APPENDIX H

Dermal Exposure Model

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A. Introduction

The exposure model for dermal contact with ground water includes the term DA_{event} , which represents the absorbed dose per unit surface area of exposed skin during a single contact event. The methodology used to calculate the DA_{event} term is presented in USEPA 2001 and is based on previous work presented in USEPA's Dermal Exposure Assessment (USEPA 1992). All chemical-specific and default inputs used in the calculation of DA_{event} and all associated references are presented in Table H-1. For a more detailed description of the theory and analysis used to develop the following equations, the reader is referred to Appendix A of USEPA 2001.

B. Estimating DA_{event} for Inorganic Compounds

For inorganic compounds, the DA_{event} term is calculated as follows:

$$DA_{event} = K_p^w \cdot C_w \cdot t_{event}$$

where,

K_{p}^{w}	=	chemical-specific permeability coefficient from water (cm/hr);
C_{w}	=	concentration of compound in water (mg/cm ³); and
t _{event}	=	duration of contact event (hr).

The input values used for each chemical evaluated are presented in Table H-1. For the K_p^w term, a default value of 0.001 cm/hr was used for inorganic chemicals for which no chemical-specific value is provided in USEPA 2001 (Exhibit B-4).

C. Estimating DAevent for Organic Compounds

For organic compounds, the DA_{event} for each chemical of potential concern is calculated according to the following series of equations:

$$\log K_{p}^{w} = -2.80 + 0.66 \cdot \log K_{o/w} - 0.0056 \cdot MW$$
$$B = K_{p}^{w} \frac{\sqrt{MW}}{2.6}$$

where,

 K_{p}^{w} = chemical-specific permeability coefficient from water (cm/hr);

K _{o/w}		octanol-water partition coefficient (unitless);
MW	=	molecular weight (g/mol); and
В	=	chemical-specific parameter (unitless).

The stratum corneum diffusion coefficient (D_{sc}) is calculated by the following:

$$\log \frac{\mathrm{D}_{\mathrm{sc}}}{\mathrm{l}_{\mathrm{sc}}} = -2.80 - 0.0056 \cdot \mathrm{MW}$$

where,

$$l_{sc}$$
 = stratum corneum length, 10^{-3} cm.

The remaining model inputs, τ and t^* (both in units of hours), are determined according to the following:

$$\tau = \frac{l_{sc}^2}{6 \cdot D_{sc}} = 0.105 \times 10^{0.0056 \text{MW}}$$

and

If
$$B \le 0.6$$
 then
 $t^* = 2.4 \cdot \tau$
Otherwise ,
 $t^* = 6 \cdot \left(b - \sqrt{b^2 - c^2}\right) \cdot \tau$

where,

$$b = \frac{2}{\pi} \cdot (1+B)^2 - c; \text{ and}$$
$$c = \frac{1+3 \cdot B + 3 \cdot B^2}{3 \cdot (1+B)}$$

where,

 D_{sc} = effective diffusion coefficient for chemical transfer through the stratum corneum (cm²/hr);

τ	=	lag time per event (hr/event);
t*	=	time to reach steady-state (hr); and
b,c	-	correlation coefficients that have been fitted to experimental data.

Finally, DA_{event} is calculated according to the following:

If
$$t_{event} < t^*$$
 then
 $DA_{event} = 2 \cdot FA \cdot K_p^w \cdot C_w \cdot \sqrt{\frac{6 \cdot \tau \cdot t_{event}}{\pi}}$
If $t_{event} > t^*$ then
 $DA_{event} = FA \cdot K_p^w \cdot C_w \cdot \left[\frac{t_{event}}{1+B} + 2 \cdot \tau \cdot \left(\frac{1+3 \cdot B + 3 \cdot B^2}{(1+B)^2}\right)\right]$

where,

FA = chemical-specific fraction adsorbed (unitless).

The chemical concentrations in water, chemical-specific inputs, and the results of the DA_{event} calculation for each applicable COPC in both the NEA and SEA are presented in Table H-1.

D. References

- Mackay, D., Shiu, W., and Ma, K. 1995. Illustrated Handbook of Physical-Chemical Properties and Environmental Fate of Organic Chemicals. Vol. 4, Oxygen, Nitrogen, and Sulfur Containing Compounds. Boca Raton, New York, London, Tokyo: CRC Press, Inc.
- U.S. Environmental Protection Agency (USEPA). 1992. Dermal Exposure Assessment Principles and Applications. Office of Health and Environmental Assessment. EPA/600/8-91/011B. January.
- U.S. Environmental Protection Agency (USEPA). 2001. Risk Assessment Guidance for Superfund, Volume 1: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment), Interim. Office of Emergency and Remedial Response, Washington, D.C. EPA/540/R/99/005. September.

				Summ	arv of Derm	TABLE H-1 al Exposure N	fodel Paran	neters					
	J		$MW^{(a,b)}$	K., ^{w(c,d)}		D _{sc} ^(c)	Tau ^(c)			(c) 1		t _{event} ()	DA _{event} ^(c)
Chemical	(ng/L)	$\log K_{o/w}^{(a,b)}$	(g/mol)	(cm/hr)	$\mathbf{B}^{(c)}$	(cm ² /hr)	(hr)	$\mathbf{b}^{(c)}$	c ^(c)	(hr)	$\mathbf{FA}^{(c)}$	(hr)	(mg/cm ² -event)
Northern Exposure Area													
Acetone	3	-0.24	58.08	5.20E-04	1.53E-03	7.49E-07	2.22E-01	3.04E-01	3.34E-01	5.34E-01	1	1	2.25E-09
Carbon tetrachloride	1.6	2.83	153.82	1.61E-02	7.67E-02	2.18E-07	7.64E-01	3.52E-01	3.86E-01	1.83E+00	1	1	6.22E-08
Chloroform	150	1.97	119.38	6.79E-03	2.85E-02	3.40E-07	4.90E-01	3.21E-01	3.53E-01	1.18E+00	1	1	1.97E-06
Tetrachloroethene	-	3.4	165.8	3.28E-02	1.62E-01	1.87E-07	8.92E-01	4.11E-01	4.49E-01	2.14E+00	1	1	8.55E-08
Toluene	0.27	2.73	92.14	3.06E-02	1.13E-01	4.83E-07	3.45E-01	3.76E-01	4.12E-01	8.28E-01	1	1	1.38E-08
Aluminum	82600			1.00E-03								1	8.26E-05
Arsenic	142			1.00E-03								1	1.42E-07
Barium	1150			1.00E-03								1	1.15E-06
Beryllium	5.1			1.00E-03								1	5.10E-09
Cadmium	3.5			1.00E-03								1	3.50E-09
Chromium (hexavalent)	97.3			1.00E-03								1	9.73E-08
Chromium (total)	85			1.00E-03								1	8.50E-08
Cobalt	0.37			1.00E-03								1	3.70E-10
Copper	71.9			1.00E-03								1	7.19E-08
Iron	68500			1.00E-03								1	6.85E-05
Lead	37			1.00E-03								1	3.70E-08
Magnesium ,	570000	,		1.00E-03								1	5.70E-04
Manganese	1130			1.00E-03								1	1.13E-06
Molybdenum	824			1.00E-03								1	8.24E-07
Nickel	63.6			1.00E-03								1	6.36E-08
Selenium	128			1.00E-03								1	1.28E-07
Silver	1.1			1.00E-03								. 1	1.10E-09
Thorium	24.1			1.00E-03								1	2.41E-08
Titanium	1830			1.00E-03								1	1.83E-06
Vanadium	158			1.00E-03								1	1.58E-07
Zinc	262			1.00E-03								1	2.62E-07
Total Cyanide	2.9			1.00E-03								1	2.90E-09

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				Summa	T ry of Derma	FABLE H-1 d Exposure M	odel Paran	neters					
	ڻ		MW ^(a,b)	K _n ^{w(c,d)}		Dse ⁽⁶⁾	Tau ^(c)			t* ^(c)		t _{event} (f)	DA _{event} (c)
Chemical	(µg/L)	$\log K_{o^{(a,b)}}$	(lom/g)	(cm/hr)	B ^(c)	(cm ² /hr)	(hr)	b ^(c)	C ^(c)	(hr)	FA ^(c)	(hr)	(mg/cm ² -event)
Southern Exposure Area													
Acetone	2.8	-0.24	58.08	5.20E-04	1.53E-03	7.49E-07	2.22E-01	3.04E-01	3.34E-01	5.34E-01	1	1	2.10E-09
Carbon tetrachloride	0.325	2.83	153.82	1.61E-02	7.67E-02	2.18E-07	7.64E-01	3.52E-01	3.86E-01	1.83E+00	1	1	1.26E-08
Chloroform	93	1.97	119.38	6.79E-03	2.85E-02	3.40E-07	4.90E-01	3.21E-01	3.53E-01	1.18E+00	1	1	1.22E-06
Tetrachloroethene	3.3	3.4	165.8	3.28E-02	1.62E-01	1.87E-07	8.92E-01	4.11E-01	4.49E-01	2.14E+00	1		2.82E-07
Toluene	0.72	2.73	92.14	3.06E-02	1.13E-01	4.83E-07	3.45E-01	3.76E-01	4.12E-01	8.28E-01		-	3.67E-08
Aluminum	844			1.00E-03								1	8.44E-07
Arsenic	86.3			1.00E-03								1	8.63E-08
Barium	12.1			1.00E-03								1	1.21E-08
Beryllium	0.05			1.00E-03								1	5.00E-11
Cadmium	1.1			1.00E-03								1	1.10E-09
Chromium (hexavalent)	82.3			1.00E-03								1	8.23E-08
Chromium (total)	60.2			1.00E-03								-	6.02E-08
Cobalt	0.03			1.00E-03								-	3.00E-11
Copper	9.75			1.00E-03								1	9.75E-09
Iron	692			1.00E-03								1	7.69E-07
Lead	0.215			1.00E-03								1	2.15E-10
Magnesium	310000			1.00E-03								1	3.10E-04
Manganese	6.1			1.00E-03								1	6.10E-09
Molybdenum	292			1.00E-03								1	2.92E-07
Nickel	24.3			1.00E-03								1	2.43E-08
Selenium	47.3			1.00E-03								1	4.73E-08
Silver	0.065			1.00E-03								1	6.50E-11
Thorium	0.48			1.00E-03								1	4.80E-10
Titanium	7.4			1.00E-03								1	7.40E-09
Vanadium	29.7			1.00E-03								1	2.97E-08
Zinc	5.6			1.00E-03								1	5.60E-09
Total Cyanide	1.25			1.00E-03								1	1.25E-09
References:													
a - Value for acetone from I	Mackay et a	l (1995)											
b - Exhibit B-2, USEPA 20	01												
c - Calculated according to	equations p	resented in USI	SPA 2001										
d - For inorganics, Exhibit l	3-4, USEP/	A 2001 (default	value = 0.0	(10									
e - Exhibit B-3, USEPA 20	JI (default	value = 1)											
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