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EMAIL REGARDING NEW U S EPA UNPUBLISHED DERMAL GUIDANCE AND SAMPLE CALCULATIONS NTC ORLANDO FL
11/29/1999
BROWN & ROOT ENVIRONMENTAL

03.09.02.0004
00563

McCoy, Steven

From: McCoy, Steven
Sent: Monday, November 29, 1999 2:31 PM
To: 'Nancy Rodriguez'
Subject: FW: OU 2 Dermal Risk Calculations

Let's try this again.
Steve

-----Original Message-----
From: McCoy, Steven
Sent: Thursday, August 26, 1999 3:44 PM
To: 'Nancy Rodriguez'
Cc: Sparks, Barbara
Subject: FW: OU 2 Dermal Risk Calculations

Nancy, attached is some feedback on the new EPA unpublished dermal guidance and the sample calc provided in July. There appear to be some discrepancies which need to be addressed by your risk assessors. If there is something that isn't clear or there are other questions regarding the calc, please feel free to contact Barbara Sparks directly at (423) 220-4746.
Steve

-----Original Message-----
From: Sparks, Barbara
Sent: Thursday, August 26, 1999 12:36 PM
To: McCoy, Steven
Subject: OU 2 Dermal Risk Calculations

Steve,

We have reviewed the complete copy of the new dermal guidance and the sample calculation provided by EPA (received 7/8/99). Although we obtained the same answer for DAevent, we have found what appears to be procedural and mathematical errors in the EPA sample calculation. Errors include:

- Comparing τevent with t* rather than comparing tevent with t*. In the example it was purely coincidental that τevent = tevent.
- Using a value for t* apparently obtained from Table B.3 of the guidance document rather than calculating t*. Default exposure conditions for Table B.3 are not appropriate for the surface water dermal pathway.
- Risk values do not correspond with consistent DAD and CSF values. Risk values do not match our calculated risk values.

Attached is the EPA calculation and our calculations. Our calculations include justification for each step as well as comments regarding what we believe to be errors in the EPA sample calculation. I would like to have EPA review our calculations and provide concurrence with or corrections to (with explanations) our calculations.

As a separate issue, as pointed out in the calculations, Kp and Kp,max for benzo(a)pyrene in Table B.2 do not match values obtained by applying the formulas stated in the table notes as those used to derive the table values. This observation and backup calculations are also included in attached document.

Barbara

Dermal Calc (New 1998 Guidance...

From EPA Region 4 7-8-99

Dermal Risk from B-a-P in surface water

MW	250
log K_{ow}	6.10
K_p	0.72 cm/hr
$K_{p,max}$	0.17 cm/hr
t*	12.3 hrs
C_w	0.341µg/L = 3.41E-07 mg/cm^2

$$\tau_{event} = \frac{I_{sc}^2}{6D_{sc}} = 0.105 \cdot 10^{(0.0056MW)} = 2.6 \frac{hr}{event}$$

If $\tau_{event} = 2.6$ hr, then $\tau_{event} < t^*$

$$DA_{event} = 2 K_p C_w \sqrt{\frac{6\tau_{event} t_{event}}{\pi}}$$

$$= 2 \cdot 0.17 \frac{cm}{hr} \cdot 3.41E-07 \frac{mg}{cm^2} \cdot \sqrt{\frac{6 \cdot 2.6 \frac{hr}{event} \cdot 2.6 \frac{hr}{event}}{\pi}}$$

$$= 4.16E-7 \frac{mg}{cm^2 - event}$$

Adolescent:	EV	1/day	Adult	EV	1/day
	EF	100/yr		EF	45/yr
	ED	10 yr		ED	24 yr
	BW	45 kg		BW	70 kg
	SA	9050 cm2		SA	7300 cm2

$$Dermally\ Absorbed\ Dose (DAD) = \frac{DA_{event}\ EV\ ED\ EF\ SA}{BW\ AT}$$

Risk = DAD x CSF

Adolescent

Risk = 2.3E-5

Adult

Risk = 1.8E-6

CALCULATION WORKSHEET Order No. 19116 (01-91) PAGE 1 OF 7

CLIENT	JOB NUMBER		
SUBJECT Dermal Risk from Benzo(a)Pyrene in Surface Water			
BASED ON	DRAWING NUMBER		
BY Barbara Sparks	CHECKED BY RAyers	APPROVED BY ~~SGM~~ for R. Jupin	DATE 8/23/99

Ref: EPA. 1998. Risk Assessment Guidance for Superfund, Volume I: Human Health Evaluation Manual, Supplemental Guidance, Dermal Risk Assessment, Interim Guidance, Peer Consultation Workshop Draft.

Benzo(a) Pyrene (BAP)

MW = 250
log Kow = 6.10 } p A-8, Table A.1

Kp = 0.72 cm/hr
Kp,max = 0.17 cm/hr } Table B.2, p. B-6.

Please note: Using the equations specified to determine Kp & Kp,max in Table B.2 (Eq 3.7 and Eq A-12, respectively), I calculated Kp = 0.77 and Kp,max = 0.14. See page 6-7 for my calculation. See page B-5 of the reference for the specified equations.
I used Kp = 0.72 cm/hr and Kp,max = 0.17 cm/hr for the remainder of the calculations for consistency

$$\tau = \frac{L_{sc}^2}{6 D_{sc}} = 0.105 * 10^{(0.0056 * MW)} \quad \text{(Eq A.4, p A-3)}$$

$$\tau = 0.105 * 10^{(0.0056 * 250)} = 2.64 \text{ hr/event}$$

τ is assumed to be τ_{event}, eq (3.2) and eq (3.3) and definition on p. 3-4 "lag time per event" [hr/event]

CLIENT	JOB NUMBER		
SUBJECT Dermal Risk from BAP in Surface Water			
BASED ON	DRAWING NUMBER		
BY B. Sparks	CHECKED BY RDA	APPROVED BY ~~BM~~ for R. Jupin	DATE 8/23/99

Calculate B:

$$B = K_p \frac{\sqrt{MW}}{2.6} \qquad \text{(Eq. A.1, p. A-2)}$$

Assume $K_{p,max}$ to be used in place of K_p (p. A-1, 1st paragraph)

$$B = \frac{K_{p,max}\sqrt{MW}}{2.6} = \frac{(0.17\ cm/hr)\sqrt{250}}{2.6} = 1.03 \quad \text{[dimensionless]}$$

$B = 1.03 > 0.6$

$$\therefore t^* = (b - \sqrt{b^2 - c^2})\frac{L_{sc}^2}{D_{sc}} \qquad \text{(Eq. A.6, p. A-3)}$$

$$C = \frac{1 + 3B + 3B^2}{3(1+B)} \qquad \text{(Eq. A.8, p. A-3)}$$

$$= \frac{1 + 3(1.03) + 3(1.03)^2}{3(1+1.03)}$$

$$= \frac{1 + 3.09 + 3.1827}{6.09} = 1.19$$

$$b = \frac{2(1+B)^2}{\pi} - C \qquad \text{(Eq. A.7, p. A-3)}$$

$$= \frac{2 * (1 + 1.03)^2}{\pi} - 1.19$$

$$= 1.43$$

$$\frac{L_{sc}^2}{D_{sc}} = 6\tau = (6)(2.64) = 15.84 \qquad \text{(Eq. A.4, p. A-3 + previous calc for } \tau\text{)}$$

CLIENT	JOB NUMBER		
SUBJECT Dermal Risk from BAP in Surface Water			
BASED ON	DRAWING NUMBER		
BY B. Sparks	CHECKED BY RDA	APPROVED BY for R. Jupin	DATE 8/23/99

$$t^* = \left(b - \sqrt{b^2 - c^2}\right) \frac{\left(\frac{2}{sc}\right)}{D_{sc}} \quad \text{(Eq. A.6, p. A-3)}$$

$$= \left(1.43 - \sqrt{(1.43)^2 - (1.19)^2}\right)(15.84)$$

$$= 10.1 \text{ hrs.}$$

Please note that the calculated value for t^* of 10.1 hrs. does not match the EPA value for t^* of 12.3 hours. It appears that the EPA value of t^* was not calculated but was taken from Table B.3, p. B-14 of the guidance. This table used default exposure conditions (listed on p. B-12) that were not appropriate for the surface water dermal pathway. For example, a tevent of 0.17 hr/event (10 min/event) is used, while the tevent for surface water exposure is 2.6 hr/event

CLIENT		JOB NUMBER	
SUBJECT Dermal Risk from BAP in Surface Water			
BASED ON		DRAWING NUMBER	
BY B. Sparks	CHECKED BY RDA	APPROVED BY SBM for R. Jupin	DATE 8/23/99

** EPA calculation compares τ_{event} and t^*; however equations 3.2 and 3.3 (p. 3-3) compare t_{event} and t^* to find the correct DA_{event} equation.

t_{event} is defined as the event duration [hr/event] on p 3-4 of the reference. t_{event} = 2.6 hr/event was used per EPA RAGS Volume I. It is simply coincidence that $\tau_{event} = t_{event}$ in this case.

t_{event} = 2.6 hrs
t^* = 10.1 hrs

$t_{event} < t^*$, ∴ eq (3.2) (p. 3-3) applies

$$DA_{event} = 2 K_p C_w \sqrt{\frac{6 \tau_{event} t_{event}}{\pi}}$$

Substitute $K_{p,max}$ for K_p

$C_w = 3.41 \times 10^{-7}$ mg/cm^3

$$DA_{event} = (2)(0.17 \text{ cm/hr})(3.41 \times 10^{-7} \text{ mg/cm}^3) * \sqrt{\frac{(6)(2.64 \text{ hr/event})(2.6 \text{ hr/event})}{\pi}}$$

$$= 4.20 \times 10^{-7} \frac{\text{mg}}{\text{cm}^2\text{-event}}$$

CLIENT	JOB NUMBER		
SUBJECT Dermal Risk from BAP in Surface Water			
BASED ON	DRAWING NUMBER		
BY B. Sparks	CHECKED BY RDA	APPROVED BY SBM for R. Jupin	DATE 8/23/99

$$DAD = \frac{DA_{event} * EV * ED * EF * SA}{BW * AT}$$ (Eq. 3.1 p. 3-3)

Using:

Adolescent:

EV = 1 event/day
EF = 100 days/yr
ED = 10 yrs
BW = 45 Kg
SA = 9050 cm^2
AT = 25,550 days

Adult

EV = 1 event/day
EF = 45 days/yr
ED = 24 yrs
BW = 70 Kg
SA = 7300 cm^2 *
AT = 25,550 days

*we used 10,000 cm^2 in HHRA

$$DAD_{adolescent} = \frac{4.20 \times 10^{-7} * 1 * 10 * 100 * 9050}{45 * 25,550}$$

$$= 3.3 \times 10^{-6} \text{ mg/Kg-day}$$

(unit check: $\frac{\frac{mg}{cm^2 \cancel{event}} \frac{event}{\cancel{day}} yrs \frac{\cancel{days}}{\cancel{yr}} cm^2}{Kg\ days}$)

$$DAD_{adult} = \frac{4.2 \times 10^{-7} * 1 * 24 * 45 * 7300}{70 * 25,550}$$

$$= 1.9 \times 10^{-6} \text{ mg/Kg-day}$$

$$Risk = DAD * CSF$$

BAP CSF = 8.1 $(mg/kg\text{-}day)^{-1}$ (EPA OU2 Comment letter)

CLIENT	JOB NUMBER		
SUBJECT: Dermal Risk from BAP in Surface Water			
BASED ON	DRAWING NUMBER		
BY: B. Sparks	CHECKED BY: ROP	APPROVED BY: SBM for E. Jappinen	DATE: 8/23/99

$Risk_{adolescent} = (3.3 \times 10^{-6})(8.1)$

$= 2.7 \times 10^{-5}$

$Risk_{adult} = (1.9 \times 10^{-6})(8.1)$

$= 1.5 \times 10^{-5}$

The above risk numbers do not match the risks shown in the EPA calculation. My DAevent value is the same as the EPA value, but the steps in the calculation differ as discussed above. See p. 7 for possible explanation of difference

* There appears to be an error in Kp and Kp,max given in Table B.2, p. B-6. The Table specifies equations 3.7 and A.12 for Kp and Kp,max.

Using equation 3.7 (p. 3-6):

$\log Kp = -2.80 + 0.67 \log K_{ow} - 0.0056\,mw$

$\log Kp = -2.80 + (0.67)(6.10) - (0.0056)(250)$

$\log Kp = -2.80 + 4.087 - 1.4$

$Kp = 10^{-0.113} = 0.77$ cm/hr

Table B.2 gives Kp of 0.72 cm/hr

Using equation A.12 (p A-9) & Kp = 0.77 cm/hr

$$Kp,max = \frac{Kp}{1+B}$$

CLIENT	JOB NUMBER		
SUBJECT Dermal Risk from BAP in Surface Water			
BASED ON	DRAWING NUMBER		
BY B Sparks	CHECKED BY RDA	APPROVED BY SBM for R. Jupin	DATE 8/23/99

Eq. A.1 (p. A-2):

$$B = \frac{Kp\sqrt{MW}}{2.6}$$

assume Kp used instead of Kp,max in this formula when substituted into Eq. A.12

By Substitution:

$$K_{p,max} = \frac{Kp}{1 + \left(\frac{Kp\sqrt{MW}}{2.6}\right)}$$

$$= \frac{0.77}{1 + \left(\frac{0.77\sqrt{250}}{2.6}\right)}$$

$$= 0.14 \text{ cm/hr}$$

∴ Therefore it appears that Kp and Kp,max for BAP should be 0.77 cm/hr and 0.14 cm/hr, respectively, rather than 0.72 cm/hr and 0.17 cm/hr, respectively.

Possible explanation of Difference in Risk Values

It appears that the values listed for risk in the EPA sample calculation (Adolescent = 2.3×10^{-5}, Adult = 1.8×10^{-6}) are actually DAD values, where the adolescent DAD value was incorrectly calculated using the ED (10 yrs = 3650 days) as the averaging time, that is:

$$DAD = \frac{(4.16 \times 10^{-7})(1)(10)(100)(9050)}{(45)(3650)} = 2.3 \times 10^{-5}$$

This is incorrect. For carcinogens, an averaging time of 70 years must be used.