1 / (k(prev)*Z(prev)));
        MT(i,next) = 1 / (1 / (k(i)*Z(i)) + 1 / (k(next)*Z(next)));

        D(i,prev) = MT(i,prev) * 24 * interfaceArea(skin(nSkin/3),blood);
        D(i,next) = MT(i,next) * 24 * interfaceArea(skin(nSkin/3),blood);
    end

    for i = skin((nSkin/3)+2):skin((nSkin*(2/3)))-1
        prev = i-1; next = i+1;
        MT(i,prev) = 1 / (1 / (k(i)*Z(i)) + 1 / (k(prev)*Z(prev)));
        MT(i,next) = 1 / (1 / (k(i)*Z(i)) + 1 / (k(next)*Z(next)));

        D(i,prev) = MT(i,prev) * 24 *
interfaceArea(skin(nSkin*2/3),blood);
        D(i,next) = MT(i,next) * 24 *
interfaceArea(skin(nSkin*2/3),blood);
    end

    for i = skin((nSkin*(2/3))+2):skin(nSkin)-1
        prev = i-1; next = i+1;
        MT(i,prev) = 1 / (1 / (k(i)*Z(i)) + 1 / (k(prev)*Z(prev)));
        MT(i,next) = 1 / (1 / (k(i)*Z(i)) + 1 / (k(next)*Z(next)));

        D(i,prev) = MT(i,prev) * 24 * interfaceArea(skin(nSkin),blood);
        D(i,next) = MT(i,next) * 24 * interfaceArea(skin(nSkin),blood);
    end

  end

% Last layer of skin to the one before
MT(skin(nSkin/3)-1,skin(nSkin/3)) = 1 / (1 /
(k(skin(nSkin/3))*Z(skin(nSkin/3))) ...
                                  + 1 / (k(skin(nSkin/3)-
1)*Z(skin(nSkin/3)-1)));
MT(skin(nSkin*(2/3))-1,skin(nSkin*(2/3))) = 1 / (1 /
(k(skin(nSkin*(2/3)))* ...
   Z(skin(nSkin*(2/3)))) + 1 / (k(skin((nSkin*(2/3)))-
1)*Z(skin((nSkin*(2/3)))-1)));
MT(skin(nSkin)-1,skin(nSkin)) = 1 / (1 / (k(skin(nSkin))*Z(skin(nSkin))) +
...
                                1 / (k(skin(nSkin)-1)*Z(skin(nSkin)-1)));

D(skin(nSkin/3)-1,skin(nSkin/3)) = MT(skin(nSkin/3)-1,skin(nSkin/3)) * 24
* ...
```

```
                                   interfaceArea(skin(nSkin/3),blood);
D(skin(nSkin*(2/3))-1,skin(nSkin*(2/3))) = MT(skin((nSkin*(2/3)))-1, ...
                   skin(nSkin*(2/3))) * 24 *
interfaceArea(skin(nSkin*(2/3)),blood);
D(skin(nSkin)-1,skin(nSkin)) = MT(skin(nSkin)-1,skin(nSkin)) * 24 * ...
                               interfaceArea(skin(nSkin),blood);

D(skin(nSkin/3),skin(nSkin/3)-1) = D(skin(nSkin/3)-1,skin(nSkin/3));
D(skin(nSkin*(2/3)),skin((nSkin*(2/3)))-1) = D(skin((nSkin*(2/3)))-1, ...
                                             skin(nSkin*(2/3)));
D(skin(nSkin),skin(nSkin)-1) = D(skin(nSkin)-1,skin(nSkin));

D(skin(nSkin/3),blood) = G(blood,skin(nSkin/3)) * Z(blood);
D(skin(nSkin*(2/3)),blood) = G(blood,skin(nSkin*(2/3))) * Z(blood);
D(skin(nSkin),blood) = G(blood,skin(nSkin)) * Z(blood);

%/( interfaceArea(skin(end),blood)*thickness(skin(end)) );
D(blood,skin(nSkin/3)) = D(skin(nSkin/3),blood);
D(blood,skin(nSkin*(2/3))) = D(skin(nSkin*(2/3)),blood);
D(blood,skin(nSkin)) = D(skin(nSkin),blood);

% kidFilmc (clothed) exchanges with persfab

adjRb = 0.016 * surfaceAreaKid / 1.8; % based on Rossbach mol/Pa-day 1.8
to adjust
                                      % for kid size

D(kidFilmc,persfab) = adjRb;

% Film on bare skin (kidFilme and kidFilmh) and persfabFilm can exchange
with surface
% films via mechanical harvesting

tc = 0.1; % transfer coefficient (m2/hr)

    for i = listSurfaceFilmsp
        D(i,kidFilme) = (surfaceArea(i) / surfaceAreaFilm) * (tc*24) * ...
                         thickness(organicFilm) * Z(i); % mol/Pa/day
        D(i,kidFilmh) = (surfaceArea(i) / surfaceAreaFilm) * (tc*24) * ...
                         thickness(organicFilm) * Z(i); % mol/Pa/day
    end

    for i = listSurfaceFilms
        D(i,persfab) = (surfaceArea(i) / surfaceAreaFilm) * (tc*24) * ...
                        thickness(organicFilm) * Z(i); % mol/Pa/day
    end

MT = makeSymmetric(MT);
D = makeSymmetric(D);

%% _________  Initial Conditions ________________________________________
f = zeros(163,1);
c = zeros(163,1);
m = zeros(163,1);
```

```
% f = zeros(nComp,1);
% c = zeros(nComp,1);
% m = zeros(nComp,1);
massExchanged=zeros(nMassExchangeComp^2,1);

%f(air) = VP;    % Pa; inital fugacity for vinyl = 3.5e-05
%c(air) = VP*Z(air) * mw(NIC);    % g/m^3
%m(air) = VP*Z(air) * V(air) * mw(NIC);    % g

yo = [f; c; m];

ndays = 365; % number of days in the simulation
      % tspan = 0:ndays; % for 1 day time steps for integration
tspan = [0 ndays]; % non-fixed integration time steps - preferred

save('modelvariables')    % saves .mat file of variables
return
```

Model

```
function ydot =
model_nicotine4(t,y,human,air,particles,vinylFilm,vinyl,wall,wallFilm,wind
owFilm,dustOnVinyl,dust,hardFloorFilm,hardFloor,fabric,fabricFilm,foam,car
petFilm,carpet,backing,persfab,persfabFilm,kidFilme,kidFilmc,kidFilmh,nMas
sExchangeComp,emitVinyl,storageCompartments,flowOut,massBalance,emitCig,sw
eep,launder,bathing,handwash,dose,nComp,nExtra,autoCalcCompartments,mw,NIC
,sweepLoss,density,V,Z,Q,transportCoeff,G,D,TSP,partFlowOut,deposition,per
centageHardFloor,percentageVinyl,sweepingLoss,launderingLoss,bathingLosse,
bathingLossc,bathingLossh,handwashingLoss,inhalation,ingDust,urineProducti
on,resuspension,rate,degRate,elimRate,lung,gut,liver,fat,fat2,tissue,blood
,lumen,bloodTotal,skinscTotal,skinveTotal,skinallTotal,storageKid,metaboli
tes,excrUrine,concUrine,excrFeces,inhVap,inhPart,absorbPart,fraction,GIabs
Dust,skinSCe,skinVEe,skinSCc,skinVEc,skinSCh,skinVEh,skine,skinc,skinh,mwR
atio,cotinine,excrRatio,massBalanceKid,bile,legendNames,skin,lastLayerSkin
e,firstLayerSkine,lastLayerSkinc,firstLayerSkinc,lastLayerSkinh,firstLayer
Skinh,absDerme,absDermc,absDermh,skinBloodFluxe,skinBloodFluxc,skinBloodFl
uxh,cig,Glucu,adjRb,launderLoss,bathLoss,handwashLoss) %#ok<INUSL>

hasSkin = true;
hasKidney = true;
filmHarvest = true;
if ~human  %(if no human)
    hasSkin = false;
    filmHarvest = false;
end
%% Split the y returned from the ODE solver into f, c, m
f = y(1:nComp);
c = y(nComp+1:2*nComp);    %#ok<*NASGU>
m = y(2*nComp+1:3*nComp);

%% ____________set up the differentials  _________
df = zeros(nComp,1);
dc = zeros(nComp,1);
dm = zeros(nComp,1);

 for i = 1:nComp
    switch i
    case air
         df(i)= 1/(Z(i)*V(i)) * (...
              + cig/mw(NIC) ...
              - D(i,flowOut)       * f(i)...
              - D(i,particles)     * (f(i)-f(particles)) ...
              - D(i,dustOnVinyl)   * (f(i)-f(dustOnVinyl)) ...
              - D(i,dust)          * (f(i)-f(dust)) ...
              - D(i,vinylFilm)     * (f(i)-f(vinylFilm)) ...
              - D(i,wallFilm)      * (f(i)-f(wallFilm)) ...
              - D(i,windowFilm)    * (f(i)-f(windowFilm)) ...
              - D(i,hardFloorFilm) * (f(i)-f(hardFloorFilm)) ...
              + D(carpetFilm,i)    * (f(carpetFilm)-f(i)) ...
              + D(fabricFilm,i)    * (f(fabricFilm)-f(i)) ...
              + D(persfabFilm,i)   * (f(persfabFilm)-f(i)) ...
              + human * ( ...
                D(lung,i)          * (f(lung)-f(i))) ...
```

```
          + hasSkin*( ...
            D(air,kidFilme)    * (f(kidFilme)-f(i))...
          + D(air,kidFilmh)    * (f(kidFilmh)-f(i)))...
            );

case vinyl
     df(i)= 1/(Z(i)*V(i))  * (...
          - D(i,vinylFilm) * (f(i)-f(vinylFilm)) ...
            );

case vinylFilm
     df(i)= 1/(Z(i)*V(i))    * (...
          - D(i,vinyl)       * (f(i)-f(vinyl)) ...
          - D(i,air)         * (f(i)-f(air)) ...
          - D(i,dustOnVinyl) * (f(i)-f(dustOnVinyl)) ...
          - filmHarvest * ( ...
            D(i,kidFilme) * (f(i)-f(kidFilme)) ...
          + D(i,kidFilmh) * (f(i)-f(kidFilmh)) ...
          + D(persfab,i)  * f(i)) ...
            );

case particles
     df(i)= 1/(Z(i)*V(i)) * ( ...
          - D(i,air)         * (f(i)-f(air)) ...
          + D(dust,i)        * f(dust) ...
          - D(i,dust)        * f(i) ...
          + D(dustOnVinyl,i) * f(dustOnVinyl) ...
          - D(i,dustOnVinyl) * f(i) ...
          - D(i,flowOut)     * f(i) ...
          + human * ( ...
          - D(particles,lung)  * f(particles) ...
          - D(particles,lumen) * f(particles)) ...
            );

case dustOnVinyl
     df(i)= 1/(Z(i)*V(i)) * ( ...
          - D(i,air)       * (f(i)-f(air)) ...
          - D(i,vinylFilm) * (f(i)-f(vinylFilm)) ...
          + D(particles,i) * f(particles) ...
          - D(i,particles) * f(i)...
          - D(i,sweep)     * f(i)...
          + human * ( ...
          - D(i,lumen) * f(i)) ...
            );

case dust
     df(i) = 1/(Z(i)*V(i)) * ( ...
           - D(i,air)           * (f(i)-f(air)) ...
           - D(i,hardFloorFilm) * (f(i)-f(hardFloorFilm)) ...
           + D(particles,i)     * f(particles) ...
           - D(i,particles)     * f(i) ...
           - D(i,sweep)         * f(i)...
           + human * ( ...
           - D(i,lumen) * f(i)) ...
             );
```

```
case wallFilm
     df(i) = 1/(Z(i)*V(i)) * ( ...
           - D(i,air)  * (f(i)-f(air)) ...
           - D(i,wall) * (f(i)-f(wall)) ...
           - filmHarvest * ( ...
             D(i,kidFilme) * (f(i)-f(kidFilme)) ...
          +  D(i,kidFilmh) * (f(i)-f(kidFilmh)) ...
          +  D(persfab,i)  * f(i)) ...
             );

case wall
     df(i) = 1/(Z(i)*V(i)) * ( ...
           - D(i,wallFilm) * (f(i)-f(wallFilm)) ...
             );

case hardFloor
     df(i)= 1/(Z(i)*V(i)) * ( ...
          - D(i,hardFloorFilm) * (f(i)-f(hardFloorFilm)) ...
            ) ;

case hardFloorFilm
     df(i)= 1/(Z(i)*V(i)) * ( ...
          - D(i,air)       * (f(i)-f(air)) ...
          - D(i,hardFloor) * (f(i)-f(hardFloor)) ...
          - filmHarvest * ( ...
            D(i,kidFilme) * (f(i)-f(kidFilme)) ...
          + D(i,kidFilmh) * (f(i)-f(kidFilmh)) ...
          + D(persfab,i)  * f(i)) ...
            );

case windowFilm
     df(i)= 1/(Z(i)*V(i)) * ( ...
          - D(i,air) * (f(i)-f(air)) ...
          - filmHarvest * ( ...
            D(i,kidFilme) * (f(i)-f(kidFilme)) ...
          + D(i,kidFilmh) * (f(i)-f(kidFilmh)) ...
          + D(persfab,i)  * f(i)) ...
            );

case carpetFilm
     df(i)= 1/(Z(i)*V(i)) * ( ...
          - D(i,air) * (f(i)-f(air)) ...
          - D(i,carpet) * (f(i)-f(carpet)) ...
          - filmHarvest * ( ...
            D(i,kidFilme) * (f(i)-f(kidFilme)) ...
          + D(i,kidFilmh) * (f(i)-f(kidFilmh)) ...
          + D(persfab,i) * f(i)) ...
            );

case carpet
     df(i) = 1/(Z(i)*V(i)) * ( ...
           - D(i,carpetFilm) * (f(i)-f(carpetFilm)) ...
           - D(i,backing)    * (f(i)-f(backing)) ...
```

```
                 );

    case backing
         df(i) = 1/(Z(i)*V(i)) * (...
               - D(i,carpet) * (f(i)-f(carpet)) ...
                 );

    case fabricFilm
         df(i) = 1/(Z(i)*V(i)) * (...
               - D(i,air) * (f(i)-f(air)) ...
               - D(i,fabric) * (f(i)-f(fabric)) ...
               - filmHarvest * ( ...
                 D(i,kidFilme) * (f(i)-f(kidFilme)) ...
               + D(i,kidFilmh) * (f(i)-f(kidFilmh)) ...
               + D(persfab,i)  * f(i)) ...
                 ); ...
    case fabric
         df(i) = 1/(Z(i)*V(i)) * ( ...
               - D(i,fabricFilm) * (f(i)-f(fabricFilm)) ...
               - D(i,foam)       * (f(i)-f(foam)) ...
                 );

    case foam
         df(i) = 1/(Z(i)*V(i)) * ( ...
               - D(i,fabric) * (f(i)-f(fabric)) ...
                 );

    case persfab
         df(i) = 1/(Z(i)*V(i)) * ( ...
                 D(i,persfabFilm) * (f(persfabFilm)-f(i)) ...
               - D(i,kidFilmc)    * (f(i)-f(kidFilmc)) ...
               + filmHarvest * ( ...
                 D(i,vinylFilm)     * f(vinylFilm) ...
               + D(i,wallFilm)      * f(wallFilm) ...
               + D(i,windowFilm)    * f(windowFilm) ...
               + D(i,hardFloorFilm) * f(hardFloorFilm)...
               + D(carpetFilm,i)    * f(carpetFilm) ...
               + D(fabricFilm,i)    * f(fabricFilm)) ...
                 );

             % - D(i,launder)     * f(i) ...

    case persfabFilm
         df(i)= 1/(Z(i)*V(i)) * ( ...
                D(i,air) * (f(air)-f(i)) ...
              - D(i,persfab) * (f(i)-f(persfab)) ...
              - D(i,launder) * f(i) ...
                ); ...

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% Human Compartments PBPK
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

       case blood
```

```
            df(i) = 1/(Z(i)*V(i)) * ( ...
                    D(lung,blood)   * (f(lung)-f(blood))  ...
                  - D(blood,gut)    * f(blood) ... % to gut
                  + D(liver,blood)  * f(liver) ...
                  - D(blood,liver)  * f(blood) ...
                  + D(fat,blood)    * (f(fat)-f(blood)) ...
                  + D(tissue,blood) * (f(tissue)-f(blood)) ...
                  - hasKidney * (...
                    D(blood,excrUrine) * f(blood))...
                  + hasSkin * ( ...
                    D(lastLayerSkine,blood) * (f(lastLayerSkine)-f(blood))
...
                  + D(lastLayerSkinc,blood) * (f(lastLayerSkinc)-f(blood))
...
                  + D(lastLayerSkinh,blood) * (f(lastLayerSkinh)-
f(blood))) ...
                    );

       case lung
            df(i) = 1/(Z(i)*V(i)) * ( ...
                    D(blood,i) * (f(blood)-f(lung)) ...
                  + human * ( ...
                    D(air,i) * f(air) ...
                  - D(i,air) * f(i) ...
                  + D(particles,i) * f(particles)) ...
                    );

      case gut
           df(i) = 1/(Z(i)*V(i)) * ( ...
                 + D(lumen,gut) * f(lumen) ...
                 - D(gut,lumen) * f(gut) ...
                 + D(bile,gut)  * f(liver) ...
                 + D(blood,gut) * f(blood) ...
                 - D(gut,liver) * f(gut) ...
                   );

      case lumen
           df(i) = 1/(Z(i)*V(i)) * ( ...
                 + D(gut,lumen) * f(gut) ...
                 - D(lumen,gut) * f(lumen) ...
                 + human * ( ...
                   D(dustOnVinyl,lumen) * f(dustOnVinyl) ...
                 + D(dust,lumen)        * f(dust) ...
                 + D(particles,lumen)   * f(particles)) ... % particles
not absorbed in lung
                   )...
                 - elimRate(lumen) * f(lumen);

      case liver
           df(i) = 1/(Z(i)*V(i)) * ( ...
                   D(blood,liver) * f(blood) ...
                 - D(liver,blood) * f(i) ...
                 + D(gut,liver)   * f(gut) ...
                 - D(bile,gut)    * f(liver)) ...
                 - degRate(liver) * f(liver);
```

```
      case fat     % (richly) perfused fat
           df(i) = 1/(Z(i)*V(i)) * ( ...
                   D(blood,i) * (f(blood)-f(i)) ...
                 + D(fat2,i) * (f(fat2)-f(i)) ...
                   );

      case fat2    % poorly perfused (or deep) fat
           df(i) = 1/(Z(i)*V(i)) * ( ...
                   D(fat,i) * (f(fat)-f(i)) ...
                   );

      case tissue
           df(i) = 1/(Z(i)*V(i)) * ( ...
                   D(blood,i) * (f(blood)-f(i)) ...
                   );

      case kidFilme
           df(i) = 1/(Z(i)*V(i)) * ( ...
                 + hasSkin * ( ...
                   D(kidFilme,firstLayerSkine) * (f(firstLayerSkine)-f(i))
...
                 + D(air,kidFilme)             * (f(air)-f(i))) ...
                 - D(kidFilme,bathing)         * f(i) ...    % bath loss
                 + filmHarvest * ( ...
                   D(windowFilm,kidFilme)    * (f(windowFilm)-f(i)) ...
                 + D(hardFloorFilm,kidFilme) * (f(hardFloorFilm)-f(i)) ...
                 + D(wallFilm,kidFilme)      * (f(wallFilm)-f(i)) ...
                 + D(carpetFilm,kidFilme)    * (f(carpetFilm)-f(i)) ...
                 + D(fabricFilm,kidFilme)    * (f(fabricFilm)-f(i))) ...
                   );

      case kidFilmc
           df(i) = 1/(Z(i)*V(i)) * ( ...
                 + hasSkin * ( ...
                   D(kidFilmc,firstLayerSkinc) * (f(firstLayerSkinc)-f(i))
...
                 + D(persfab,kidFilmc)         * (f(persfab)-f(i))) ...
                 - D(kidFilmc,bathing)         * f(i) ...    % bath loss
                   );

      case kidFilmh
           df(i) = 1/(Z(i)*V(i)) * ( ...
                 + hasSkin * ( ...
                   D(kidFilmh,firstLayerSkinh) * (f(firstLayerSkinh)-f(i))
...
                 + D(air,kidFilmh) * (f(air)-f(i))) ...
                 - D(kidFilmh,handwash)        * f(i) ...    % handwash
loss
                 - D(kidFilmh,bathing)         * f(i) ...    % bath loss
                 + filmHarvest * ( ...
                   D(windowFilm,kidFilmh)    * (f(windowFilm)-f(i)) ...
                 + D(hardFloorFilm,kidFilmh) * (f(hardFloorFilm)-f(i)) ...
                 + D(wallFilm,kidFilmh)      * (f(wallFilm)-f(i)) ...
                 + D(carpetFilm,kidFilmh)    * (f(carpetFilm)-f(i)) ...
```

```
                 + D(fabricFilm,kidFilmh)    * (f(fabricFilm)-f(i))) ...
                   ) ;

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
    end % of the switch statement
    if isnan(df(i)), error('df(%i) isnan',i), end
    if isinf(df(i)), error('df(%i) isinf',i), end
end % of the for loop that increments through all compartments
%%   The Skin (exposed or e)
if hasSkin
   % First layer e
   i = firstLayerSkine; secondLayerSkine = i+1;
   df(i) = 1/(V(i)*Z(i)) * (...
           hasSkin * ( ...
           D(kidFilme,i)         * (f(kidFilme)-f(i)) ...
         + D(i,secondLayerSkine) * (f(secondLayerSkine)-f(i))) ...
           );

         % - D(i,bathing)          * f(i)) ...    % bath loss?

   %  Middle layers of skin e
   if length(skin) > 2
      for i = skin(2):(lastLayerSkine-1)
              prev = i-1; next = i+1;
              df(i) = 1/(V(i)*Z(i)) * ( ...
                     D(prev,i) * (f(prev)-f(i)) ...
                   + D(i,next) * (f(next)-f(i)) ...
                     );
      end
   end
   % Last layer of skin e
   i = lastLayerSkine; prev = i-1;
   df(i) = 1/(V(i)*Z(i)) * ( ...
         + hasSkin * (...
           D(prev,i)               * (f(prev)-f(i)) ...
         + D(lastLayerSkine,blood) * (f(blood)-f(lastLayerSkine)))...
           );
end
%%   The Skin (clothed or c)
if hasSkin
   % First layer c
   i = firstLayerSkinc; secondLayerSkinc = i+1;
   df(i) = 1/(V(i)*Z(i)) * ( ...
           hasSkin * ( ...
           D(kidFilmc,i)         * (f(kidFilmc)-f(i)) ...
         + D(i,secondLayerSkinc) * (f(secondLayerSkinc)-f(i))) ...
           );

         % - D(i,bathing)          * f(i)) ...    % bath loss?

   % Middle layers of skin c
   if length(skin) > 2
      for i = skinSCc(2):(lastLayerSkinc-1)
              prev = i-1; next = i+1;
              df(i) = 1/(V(i)*Z(i)) * ( ...
```

```
                      D(prev,i) * (f(prev)-f(i)) ...
                    + D(i,next) * (f(next)-f(i)) ...
                      );
      end
   end

   % Last layer of skin c
   i = lastLayerSkinc; prev = i-1;
   df(i) = 1/(V(i)*Z(i)) * ( ...
         + hasSkin * ( ...
           D(prev,i)               * (f(prev)-f(i)) ...
         + D(lastLayerSkinc,blood) * (f(blood)-f(lastLayerSkinc))) ...
           );
end
%%   The Skin (hands or h)
if hasSkin
   % First layer h
   i = firstLayerSkinh; secondLayerSkinh = i+1;
   df(i) = 1/(V(i)*Z(i)) * ( ...
           hasSkin * ( ...
           D(kidFilmh,i)         * (f(kidFilmh)-f(i)) ...
         + D(i,secondLayerSkinh) * (f(secondLayerSkinh)-f(i))) ...
           );

         % - D(i,handwash)         * f(i) ...    % handwashing loss?
         % - D(i,bathing)          * f(i)) ...    % bath loss?

   %  Middle layers of skin c
   if length(skin) > 2
      for i = skinSCh(2):(lastLayerSkinh-1)
              prev = i-1; next = i+1;
              df(i) = 1/(V(i)*Z(i)) * ( ...
              D(prev,i) * (f(prev)-f(i)) ...
            + D(i,next) * (f(next)-f(i)) ...
              );
      end
   end
   % Last layer of skin c
   i = lastLayerSkinh; prev = i-1;
   df(i)= 1/(V(i)*Z(i)) * ( ...
        + hasSkin * ( ...
          D(prev,i)               * (f(prev)-f(i)) ...
        + D(lastLayerSkinh,blood) * (f(blood)-f(lastLayerSkinh))) ...
          );
end
%% ____________ Automatically Calculate Concentration and Mass
____________
for i = autoCalcCompartments    % environmental, body, and skin
compartments, but not special mass compartments
        dc(i)= mw(NIC)        * Z(i) * df(i);        % g/m3/day
        dm(i)= mw(NIC) * V(i) * Z(i) * df(i);        % g/day
end

%% Environment Analysis Equations
dm(emitVinyl) = mw(NIC) * D(vinyl,vinylFilm) * (f(vinyl)-f(vinylFilm));
```

```
dm(storageCompartments) = dm(vinyl) ...
                        + dm(vinylFilm) ...
                        + dm(air) ...
                        + dm(particles) ...
                        + dm(dustOnVinyl) ...
                        + dm(dust) ...
                        + dm(hardFloorFilm) ...
                        + dm(hardFloor) ...
                        + dm(wallFilm) ...
                        + dm(wall) ...
                        + dm(windowFilm) ...
                        + dm(fabric) ...
                        + dm(fabricFilm) ...
                        + dm(foam) ...
                        + dm(carpetFilm) ...
                        + dm(carpet) ...
                        + dm(backing) ...
                        + dm(persfab) ...
                        + dm(persfabFilm);

dm(flowOut) = mw(NIC) * ( ...
              D(air,flowOut)       * f(air) ...
            + D(particles,flowOut) * f(particles) ...
              );

dm(sweep) = mw(NIC)* ( ...
            D(dustOnVinyl,sweep) * f(dustOnVinyl) ...
          + D(dust,sweep)        * f(dust) ...
            );

dm(launder) = mw(NIC)* ( ...
            + D(persfabFilm,launder) * f(persfabFilm) ...
              );

%               D(persfab,launder)     * f(persfab) ...

dm(emitCig) = 0.0057; % g/day
%% _____________________PBPK Analysis Equations ______________________
dm(storageKid) = dm(lung) ...
               + dm(gut) ...
               + dm(liver) ...
               + dm(lumen) ...
               + dm(fat) ...
               + dm(fat2) ...
               + dm(tissue) ...
               + dm(blood) ...
               + dm(kidFilme) ...
               + dm(kidFilmc) ...
               + dm(kidFilmh) ...
               + sum(dm(skin));

% Mass of NIC which has been metabolized and excreted
dm(excrUrine) = hasKidney * mw(NIC) * D(blood,excrUrine) * f(blood);
```

```
dm(excrFeces) = elimRate(lumen) * m(lumen);

% Loss of NIC due to bathing and handwashing

dm(bathing) = mw(NIC)* ( ...
               D(kidFilme,bathing) * f(kidFilme) ...
             + D(kidFilmc,bathing) * f(kidFilmc) ...
             + D(kidFilmh,bathing) * f(kidFilmh) ...
               );

dm(handwash) = mw(NIC)* ( ...
               D(kidFilmh,handwash) * f(kidFilmh) ...
               );

% Dermal Absorption
dm(absDerme) = hasSkin * mw(NIC)* ( ...
                D(kidFilme,skinSCe(1)) * (f(kidFilme)-f(skinSCe(1))) ...
                );

dm(absDermc) = hasSkin * mw(NIC)* ( ...
                D(kidFilmc,skinSCc(1)) * (f(kidFilmc)-f(skinSCc(1))) ...
                );

dm(absDermh) = hasSkin * mw(NIC) * ( ...
                D(kidFilmh,skinSCh(1)) * (f(kidFilmh)-f(skinSCh(1))) ...
                );

% Flux into blood from last layer of exposed skin  (convert to ug/cm2/h)
dm(skinBloodFluxe) = hasSkin * mw(NIC) * ( ...
                     D(lastLayerSkine,blood)*(f(lastLayerSkine)-f(blood))
...
                     );

dm(skinBloodFluxc) = hasSkin * mw(NIC) * ( ...
                     D(lastLayerSkinc,blood)*(f(lastLayerSkinc)-f(blood))
...
                     );

dm(skinBloodFluxh) = hasSkin * mw(NIC) * ( ...
                     D(lastLayerSkinh,blood)*(f(lastLayerSkinh)-f(blood))
...
                     );

% Inhalation from vapor
dm(inhVap)= human * mw(NIC) * ( ...
            D(air,lung)* (f(air) - f(lung)) ...
            );

% Inhalation of particles
dm(inhPart) = human * mw(NIC) * ( ...
               D(particles,lung)  * f(particles)...
             + D(particles,lumen) * f(particles)...
               );
```

```
% Ingestion of dust
dm(ingDust) = human * mw(NIC) * ( ...
              D(dust,lumen)        * f(dust) ...
            + D(dustOnVinyl,lumen) * f(dustOnVinyl) ...
              );

% Dose to kid:
dm(dose) = dm(inhVap) + dm(inhPart) + dm(ingDust) + dm(absDerme) +
dm(absDermc) + dm(absDermh);

% Mass of NIC equivalents metabolized
dm(metabolites) = degRate(liver) * m(liver);

% Concentration in urine of metabolites cotinine and glucuronides
[ug/l/day]
dm(concUrine) = 1E+6 * dm(metabolites) * (... % converted to ug
                (mwRatio(cotinine) * excrRatio(cotinine)) ...
                )...
              / rate(urineProduction);
%% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%% ____________ Mass Balance _________________________________________
% Overall mass balance [g/day]
dm(massBalance) = dm(emitCig) ...
                - dm(storageCompartments) ...
                - dm(flowOut) ...
                - dm(sweep) ...
                - dm(launder) ...
                - dm(excrUrine) ...
                - dm(excrFeces) ...
                - dm(storageKid) ...
                - dm(bathing) ...
                - dm(handwash);

% Human mass balance
dm(massBalanceKid) = dm(inhVap) ...
                   + dm(inhPart) ...
                   + dm(ingDust) ...
                   + dm(absDerme) ...
                   + dm(absDermc) ...
                   + dm(absDermh) ...
                   - dm(excrUrine) ...
                   - dm(excrFeces) ...
                   - dm(storageKid) ...
                   - dm(bathing) ...
                   - dm(handwash);

%% Create ydot
ydot = [df; dc; dm];
ydot(isnan(ydot)) = 0;

return
```

Run Only

```
function runOnly_nicotine4(human)
% Runs the model
if nargin<1 % this means "if number of inputs < 1"
    human = 1;
    fprintf('Default run: human in room')
end
human=(human==1);

%% Load/calculate initial parameters
parameters_nicotine4();
load modelvariables  %recalculate parameters and load them
functionHandle = @(t,y)
model_nicotine4(t,y,human,air,particles,vinylFilm,vinyl,wall,wallFilm,wind
owFilm,dustOnVinyl,dust,hardFloorFilm,hardFloor,fabric,fabricFilm,foam,car
petFilm,carpet,backing,persfab,persfabFilm,kidFilme,kidFilmc,kidFilmh,nMas
sExchangeComp,emitVinyl,storageCompartments,flowOut,massBalance,emitCig,sw
eep,launder,bathing,handwash,dose,nComp,nExtra,autoCalcCompartments,mw,NIC
,sweepLoss,density,V,Z,Q,transportCoeff,G,D,TSP,partFlowOut,deposition,per
centageHardFloor,percentageVinyl,sweepingLoss,launderingLoss,bathingLosse,
bathingLossc,bathingLossh,handwashingLoss,inhalation,ingDust,urineProducti
on,resuspension,rate,degRate,elimRate,lung,gut,liver,fat,fat2,tissue,blood
,lumen,bloodTotal,skinscTotal,skinveTotal,skinallTotal,storageKid,metaboli
tes,excrUrine,concUrine,excrFeces,inhVap,inhPart,absorbPart,fraction,GIabs
Dust,skinSCe,skinVEe,skinSCc,skinVEc,skinSCh,skinVEh,skine,skinc,skinh,mwR
atio,cotinine,excrRatio,massBalanceKid,bile,legendNames,skin,lastLayerSkin
e,firstLayerSkine,lastLayerSkinc,firstLayerSkinc,lastLayerSkinh,firstLayer
Skinh,absDerme,absDermc,absDermh,skinBloodFluxe,skinBloodFluxc,skinBloodFl
uxh,cig,Glucu,adjRb,launderLoss,bathLoss,handwashLoss);

%fprintf('\nParameters loaded.  ');
clear t y f m c             %remove old results from prior runs

%% Set Absolute Tolerance for Matlab
    abstol=1e-10;
    fprintf('\n Absolute Tolerance %6.0e',abstol)
    options = odeset('AbsTol',abstol);
  %options = []; %comment this out to set the absolute tolerance limit
                 %(Matlab default is 1E-6)
%% Run model
fprintf('\nModel running...    ');

    tic; [t,y] = ode15s(functionHandle,tspan,yo,options); runtime = toc;

%% Print runtime
    if runtime < 90
fprintf('\n  Done. %3.0f s    \n',runtime);
    else
        rtMin = floor(runtime/60);
        rtSec = rem(runtime,60);
        fprintf('\n  Done. %3.0f min %3.0f s    \n',rtMin,rtSec);
    end
```

```
%% Round off results below absolute tolerance to zero
    y=roundOff(y,abstol);

%% Define Fugacity,Mass,Concentration and others from y
% The ode solver returns a y value, this renames the various parts:
f=y(:,1:nComp);   % fugacity results
c=y(:,nComp+1:2*nComp); % concentration results
m=y(:,2*nComp+1:3*nComp);  % mass results

%% Other calculations
last = size(t,1); % the final  ODE  step at t=tspan(end) (#days)
mm = m(last,:);

% concentrations by mass in air, dust and particles
cmAir = zeros(last,nComp);
cmAir(:,air) = c(:,air)*1E6; %ug/m3 in air
cmAir(:,particles) = c(:,particles)/density(particles)*TSP*1E6; %ug  in
particles/m3 air
cmAir(:,dust) = c(:,dust)/density(dust) * 1000; %ug /g dust
cmAir(:,dustOnVinyl) = c(:,dustOnVinyl)/density(dustOnVinyl)*1000;
dustAverage = zeros(last,1);
dustAverage(:,1) = percentageHardFloor* cmAir(:,dust)+
percentageVinyl*cmAir(:,dustOnVinyl);

%cumulative dose/days of exposure
daily = zeros(1,nComp); dailyPercent = zeros(1,nComp);
clear i
for i = [dose, absDerme, absDermc, absDermh, inhVap, inhPart, ingDust,
excrFeces, excrUrine];
daily(i) = m(last,i) / (t(last))*1e6;
dailyBW(i) = daily(i)/BW;
dailyPercent(i) = daily(i)/daily(dose)*100;
end

% flux into the film on the kid averaged over runtime % ug/cm2/h
skinFlux= m(last,absDerme)/(surfaceArea(skin(1))*100^2 *t(last)*24)*1e6;
sbFluxe= m(last,skinBloodFluxe)/(surfaceArea(skin(1))*100^2
*t(last)*24)*1e6;
sbFluxc=
m(last,skinBloodFluxc)/(surfaceArea(skin(nSkin/3+1))*100^2*t(last)*24)*1e6
;
sbFluxh=
m(last,skinBloodFluxh)/(surfaceArea(skin(nSkin*(2/3)+1))*100^2*t(last)*24)
*1e6;

% Mass excreted  ug/day
massExcreted = sum(mm([excrUrine,excrFeces]))/t(last)*1e6;
massExcretedBW = massExcreted/BW;
massRetained = sum(mm(bodyList))*1e6;
percentDoseRetained = (massRetained-massExcreted)/massRetained;
kidFilmLoading = mm(kidFilme)*1E6/(surfaceArea(kidFilme)*100^2); %ug/cm2
massAir = mm(air);
% massFilms = sum(mm(film));
```

```
massSubs = sum(mm(filmSubs));

fprintf('Mass Balance: %6.2e\n MB Kid:
%6.2e\n\n',mm(massBalance),mm(massBalanceKid))

fprintf('\n---\nDermal Dose: \n\t %6.3g ug/kg/d \nPercentage Total Dose:
\n\t
%6.1f',dailyBW(absDerme)+dailyBW(absDermc)+dailyBW(absDermh),dailyPercent(
absDerme)+dailyPercent(absDermc)+dailyPercent(absDermh));
fprintf('\n---\nDust Dose: \n\t %6.3g ug/kg/d \nPercentage Total Dose:
\n\t %6.1f',dailyBW(ingDust),dailyPercent(ingDust));
fprintf('\n---\nInhalation Dose: \n\t %6.3g ug/kg/d \nPercentage Total
Dose: \n\t
%6.1f',dailyBW(inhVap)+dailyBW(inhPart),dailyPercent(inhVap)+dailyPercent(
inhPart));
fprintf('\n---\nTotal Dose: \n\t %6.3g ug/kg/d \nCotinine Dose: \n\t %6.1f
ug/l
\n\n',dailyBW(absDerme)+dailyBW(absDermc)+dailyBW(absDermh)+dailyBW(ingDus
t)+dailyBW(inhVap)+dailyBW(inhPart),(dailyBW(absDerme)+dailyBW(absDermc)+d
ailyBW(absDermh)+dailyBW(ingDust)+dailyBW(inhVap)+dailyBW(inhPart))*BW/0.3
8*0.13);

%% Save and done
save('results.mat')
%delete modelvariables.mat          %delete temporary storage
```

Appendix C.

Table C. 1 Fugacity, Mass and Concentration in Environmental Compartments

Index	Compartment	Mass (g)	Fugacity (Pa)	Concentration (g/m^3)
1	Vinyl	2.03E-03	5.88E-05	2.03E-01
2	vinylFilm	6.10E-05	5.88E-05	1.52E+02
3	air	9.25E-04	5.88E-05	3.85E-06
4	particles	9.79E-08	5.88E-05	2.04E+01
5	dustOnVinyl	1.45E-03	5.83E-05	7.27E+01
6	dust	2.90E-03	5.82E-05	7.25E+01
7	hardFloorFilm	1.22E-04	5.88E-05	1.52E+02
8	hardFloor	3.97E-04	5.88E-05	1.98E-03
9	wallFilm	5.68E-04	5.88E-05	1.52E+02
10	wall	1.85E-03	5.88E-05	1.98E-03
11	windowFilm	2.99E-05	5.88E-05	1.52E+02
12	fabric	7.11E-04	5.88E-05	1.73E-02
13	fabricFilm	1.39E-04	5.88E-05	1.52E+02
14	foam	4.33E-02	5.88E-05	1.73E-02
15	carpetFilm	6.10E-03	5.88E-05	1.52E+02
16	carpet	1.86E-01	5.88E-05	9.30E-03
17	backing	1.66E-03	5.88E-05	1.73E-02
18	persFab	3.21E-05	4.48E-05	1.29E-01
19	persFabFilm	1.29E-06	4.49E-05	1.16E+02
20	kidFilme	2.35E-09	4.44E-07	1.15E+00
21	kidFilmc	1.29E-08	4.50E-07	1.17E+00
22	kidFilmh	4.02E-10	3.00E-07	7.78E-01
23	lung	8.27E-08	8.80E-09	6.95E-04
24	liver	2.30E-06	9.90E-09	5.21E-03
25	lumen	1.18E-06	0.00E+00	4.95E-07
26	gut	1.65E-07	8.80E-09	6.95E-04
27	fat	6.90E-05	8.72E-09	6.88E-02
28	fat2	1.99E-04	8.71E-09	6.88E-02
29	tissue	7.44E-06	8.72E-09	6.88E-04
30	blood	8.66E-07	8.72E-09	6.88E-04

Table C. 2 Fugacity, Mass and Concentration in Skin Compartments

Index	Compartment	Mass (g)	Fugacity (Pa)	Concentration (g/m^3)
59	SkinSCe1	1.46E-07	3.67E-07	1.44E+00
60	SkinSCe2	1.37E-07	3.43E-07	1.34E+00
61	SkinSCe3	1.28E-07	3.20E-07	1.25E+00
62	SkinSCe4	1.19E-07	2.97E-07	1.16E+00
63	SkinSCe5	1.09E-07	2.73E-07	1.07E+00
64	SkinSCe6	9.99E-08	2.50E-07	9.79E-01
65	SkinSCe7	9.06E-08	2.27E-07	8.88E-01
66	SkinSCe8	8.12E-08	2.03E-07	7.96E-01
67	SkinSCe9	7.19E-08	1.80E-07	7.05E-01
68	SkinSCe10	6.26E-08	1.57E-07	6.14E-01
69	SkinSCe11	5.33E-08	1.33E-07	5.22E-01
70	SkinSCe12	4.40E-08	1.10E-07	4.31E-01
71	SkinSCe13	3.46E-08	8.66E-08	3.40E-01
72	SkinSCe14	2.53E-08	6.33E-08	2.48E-01
73	SkinSCe15	1.60E-08	4.00E-08	1.57E-01
74	SkinVEe1	7.70E-09	2.83E-08	1.51E-02
75	SkinVEe2	7.67E-09	2.82E-08	1.50E-02
76	SkinVEe3	7.64E-09	2.81E-08	1.50E-02
77	SkinVEe4	7.62E-09	2.80E-08	1.49E-02
78	SkinVEe5	7.59E-09	2.79E-08	1.49E-02
79	SkinVEe6	7.56E-09	2.78E-08	1.48E-02
80	SkinVEe7	7.54E-09	2.77E-08	1.48E-02
81	SkinVEe8	7.51E-09	2.76E-08	1.47E-02
82	SkinVEe9	7.48E-09	2.75E-08	1.47E-02
83	SkinVEe10	7.46E-09	2.74E-08	1.46E-02
84	SkinVEe11	7.43E-09	2.73E-08	1.46E-02
85	SkinVEe12	7.40E-09	2.72E-08	1.45E-02
86	SkinVEe13	7.37E-09	2.71E-08	1.45E-02
87	SkinVEe14	7.35E-09	2.70E-08	1.44E-02

Index	Compartment	Mass (g)	Fugacity (Pa)	Concentration (g/m^3)
88	SkinVEe15	7.32E-09	2.69E-08	1.44E-02
89	SkinVEe16	7.29E-09	2.68E-08	1.43E-02
90	SkinVEe17	7.27E-09	2.67E-08	1.42E-02
91	SkinVEe18	7.24E-09	2.66E-08	1.42E-02
92	SkinVEe19	7.21E-09	2.65E-08	1.41E-02
93	SkinVEe20	7.19E-09	2.64E-08	1.41E-02
94	SkinSCc1	9.35E-07	4.32E-07	1.69E+00
95	SkinSCc2	8.73E-07	4.03E-07	1.58E+00
96	SkinSCc3	8.11E-07	3.75E-07	1.47E+00
97	SkinSCc4	7.48E-07	3.46E-07	1.36E+00
98	SkinSCc5	6.86E-07	3.17E-07	1.24E+00
99	SkinSCc6	6.24E-07	2.88E-07	1.13E+00
100	SkinSCc7	5.62E-07	2.60E-07	1.02E+00
101	SkinSCc8	4.99E-07	2.31E-07	9.05E-01
102	SkinSCc9	4.37E-07	2.02E-07	7.92E-01
103	SkinSCc10	3.75E-07	1.73E-07	6.79E-01
104	SkinSCc11	3.13E-07	1.45E-07	5.66E-01
105	SkinSCc12	2.51E-07	1.16E-07	4.54E-01
106	SkinSCc13	1.88E-07	8.70E-08	3.41E-01
107	SkinSCc14	1.26E-07	5.83E-08	2.28E-01
108	SkinSCc15	6.38E-08	2.95E-08	1.16E-01
109	SkinVEc1	2.22E-08	1.51E-08	8.04E-03
110	SkinVEc2	2.20E-08	1.49E-08	7.98E-03
111	SkinVEc3	2.18E-08	1.48E-08	7.91E-03
112	SkinVEc4	2.17E-08	1.47E-08	7.85E-03
113	SkinVEc5	2.15E-08	1.46E-08	7.78E-03
114	SkinVEc6	2.13E-08	1.45E-08	7.72E-03
115	SkinVEc7	2.11E-08	1.43E-08	7.65E-03
116	SkinVEc8	2.09E-08	1.42E-08	7.59E-03
117	SkinVEc9	2.08E-08	1.41E-08	7.52E-03
118	SkinVEc10	2.06E-08	1.40E-08	7.45E-03

Index	Compartment	Mass (g)	Fugacity (Pa)	Concentration (g/m^3)
119	SkinVEc11	2.04E-08	1.38E-08	7.39E-03
120	SkinVEc12	2.02E-08	1.37E-08	7.32E-03
121	SkinVEc13	2.00E-08	1.36E-08	7.26E-03
122	SkinVEc14	1.99E-08	1.35E-08	7.19E-03
123	SkinVEc15	1.97E-08	1.34E-08	7.13E-03
124	SkinVEc16	1.95E-08	1.32E-08	7.06E-03
125	SkinVEc17	1.93E-08	1.31E-08	7.00E-03
126	SkinVEc18	1.91E-08	1.30E-08	6.93E-03
127	SkinVEc19	1.90E-08	1.29E-08	6.87E-03
128	SkinVEc20	1.88E-08	1.27E-08	6.80E-03
129	SkinSCh1	1.78E-08	1.75E-07	6.87E-01
130	SkinSCh2	1.68E-08	1.66E-07	6.50E-01
131	SkinSCh3	1.58E-08	1.56E-07	6.13E-01
132	SkinSCh4	1.49E-08	1.47E-07	5.76E-01
133	SkinSCh5	1.39E-08	1.37E-07	5.39E-01
134	SkinSCh6	1.30E-08	1.28E-07	5.01E-01
135	SkinSCh7	1.20E-08	1.18E-07	4.64E-01
136	SkinSCh8	1.10E-08	1.09E-07	4.27E-01
137	SkinSCh9	1.01E-08	9.95E-08	3.90E-01
138	SkinSCh10	9.12E-09	9.00E-08	3.53E-01
139	SkinSCh11	8.16E-09	8.06E-08	3.16E-01
140	SkinSCh12	7.20E-09	7.11E-08	2.79E-01
141	SkinSCh13	6.24E-09	6.16E-08	2.41E-01
142	SkinSCh14	5.28E-09	5.21E-08	2.04E-01
143	SkinSCh15	4.32E-09	4.26E-08	1.67E-01
144	SkinVEh1	2.61E-09	3.79E-08	2.02E-02
145	SkinVEh2	2.61E-09	3.78E-08	2.02E-02
146	SkinVEh3	2.61E-09	3.78E-08	2.02E-02
147	SkinVEh4	2.60E-09	3.77E-08	2.01E-02
148	SkinVEh5	2.60E-09	3.77E-08	2.01E-02
149	SkinVEh6	2.60E-09	3.77E-08	2.01E-02

Index	Compartment	Mass (g)	Fugacity (Pa)	Concentration (g/m^3)
150	SkinVEh7	2.59E-09	3.76E-08	2.01E-02
151	SkinVEh8	2.59E-09	3.76E-08	2.01E-02
152	SkinVEh9	2.59E-09	3.75E-08	2.00E-02
153	SkinVEh10	2.59E-09	3.75E-08	2.00E-02
154	SkinVEh11	2.58E-09	3.75E-08	2.00E-02
155	SkinVEh12	2.58E-09	3.74E-08	2.00E-02
156	SkinVEh13	2.58E-09	3.74E-08	2.00E-02
157	SkinVEh14	2.57E-09	3.73E-08	1.99E-02
158	SkinVEh15	2.57E-09	3.73E-08	1.99E-02
159	SkinVEh16	2.57E-09	3.73E-08	1.99E-02
160	SkinVEh17	2.57E-09	3.72E-08	1.99E-02
161	SkinVEh18	2.56E-09	3.72E-08	1.98E-02
162	SkinVEh19	2.56E-09	3.71E-08	1.98E-02
163	SkinVEh20	2.56E-09	3.71E-08	1.98E-02