Attachment 5

METHODOLOGY FOR DERIVING TEMPORARY EMERGENCY EXPOSURE LIMITS (TEELs) (U)

Douglas K Craig and C. Ray Lux, Westinghouse Safety Management Solutions

Westinghouse Savannah River Company
Project Engineering & Construction Division
Aiken, SC 29808

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PREPARED FOR THE U.S. DEPARTMENT OF ENERGY UNDER CONTRACT NO. DE-AC09-96SR18500

APPROVAL SHEET

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ABSTRACT

Exposure limits for chemicals are required throughout the Department of Energy Complex for emergency planning, for the performance of hazard assessments, and for safety analysis. DOE's Subcommittee on Consequence Assessment and Protective Actions (SCAPA) has adopted methodology for deriving TEELs for chemicals where approved Emergency Response Planning Guidelines (ERPGs) do not exist. This methodology is based on hierarchies of existing concentration limits for other standards of exposure, e.g., Permissible Exposure Limits (PELs), and Immediately Dangerous to Life or Health (IDLH) levels. Since many chemicals lack such limits, this methodology was expanded to include use of published toxicity parameters (e.g., LD_{50}, LD_{LO}, TD_{LO}, LC_{50}, LC_{LO}, and TC_{LO}, where L= lethal, T = toxic, LO = low, D = dose, and C = concentration). This expanded methodology was based on the results of statistical analyses of existing ERPGs and human-equivalent concentrations calculated from the above toxicity parameters. The objective of this work is to automate the integrated methodology, combining hierarchy-based and toxicity-based TEELs into procedure-derived TEELs, to facilitate its use by anyone requiring concentration limits for chemicals. Data for each chemical for which concentration limits are required are entered on a Microsoft Excel worksheet. These data include the chemical name, its Chemical Abstract Service (CAS) Registry Number, molecular weight, units of concentration limits (ppm or mg/m^3), and all available toxicity data for six toxicity parameters. The Excel spreadsheet calculates procedure-derived TEELs from these data. This methodology has been successfully applied to about 680 chemicals. Most of the required input data parameters are already available on CD ROM diskettes.

INTRODUCTION

ERPGs are being developed under the auspices of an American Industrial Hygiene Association[1] technical committee for use in evaluating the effects of accidental chemical releases on the general public. They are estimates of concentration ranges for specific chemicals above which acute exposure would be expected to lead to adverse health effects of increasing severity for ERPG-1, ERPG-2, and ERPG-3. DOE's Subcommittee on Consequence Assessment and Protective Actions (SCAPA) has recently published methodology[2] to derive TEELs for chemicals of interest until ERPGs are available. It involves hierarchies of commonly available published and documented concentration-limit parameters, to be used in the order presented, based on availability for the

chemical of interest. When no other concentration limits were available for chemicals likely to be released as aerosols, the value of 10 mg/m^3 recommended by ACGIH[3] as the Time-Weighted Average Threshold Limit Value (TLV-TWA) for Particulates Not Otherwise Classified (PNOC), was invoked to derive TEEL-1 (3 x TLV-TWA) and TEEL-2 (5 x TLV-TWA) values. In addition, in the absence of other information, a TEEL-3 of 500 mg/m^3 was used for aerosols, based on the assumption that this is the upper bound for a stable cloud of inhalable dust.

This hierarchy methodology was approved by DOE and has been incorporated into their revised Emergency Management Guidelines[4]. This hierachy methodology has been enhanced to use other published concentration limits, including NIOSH recommended exposure limits[7,8] (RELs), AIHA workplace environmental exposure limits[1] (WEELs), Federal Republic of Germany maximum allowable concentrations[8] (MAKs), etc.[12].

Since there are no published concentration limits for many chemicals, this methodology was further expanded to include the use of published toxicity parameters[5]. The parameters used include lowest (lo) observed toxic (T) and lethal (L) dose (D) and concentration (C) values, as well as 50% lethality values. TD_{lo} and TC_{lo} values were used to estimate TEEL-2s and LD_{50}, LC_{50}, LD_{lo}, and LC_{lo} were used to estimate TEEL-3s. Human data was given primary consideration, and rat data were preferred over that for other species. Inhalation data were preferred over data from other routes of uptake. Data were extracted for all chemicals for which ERPG were available (74 as of 2/26/97). All toxicity data were first reduced to human-equivalent concentrations in mg/m^3, using default average values to adjust for body weight, quantity of air inhaled per unit time, and route of entry into the body. Statistical correlations were carried out between all and rat-only LD_{50} and LC_{50} data, all and human-only LD_{lo} and LC_{lo} data, and the corresponding ERPG-3 concentrations. These statistical analyses were done first for all values, and then repeated for restricted ranges of ratios to eliminate ratios considered to be outliers in the sense that they distorted the means and standard deviations of most of the data. Similar statistical correlations were carried out between TD_{lo} and TC_{lo} data, and the corresponding ERPG-2 concentrations.

Using only the restricted-range data, mean ratios of LC_{50} to ERPG-3s were approximately 100 for both all the data and for rat data only. Mean ratios of LC_{lo} to ERPG-3s were approximately 100 for all the data and 50 for the human data only. Mean ratios of LD_{50} to ERPGs for all the data and for the rat data only were both about 2, while mean ratios of LD_{lo} to ERPG-3s for all data and for human data only were both close to unity. The results were used to estimate TEEL-3 values. Mean ratios of TC_{lo} to ERPG-2s were about 15 for all the data and 10 for the human data only. Mean ratios of TD_{lo} to ERPG-2s were around 1.5 for all the data and about 1 for rat data only. The results were used to estimate TEEL-2 values.

METHODS

Input:

The name of the chemical compound requiring emergency exposure limits (ERPGs or TEELs) was entered on the first worksheet of an Excel workbook named "TEEL calc", along with its CAS number, SAX number[5], molecular weight (MW) and the primary units of available concentration limits (e.g., PELs, TLVs, ERPGs, etc.). These units are usually parts per million for gases and volatile liquids, milligrams per cubic meter for other liquids and solids. All available concentration limits required for implementation of the hierarchy methodology (see Appendix 1, Table 1) were also entered on this input worksheet. Finally, LD_{50}, LD_{lo}, TD_{lo}, LC_{50}, LC_{lo}, and TC_{lo} data from SAX[5], required for the computation of toxicity-based TEELs, were entered (see Appendix 1, "Input" Worksheet). These included dose (mg/kg), animal species, route of administration, and for TD_{lo}, sex and nature of test, and the number of exposure days. For inhalation exposures, exposure time and whether toxic effects of the chemical are concentration-dependent were also entered. When data for more than one species were available, human data were preferred, followed by rat, mouse and other species in order. The lowest reported dose or concentration reported for a given parameter (e.g., TD_{lo}) was used. Default values for mean body weight (BW in kg), breathing rate (BR in m^3/d), and an adjustment factor for route of administration (RAF) are included in two separate worksheets as lookup tables.

Calculations:

All subsequent "TEEL calc" worksheets in this file are linked to the "Input" worksheet, extracting values or performing calculations to derive hierarchy-based TEELs ("H-s" and "H-Ts min"), toxicity-based TEELs ("Tcalcs", "t-Ts" and "Proc t-Ts"), and procedure-derived TEELs ("Proc Ts").

Appendix 1 calculations: Direct application of the hierarchy methodology to these chemicals yields the hierarchy-based TEELs in the "H-Ts" worksheet. The "H-Ts min" worksheet provides the minimum hierarchy-based values for procedure-based TEELs. It also provides factors used to convert ppm units to mg/m^3 at 25^oC and 760 mmHg for use in subsequent worksheets.

Appendix 2 calculations: The "Tcalcs" worksheet calculates human-equivalent concentrations from the toxicity data, applying simple body weight and breathing rate animal to human conversions, as well as a route adjustment factor to account for differences in uptake for different routes of exposure. For example, intravenous administration (iv) has been assumed to have an RAF of 1.00, since the material is injected directly into the blood stream, whereas oral administration (os) has been assigned an arbitrary RAF = 0.25. These factors are presented in Tables 2 and 3. These computations yield human-equivalent LC_{50}, LC_{lo}, and TC_{lo} values in mg/m^3 from doses given in mg/kg, for all routes of administration except inhalation. No route of administration adjustment is required for inhaled material. However, consideration must be given to whether the toxic consequences of exposure to a chemical may be concentration-dependent (e.g., hydrogen sulfide), dose-dependent (e.g., quartz), or both (e.g., benzene). All toxic concentration data are reduced to a

15-minute exposure time. If the exposure time was not given, 15 minutes was assumed for concentration-dependent chemicals, and 60 minutes was assumed for dose-dependent chemicals[11].

Appendix 3 calculations: The "t-Ts" worksheet calculates toxicity-based TEELs using mean ratios of the human-equivalent concentrations for LC_{50}, LC_{lo}, LD_{50}, and LD_{lo} data to ERPG-3s for TEEL-3 values, and mean ratios of the human-equivalent concentrations for TC_{lo} and TD_{lo} to ERPG-2s for TEEL-2 values. The mean ratios used were based on statistical correlations carried out between matched pairs (i.e., both toxicity and ERPG data were available for a chemical) for all and rat-only LC_{50}, LD_{50}, and TD_{lo} data, all and human-only LC_{lo}, LD_{lo}, and TC_{lo} and ERPGs. Correlations were conducted on all matched pairs and repeated for pairs within selected ratio ranges. The statistical results are summarized in Table 4. The rounded ratios used to estimate TEELs are presented in Table 5.

Ratios of all existing ERPG-3 to ERPG-2 values, and ERPG-2 to ERPG-1 values, were calculated. The means, standard deviations, and coefficients of variation of these ratios were calculated. This analysis was conducted for all available ratios (n = N), and then repeated after eliminating a few outlier ratios (n < N). The mean ratio of ERPG-3 to ERPG-2 (~5) was used to estimate TEEL-3s from TEEL-2s, or vice versa, if there were neither hierarchy-based nor toxicity-based TEEL-2 or TEEL-3 values. The mean ratio of ERPG-2 to ERPG-1 (~7) was used to estimate TEEL-1s from TEEL-2s if no hierarchy-based TEEL-1 was available.

The "Proc Ts" worksheet computes procedure-based TEELs, invoking a rounding protocol similar to that used by others (OSHA, ACGIH and AIHA). Procedure based TEELs are factors or multples of ten of 1.0, 1.25, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 5.0, 6.0, or 7.5. The "Rec TEELs" worksheet adjusts procedure-based TEELs to ensure that all TEELs are at least equal to the minimum values calculated in the "H-Ts min" worksheet, that $T_0 \leq T_1 \leq T_2 \leq T_3$, and that all TEELs in units of $mg/m^3 \leq 500$. All the user has to do is enter all required, available data for a chemical on the "Input" worksheet, and press the "calculate" keys, to obtain the desired TEELs for that chemical.

RESULTS

TEELs for 754 chemicals, including seventy-eight for which "official" ERPGs had been published on the SCAPA home page, http://www.sep.bnl.gov/scapa, by September 30, 1997, were included in the document WSMS-SAE-97-0041: ERPGs and TEELs for Chemicals of Concern: Rev. 13 Detail (December 31, 1997). An abbreviated version of this document, WSMS-SAE-98-0001, is available on DOE EH's Chemical Safety home page: http://tis-hq.eh.gov/web/chem_safety/ , under "Requirements and Guidelines". The methodology described in this document was incomplete when Rev. 12 was issued (July 9, 1997) in that it had been only partly automated. The "TEEL calc" automated methodology has been applied to all 471 chemicals in that list (Rev. 12), and over 300 additional chemicals. Most of these (283) are included in Rev. 13.

Results of the statistical analysis of the available toxicity and ERPGs are presented in Appendix 3: Procedure-derived toxicity-based TEELs, Table 4. The rounded mean ratios of human-equivalent toxicity parameters to ERPG-3s (lethality) and ERPG-2s (toxicity) from Table 4 are presented in

Table 5.

TEELs estimated from human-equivalent toxicity concentrations are computed in the "Tcalcs" and "t-Ts" worksheets 9 (Appendix 2), while procedure-derived TEEL-2 and TEEL-3 values are calculated in the "Proc t-Ts" worksheet (Appendix 3). This selects hierarchy-based values from the "H-Ts" and "H-Ts min" worksheets, if available, followed by toxicity-based values in order. i.e., TC_{lo} and TD_{lo} for TEEL-2, LC_{50}, LC_{lo}, LD_{50}, and LD_{lo} for TEEL-3. However, human toxicity data take precedence over animal data, over-riding the order of toxicity-parameter selection. Procedure-derived TEELs at all levels (i.e., TEEL-0, TEEL-1, TEEL-2, and TEEL-3) are calculated in the "Proc Ts" worksheet (Appendix 3). This returns the raw numbers, rounded to factors of ten of 1.0, 1.25, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 5.0, 6.0 and 7.5, unless the value is within five per cent of the next higher value. The "Rec TEELs" worksheet modifies these procedure-based TEELs to ensure that there are no blanks, and that TEEL-3 ≥ TEEL-2 ≥ TEEL-1 ≥ TEEL-0. It also reduces all TEEL values for materials in aerosol form (mg/m^3 units) to a maximum of 500 mg/m^3. A sample of the output for five chemicals for which differing input data are available is included in the appendices.

DISCUSSION

Data for each chemical for which concentration limits are required are entered on the first worksheet of the "TEEL calc" Excel workbook. These data include the chemical name, its Chemical Abstract Service Registry Number (CASRN), molecular weight (MW), units of concentration limits (ppm or mg/m^3), and toxicity data for six toxicity parameters. If there are data for the same parameter (e.g., LC_{LO}) for more than one species, human data are used first, followed by rat data, mouse data, and data for other species in order. The program then calculates procedure-derived TEELs from these data. This methodology has been successfully applied to over 700 chemicals lacking ERPGs. Most of the required input data parameters are already available on CD ROM diskettes.

The ultimate objective is to develop methodology so that, for example, only a CASRN need be entered, following which all the required input data will be extracted for the automatic computation of hierarchy-based, toxicity-based, and procedure-derived TEELs. Since the CD ROMs are propriety items, it may be necessary to enter the diskette data in a separate data base in order to accomplish this, or we may have to acquire extractable diskettes. Trial disks containing the completed methodology will be distributed to a limited number of qualified individuals for testing. The published[2] hierarchy methodology for deriving TEELs is already in use, but must be carried out manually by qualified individuals. It is also included in the United States Department of Energy Emergency Management Guidance.

CONCLUSIONS

Application of the methodology described in this document to additional chemicals requiring temporary emergency exposure limits requires only that the chemical name, its CASRN and molecular weight, available concentration limits and toxicity parameters, be entered on the first worksheet of the "TEEL calc" Excel workbook. At the "calculate" command, these data are used to produce procedure-derived TEELs, which are then rounded down (unless the value is within 5% of

the next higher value) according to the given protocol to produce recommended TEELs for those chemicals. . The work described greatly expands the number of chemicals for which TEELs can be derived, and its application will ensure consistency of TEEL values from one DOE site to another.

SUMMARY

Methodology is described to fulfil the need for exposure limits for chemicals for emergency planning, for the performance of hazard assessments, and for safety analysis. DOE's Emergency Management Advisory Committee's SCAPA has adopted methodology for deriving TEELs for chemicals where approved ERPGs do not exist. This methodology is based on hierarchies of existing concentration limits, e.g., Permissible Exposure Limits (PELs), and Immediately Dangerous to Life or Health (IDLH) levels. Many chemicals in use, waste storage, or at remediation sites, lack such limits. Therefore, this methodology was expanded to include other available concentration limits (RELs, WEELs, MAKs), as well as published toxicity parameters (e.g., LD_{50}, LD_{LO}, TD_{LO}, LC_{50}, LC_{LO}, and TC_{LO}, where L= lethal, T = toxic, LO = low, D = dose, and C = concentration), based on statistical analyses of existing ERPGs and human-equivalent concentrations calculated from these toxicity parameters. This integrated methodology has been automated, combining hierarchy-based and toxicity-based TEELs into procedure-derived TEELs, to facilitate its use by anyone requiring concentration limits for chemicals. Data for each chemical for which concentration limits are required are entered in the "TEEL calc" Microsoft Excel workbook. The Excel program calculates procedure-derived and recommended TEELs from these data. This methodology has been successfully applied to over 700 chemicals. Most of the required input data parameters are already available on CD ROM diskettes, but must be manually entered on the first worksheet.

REFERENCES

1 Emergency Response Planning Guidelines: Published periodically by the American Industrial Hygiene Association. The latest available list of approved ERPGs, dated 9/30/97, is available on SCAPA's home page (http://www.sep.bnl.gov/scapa). This includes 78 chemicals.

2 Craig, D.K., J.S. Davis, R. DeVore, D.J. Hansen, A.J. Petrocchi, and T.J. Powell. Alternative Guideline Limits for Chemicals without ERPGs. Amer. Ind. Hyg. Assoc J. V 56, No. 9, pp 919-925 (1995).

3 1996 Threshold Limit Values (TLV) for Chemical Substances and Physical Agents and Biological Exposure Indices: The American Conference Of Governmental Industrial Hygienists (ACGIH) . Cincinnati, OH (ISBN: 1-882417-13-5). (1996; updated annually).

4 Emergency Management Guidelines(1997). U.S. Department of Energy *Hazards Surveys and Hazards Assessments*, DOE G 151.1-1, Volume II, U. S. Department of Energy, August 21,1997

5 SAX's Dangerous Properties of Industrial Materials, Ninth Edition, Editor: Richard J. Lewis, Sr. Van Nostrand Reinhold, New York (1996). These data are now available on a CD ROM, which is

updated regularly.

6 Code of Federal Regulations, Title 29 - Labor, Part 1910.1000, Chapter XVII - Occupational Safety and Health Administration: Subpart Z - Toxic and Hazardous Substances, Tables Z-1 and Z-2. (1993).

7 NIOSH Pocket Guide to Chemical Hazards, Department of Health and Human Services, Public Health Service, National Institute for Occupational Safety and Health, Washington, DC (June 1994 Edition).

8 Guide to Occupational Exposure Values - 1996, Compiled by the American Conference of Governmental Industrial Hygienists. ISBN: 1-882417-14-3. Cincinnati, OH (1996).

9 Emergency and Continuous Exposure Guidance Levels for Selected Airborne Contaminants, Committee on Toxicology, Board on Environmental Studies and Toxicology, National Research Council, National Academy Press, Washington, DC (1985).

10 Technical Guidance for Hazards Analysis. Emergency Planning for Extremely Hazardous Substances. U.S. Environmental Protection Agency, Federal Emergency Management Agency, and U.S. Department of Transportation: EPA-OSWER-88-0001 (December 1987)

11 WSRC-MS-92-206, REV. 2: Toxic Chemical Hazard Classification and Risk Acceptance Guidelines for Use in D.O.E. Facilities (U). Recommendations of the Westinghouse M & O Nuclear Facility Safety Committee Subcommittee on Nonradiological Risk Acceptance Guidelines Development (March 24, 1995).

12 Occupational Exposure Limits for Airborne Toxic Substances, Third Edition: Values of Selected Countries prepared from the ILO-CIS Data Base of Exposure Limits. International Labor Office, Geneva. ISBN 92—2-107293-2. (1991)

APPENDICES

The Excel Spreadsheet used in the computation of TEELs comprises a number of different **Worksheets** are presented below in the order in which they appear in the spreadsheet. The column headings are presented first, followed by the formulae in the first row for which chemical data are Input.

Appendix 1: Derivation of Hierarchy-based TEELs

The expanded (to include RELs, WEELs, MAKs, etc.) hierarchy of concentration-limits (parameters) used for deriving TEELs is presented in Table 1.
Concentration limits are tabulated for chemicals requiring TEELs. The Chemical Abstract Service (CAS) Registry Number is used for the unique identification of each chemical. The hierarchy is then used to derive H-T values. The American Conference Of Governmental Industrial Hygienists (ACGIH) Threshold Limit Value (TLV) Committee recommends use of the term "Particulates Not Otherwise Classified (PNOC)" for chemicals likely to be released as aerosols[3]. A time-weighted average threshold limit value (TLV-TWA) of 10 mg/m^3 for inhalable (3 mg/m^3 for respirable) particulate material is recommended by ACGIH as the PNOC limit. This 10 mg/m^3 TLV-TWA was invoked to derive TEEL-1 (3 x TLV-TWA) and TEEL-2 (5 x TLV-TWA) values when no other concentration limits were available. In the absence of toxicity information indicating more restrictive values, a TEEL-3 of 500 mg/m^3 was used for particulate materials. This upper bound is based on the assumption that this is the maximum stable concentration for a cloud of inhalable dust.

Table 1: Hierarchy of Alternative Concentration-Limit Parameters*

Primary Guideline	Hierarchy of Alternative Guidelines	Source of Concentration Parameter
ERPG-3		AIHA 1997[1]
	EEGL (30-min)	NAS 1985[9]
	IDLH	NIOSH 1994[7]
ERPG-2		AIHA 1997[1]
	EEGL (60-min)	NAS 1985[9]
	LOC	EPA 1987[10]
	PEL-C	29:1910.1000[6]
	TLV-C	ACGIH 1996[3]
	REL-C*	NIOSH 1996[8]
	WEEL-C*	AIHA-C[1]
	TLV-TWA x 5	ACGIH 1996[3]
ERPG-1		AIHA 1997[1]
	PEL-STEL	CFR 29:1910.1000[6]
	TLV-STEL	ACGIH 1996[3]
	REL-STEL*	NIOSH 1996[8]
	WEEL-STEL*	AIHA 1996[1]
	OTHER-STEL*	e.g.,German, Russian[12]
	TLV-TWA x 3	ACGIH 1996
PEL-TWA		CFR 29:1910.1000[6]
	TLV-TWA	ACGIH 1996[3]
	REL-TWA*	NIOSH 1996[8]
	WEEL-TWA*	AIHA-1996[1]
	MAK-TWA*	German Fed. Republic 1996[8]
	OTHER-TWA*	e.g. Russian[12]
	CEGL	NAS 1985[9]

Note: If application of this hierarchy to a particular chemical gives rise to a value for a lower hazard class that is higher than the value for the next higher hazard class then that value should be adjusted downwards to match that of the next higher hazard class.

* Parameters added since publication of the hierarchy methodology[2].

"Input" Worksheet (Hierarchy data)

A	B	C	D	E	F
No.	Chemical Compound	CAS Number	SAX Number	Molecular Weight MW	Units of Original limits
1	Chemical with ERPGs	00107-13-1	ADX500	53.07	ppm
2	Chemical with toxicity data only	00105-60-2	CBF700	115.18	mg/m3
3	Chemical with HT-3, toxicity data, but no HT-2	00140-88-5	EFT000	100.13	ppm
4	Chemical with no HTs and only LC_{50} data	28182-81-2	HEG300		mg/m3
5	Chemical with HT-2 and some toxicity data	01310-65-2	LHI100	23.95	mg/m3

A	B	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U
		TEEL-0								TEEL-1						
No.	Chemical	Time-weighted Average Concentration (TWA)								ERPG	Short-term Exposure Limit (STEL)					3*TLV
	Compound	PEL	Note	TLV	Note	REL	WEE	Other	Note	1	PEL	TLV	REL	WEE	Other	TWA
1	ERPGs	2		2		1				10						
2	Tox data only			1	A4	1		5	DFG			3	3			
3	HT-3, tox data	25	68	5	A4			5	DFG			15				
4	No HTs, LC_{50}															
5	HT-2, some tox															

A	B	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF
		TEEL-2								TEEL-3		
No.	Chemical	ERPG	EEGL	EPA	15-min Ceiling Concentration (C)				5*TLV	ERPG	EEGL	IDLH
		2	60min	LOC	PEL	TLV	REL	WEEL	TWA	3	30min	
1	ERPGs	35		50	10					75		85
2	Tox data only											
3	HT-3, tox data											300
4	No HTs, LC_{50}											
5	HT-2, some tox							1				

"Input" Worksheet (Toxicity data)

A	B	AG	AH	AI	AJ	AK	AL	AM	AN	AO	AP	AQ
		LD50			LDlo			TDlo				
No.	Chemical Compound	Dose mg/kg	Spec	Rte	Dose mg/kg	Spec	Rte	Dose mg/kg	Spec	Rte	Sex and exp	Days
1	ERPGs	78	r	os	2015	chd	sk	650	r	os	f post	10
2	Tox data only	930	r	os	800	r	ip					
3	HT-3, tox data	800	r	os	1800	r	sk	51500	r	os	2yr-I	260
4	No HTs, LC_{50}											
5	HT-2, some tox				200	mu	os					

A	B	AR	AS	AT	AU	AV	AW	AX	AY
		LC50				LClo			
No.	Chemical Compound	Dose ppm	Dose mg/m3	Spec	Exp T/d min	Dose ppm	Dose mg/m3	Spec	Exp T/d min
1	ERPGs	425		r	240		1000	hmn	60
2	Tox data only		300	r	120				
3	HT-3, tox data	2180		r	240	1204		rb	420
4	No HTs, LC_{50}		18500	r	60				
5	HT-2, some tox		960	r	240				

A	B	AZ	BA	BB	BC	BD	BE	BF	BG	BH
		TClo								Toxicity Concentration dependent
No.	Chemical Compound	Dose ppm	Dose mg/m3	Spec	Exposure regimen y	w	d	min	Exp T/d min	
1	ERPGs	16		hmn				20	20	Y
2	Tox data only		21.2	hmn					15	Y
3	HT-3, tox data	50		hmn					15	Y
4	No HTs, LC_{50}									Y
5	HT-2, some tox									Y

"H-Ts" Worksheet (calculates hierarchy-based TEELs from "Input" data)

A	B	C	D	E	F	G	H	I	J	K
No.	Chemical	Hierarchy-based Values Unadjusted input values (Hua)				Hierarchy-derived TEELs Adjusted for Tx <= Ty <= Tz				Units of original limits
		Htua-0	Htua-1	Htua-2	Htua-3	HT-0	HT-1	HT-2	HT-3	
1	ERPGs	2	10	35	75	2	10	35	75	ppm
2	Tox data only	1	3			1	3			mg/m^3
3	HT-3, tox data	25	15		300	15	15		300	ppm
4	No HTs, LC_{50}									mg/m^3
5	HT-2, some tox			1				1		mg/m^3

Note: Unadjusted hierarchy-based TEELs are taken straight from the "Input" Worksheet, in the order specified by Table 1, without regard to magnitude. Hierarchy-derived TEELs are adjusted to ensure that TEEL-3 ≥ TEEL-2 ≥ TEEL-1 ≥ TEEL-0

Column

A = Input!A4

B = Bring(Input!B4)

C = IF(MIN(Input!G4:M4)=0,"",MIN_Num(First_Num(Input!G4:M4), MIN_Num(Input!Y4:Z4)))

D = IF(MIN(Input!O4:U4)=0,"",First_Num(Input!O4,MIN_Num(First_Num (Input!P4:U4),MIN_Num(Input!Y4:Z4))))

E = First_Num(Input!V4:AC4)

F = First_Num(Input!AD4:AF4)

G = IF(Bring(C4)'="","",MIN_Num(C4:F4))

H = IF(Bring(D4)'="","",MIN_Num(D4:F4))

I = IF(Bring(E4)'="","",MIN_Num(E4,F4))

J = IF(Bring(F4)'="","",MIN_Num(F4))

K = Bring(Input!$F4)

"H-Ts min" Worksheet (provides minimum values for procedure-based TEELs)

The factor by which concentration in ppm is converted to concentration in mg/m^3 at 25°C and 760 mmHg is given in Column C below. This is calculated form the equation

$$C(ppm) = \frac{22.414}{M.W.} x \frac{T}{273} x \frac{760}{P} xC(mg/m3) = \frac{24.467}{M.W.} xC(mg/m3)$$

or

$$C(mg/m3) = \frac{M.W.}{24.467} xC(ppm)$$

P is assumed to be close to normal atmospheric pressure, but obviously decreases as altitude increases above sea level. Thus, at an atmospheric pressure of 625 mmHg, the value of 24.467 would become about 29.75, an increase of about 22%.

A	B	C	D	E	F	G	H
		Conversion	H-TEELs (min)				Units of
No.	Chemical	Factor	Minimum HTs to override Procedure-based TEELs				original
		ppm:mg/m3	h-TEEL-0	h-TEEL-1	h-TEEL-2	h-TEEL-3	limits
1	ERPGs	2.17	2.00E+0	1.00E+1	3.50E+1	7.50E+1	ppm
2	Tox data only	4.71	1.00E+0	3.00E+0	3.00E+0	3.00E+0	mg/m^3
3	HT-3, tox data	4.09	1.50E+1	1.50E+1	1.50E+1	3.00E+2	ppm
4	No HTs, LC_{50}						mg/m^3
5	HT-2, some tox	0.98	5.00E-2	5.00E-2	1.00E+0	1.00E+0	mg/m^3

Column

A = Input!A4

B = Bring(Input!B4)

C = Bring(Input!E4/24.467)

D = MgLimit(First_Num('H-Ts'!G4,chem_round(First_Num('H-Ts'!H4/T0_1, 'H-Ts'!I4/(T0_1*T1_2),'H-Ts'!J4/(T0_1*T1_2*T2_3)),'H-Ts'!G4)),H4)

E = MgLimit(Max_Num(First_Num('H-Ts'!H4,chem_round('H-Ts'!I4/T1_2,'H-Ts'!G4*T0_1, 'H-Ts'!J4/(T1_2*T2_3),'H-Ts'!G4)),D4),H4)

F = MgLimit(Max_Num(First_Num('H-Ts'!I4,chem_round('H-Ts'!J4/T2_3,'H-Ts'!H4*T1_2, 'H-Ts'!G4*T0_1*T1_2,'H-Ts'!H4)),E4),H4)

G = MgLimit(Max_Num(First_Num('H-Ts'!J4,chem_round('H-Ts'!I4*T2_3, 'H-Ts'!H4*(T2_3*T1_2),'H-Ts'!G4*(T0_1*T1_2*T2_3),'H-Ts'!I4)),F4),H4)

H = Bring(Input!$F4)

Appendix 2: Toxicity Calculations

Table 2: Default mean body weight and breathing rate values for different species

Row number	A	B	C	D
	Species	Abbreviation (Sp)	Mean ABW (kg)	Mean ABR (m^3/d)
4	Child	chd	20	8.64
5	Cat	ct	2	1.25
6	Dog	dg	10	3.66
7	Frog	frg	0.033	1.51
8	Guinea pig	gp	0.5	0.283
9	Hamster	ham	0.125	0.1
10	Human/man	hmn	70	20
11	Infant	inf	5	25
12	Monkey	mo	5	3.94
13	Mouse	mu	0.025	0.035
14	Pig	pg	60	20
15	Rat	r	0.2	0.153
16	Rabbit	rb	2	1.3
17	Women	wmn	50	16

Notes: The default body weight data in the left-hand table is from SAX (Reference 2). The daily inhalation rates are commonly used values for human males, females, children and infants, and laboratory animals. Similar sets of default values, for a more limited list of species, are presented by: Calabrese, E.J. and E.M. Kenyon: Air Toxics and Risk Assessment, Lewis Publishers, Inc., Chelsea, MI (1991), and Hayes, A.W. (Editor): Principles and Methods of Toxicology, Second Edition, Raven Press, New York, NY (1989).

Table 3: Adjustment factors used for different routes of administration.

Row Number	A	B	C
3	Route of administration	Abbreviation (Rte)	RAF
4	eye	eye	0.20
5	inhalation-gas	ih-g	0.50
6	inhalation-particles	ih-p	0.25
7	intracerebral	ice	0.50
8	intradermal	idr	0.10
9	intramuscular	im	0.25
10	intraperitoneal	ip	0.75
11	intrapleural	ipl	0.50
12	intratesticular	itt	0.25
13	intratracheal	it	0.25
14	intravenous	iv	1.00
15	oral	os	0.25
16	skin-insoluble	sk-i	0.10
17	skin-soluble	sk-s	0.20
18	subcutaneous	sc	0.10
19	unknown	uk	0.25

Note: The route of administration adjustment factors presented are rough estimates used to partially account for the differences between administered dose and absorbed dose. In practice, these values would be expected to vary from chemical to chemical, depending upon solubility in body fluids, metabolic changes, and other factors.

The Worksheet headings and formulae used to calculate the human-equivalent concentrations, using linear body weight and breathing rate adjustments, from the toxicity input data are given below.

For example, the equations used to convert an animal LD_{50} dose in mg/kg to a human-equivalent concentration (HLC-eq) in mg/m^3 are:

$$ALC_{50} = LD_{50} \times (ABW/ABR) \times RAF$$

$$HLC_{50}\text{-eq} = ALC_{50} \times (HBW/ABW) \times (ABR/HBR)$$

where A = animal, H = human, BW = body weight and BR = breathing rate (both in Table 2), and RAF = route adjustment factor (Table 3).

Equations of the same form were used to calculate human LC_{LO} and TC_{LO}-equivalent concentrations from LD_{LO} and TD_{LO} values. Data for infants (inf), children (chd), and women (wmn) were treated the same way. Toxicity data specified as "human" (hmn) were assumed to be for men.

The equations used to convert an animal LC_{50} concentration to human-equivalent concentrations (both in mg/m^3) make different adjustments for exposure time (t), depending upon whether the acute toxic effects were concentration-dependent ("Y" in "Input" column BH) or dose-dependent ("N" in 'Input" column BH). The reason for this is that exposure time is not the primary factor in determining the toxic consequence of chemicals whose effects are concentration dependent[1]. The choice of the square root is somewhat arbitrary, but the intention is to reduce the influence of exposure time for chemicals whose primary acute effect is primarily determined by the concentration.

For "Y" chemicals:

$$HLC_{50}\text{-eq} = ALC_{50} \times (t/15)^{0.5} \times (HBW/ABW) \times (ABR/HBR)$$

For "N" chemicals:

$$HLC_{50}\text{-eq} = ALC_{50} \times (t/15) \times (HBW/ABW) \times (ABR/HBR)$$

"Tcalcs" Worksheet

A	B	C	D	E	F	G	H	I	J	K	L
		LC_{50}					LC_{Lo}				
No.	Chemical	BW	RAF	ABR	$ALC_{50}adj$	$HLC_{50}eq$	BW	RAF	ABR	$ALC_{Lo}adj$	$HLC_{Lo}eq$
		kg		m^3/d	mg/m^3	mg/m^3	kg		m^3/d	mg/m^3	mg/m^3
1	ERPGs	0.2	0.25	0.153	2.55E+1	6.83E+1	20	0.25	8.64	1.17E+3	1.76E+3
2	Tox data only	0.2	0.25	0.153	3.04E+2	8.14E+2	0.2	0.75	0.153	7.84E+2	2.10E+3
3	HT-3, tox data	0.2	0.25	0.153	2.61E+2	7.00E+2	0.2	0.25	0.153	5.88E+2	1.58E+3
4	No HTs, LC_{50}										
5	HT-2, some tox						0.025	0.25	0.035	3.57E+1	1.75E+2

Column

A = Input!A4

B = Bring(Input!B4)

C = First_Num(INDEX(SPECIES_DATA,MATCH(Input!AH4,'Species data'!$B$4:$B$17),2))

D = First_Num(INDEX(ROUTE_DATA,MATCH(Input!AI4,'Route data'!$B$4:$B$19),2))

E = First_Num(INDEX(SPECIES_DATA,MATCH(Input!AH4,'Species data'!$B$4:$B$17),3))

F = First_Num((Input!AG4*C4/E4)*D4)

G = First_Num(IF(Input!AH4="hmn",F4,F4*(70*E4)/(20*C4)))

H = First_Num(INDEX(SPECIES_DATA,MATCH(Input!AK4,'Species data'!$B$4:$B$17),2))

I = First_Num(INDEX(ROUTE_DATA,MATCH(Input!AL4,'Route data'!$B$4:$B$19),2))

J = First_Num(INDEX(SPECIES_DATA,MATCH(Input!AK4,'Species data'!$B$4:$B$17),3))

K = First_Num((Input!AJ4*H4/J4)*I4)

L = First_Num(IF(Input!AK4="hmn",K4,K4*(70*J4)/(20*H4)))

"Tcalcs" Worksheet (continued)

A	B	M	N	O	P	Q	R	S	T	U	V
No.	Chemical	Dose	BW	RAF	ABR	.ATC$_{lo}$adj	HTCloeq	Conc.	BW	ABR	HLC$_{50}$eq
		mg/kg	kg		m^3/d	mg/m^3	mg/m^3	mg/m^3	kg	m^3/d	mg/m^3
1	ERPGs	6.50E+1	0.2	0.25	0.153	2.12E+1	5.69E+1	9.22E+2	0.2	0.153	9.87E+3
2	Tox data only							3.00E+2	0.2	0.153	2.27E+3
3	HT-3, tox data	1.98E+2	0.2	0.25	0.153	6.47E+1	1.73E+2	8.92E+3	0.2	0.153	9.55E+4
4	No HTs, LC$_{50}$							1.85E+4	0.2	0.153	9.91E+4
5	HT-2, some tox							9.60E+2	0.2	0.153	1.03E+4

Column

A = Input!A4

B = Bring(Input!B4)

M = First_Num(Input!AM4/Input!AQ4,Input!AM4)

N = First_Num(INDEX(SPECIES_DATA,MATCH(Input!AN4,'Species data'!$B$4:$B$17),2))

O = First_Num(INDEX(ROUTE_DATA,MATCH(Input!AO4,'Route data'!$B$4:$B$19),2))

P = First_Num(INDEX(SPECIES_DATA,MATCH(Input!AN4,'Species data'!$B$4:$B$17),3))

Q = First_Num((M4*N4/P4)*O4)

R = First_Num(IF(Input!AN4="hmn",Q4,Q4*(70*P4)/(20*N4)))

S = First_Num(Input!AR4*'H-Ts min'!C4,Input!AS4)

T = First_Num(INDEX(SPECIES_DATA,MATCH(Input!AT4,'Species data'!$B$4:$B$17),2))

U = First_Num(INDEX(SPECIES_DATA,MATCH(Input!AT4,'Species data'!$B$4:$B$17),3))

V = First_Num(Input!AT4="hmn",IF(Input!BH4="Y",SQRT(Input!AU4/15)), IF(Input!BH4="Y", S4*SQ SQRT(Input!AU4/15)*((70*U4)/(20*T4)),S4*(Input!AU4/15)*((70*U4)/(20*T4)))))

"Tcalcs" Worksheet (continued)

A	B	W	X	Y	Z	AA	AB	AC	AD
		LCl				TCl			
No.	Chemical	Conc. mg/m^3	BW kg	ABR m^3/d	HLClo.eq mg/m^3	Conc. mg/m^3	BW kg	ABR m^3/d	HTClo.eq mg/m^3
1	ERPGs	1.00E+3	70	20	2.00E+3	3.47E+1	70	20	4.01E+1
2	Tox data only					2.12E+1	70	20	2.12E+1
3	HT-3, tox data	4.93E+3	2	1.3	5.93E+4	2.05E+2	70	20	2.05E+2
4	No HTs, LC_{50}								
5	HT-2, some tox								

Column

A = Input!A4

B = Bring(Input!B4)

W = First_Num(Input!AV4*'H-Ts min'!C4,Input!AW4)

X = First_Num(INDEX(SPECIES_DATA,MATCH(Input!AX4,'Species data'!$B$4:$B$17),2))

Y = First_Num(INDEX(SPECIES_DATA,MATCH(Input!AX4,'Species data'!$B$4:$B$17),3))

Z = First_Num(IF(Input!AX4="hmn",IF(Input!BH4="Y",W4*SQRT(Input!AY4/15),W4*(Input!AY4/15)), IF(Input!BH4="Y",W4*SQRT(Input!AY4/15)*((70*Y4)/(20*X4)),W4*(Input!AY4/15)*((70*Y4)/(20*X4)))))

AA = First_Num(Input!AZ4*'H-Ts min'!C4,Input!BA4)

AB = First_Num(INDEX(SPECIES_DATA,MATCH(Input!BB4,'Species data'!$B$4:$B$17),2))

AC = First_Num(INDEX(SPECIES_DATA,MATCH(Input!BB4,'Species data'!$B$4:$B$17),3))

AD = First_Num(IF(Input!AB4'="hmn",IF(Input!AH4'="Y",AA4*SQRT(Input!AG4/15), AA4*(Input!AG4/15)),IF(Input!AH4'="Y",AA4*SQRT(Input!AG4/15)*((70*AC4)/ (20*AB4)),AA4*(Input!AG4/15)*((70*AC4)/(20*AB4)))))

Appendix 3: Procedure-derived toxicity-based TEELs

Table 4: Results of statistical correlations between toxicity parameters and ERPGs

	Regression parameters			n = N (Data from all matched pairs)						n < N (Restricted ratio range data)							
N	Lim	Toxicity	Data	mean	sd	cv	df	r^2	r	Range	n	mean	sd	cv	df	r^2	r
51	E3	LD50	All	26.7	105	395	49	0.219	0.468	10 to 0.01	41	**1.29**	1.84	142	39	0.485	0.696
45	E3	LD50	Rat	13.8	42	305	43	0.231	0.481	10 to 0.01	37	**1.29**	1.82	141	35	0.496	0.704
51	E3	Log LD50	All				49	0.303	0.551	10 to 0.01	41				39	0.454	**0.674**
45	E3	Log LD50	Rat				43	0.321	0.566	10 to 0.01	37				35	0.434	**0.659**
37	E3	LDLo	All	32.9	32.9	552	35	0.004	-0.067	5 to 0.005	31	**0.75**	1.12	150	29	0.036	0.189
18	E3	LDLo	Human	2.55	6.30	247	16	0.077	0.278	5 to 0.005	16	**0.61**	1.16	192	14	0.110	0.331
37	E3	Log LDLo	All				35	0.052	0.228	5 to 0.005	31				29	0.263	**0.513**
18	E3	Log LDLo	Human				16	0.163	0.404	5 to 0.005	16				14	0.354	**0.595**
66	E3	LC50	All	772	3896	505	64	0.563	0.750	300 to 3	51	**103**	73.5	71.5	49	0.852	0.923
53	E3	LC50	Rat	841	4345	516	51	0.560	0.748	300 to 3	43	**96.4**	67.2	69.8	41	0.855	0.925
66	E3	Log LC50	All				64	0.606	0.778	300 to 3	51				49	0.876	**0.936**
53	E3	Log LC50	Rat				51	0.638	0.799	300 to 3	43				41	0.896	**0.946**
38	E3	LCLo	All	323	832	257	36	0.116	0.341	300 to 3	27	**71.2**	68.9	96.7	25	0.502	0.708
20	E3	LCLo	Human	86.9	191	220	18	5E-5	-0.007	300 to 3	15	**58.9**	72.0	122	13	0.569	0.754
38	E3	Log LCLo	All				36	0.488	0.699	300 to 3	27				25	0.801	**0.895**
20	E3	Log LCLo	Human				18	0.472	0.687	300 to 3	15				13	0.636	**0.798**
33	E2	TDLo	All	32.3	158	489	31	0.074	0.272	10 to 0.01	28	**1.4**	1.41	125	26	0.163	0.404
18	E2	TDLo	Rat	56.0	214	382	16	0.003	-0.059	10 to 0.01	14	**1.1**	1.79	162	12	0.039	0.198
33	E2	Log TDLo	All				31	0.267	0.517	10 to 0.01	28				26	0.567	**0.753**
18	E2	Log TDLo	Rat				16	0.050	0.223	10 to 0.01	14				12	0.265	**0.515**
37	E2	TCLo	All	1622	7885	486	35	0.002	-0.048	100 to 0.1	27	**14.1**	19.5	138	25	0.037	0.194
29	E2	TCLo	Human	1678	8909	531	27	0.006	0.076	100 to 0.1	24	**10.6**	14.1	134	22	0.037	0.192
37	E2	Log TCLo	All				35	0.221	0.470	100 to 0.1	27				25	0.595	**0.771**
29	E2	Log TCLo	Human				27	0.318	0.564	100 to 0.1	24				22	0.652	**0.807**

Notes:
N = Total number of data points for the parameter of interest
n = Number of data points within the stated range
E3 = ERPG-3 and E2 = ERPG-2
SD = standard deviation of the mean
CV = Coefficient of variation (= SD * 100/mean)
r^2 = Coefficient of determination
r = Correlation coefficient

For Y = mX + b
where
X = ERPG-2, ERPG-3, Log ERPG-2, or Log ERPG-3
and
Y = Stated toxicity parameter or Log of toxicity parameter

Means and CVs are on toxicity parameter to ERPG ratios.
Correlations on toxicity parameter versus ERPGs

Table 5

Adjustment factors to derive toxicity-based TEELs from human-equivalent toxicity concentration values

Species	ERPG-3				ERPG-2	
	LC_{50}	LC_{lo}	LD_{50}	LD_{lo}	TC_{lo}	TD_{lo}
Human only	-	50	-	1	10	-
Rat only	100	-	2	-	-	1
All data	100	100	2	1	15	1.5

Notes:

Factors are rounded from the mean of the restricted range human-equivalent toxicity concentration to ERPG ratios (see Table 4).

The human-equivalent toxicity concentration is divided by the appropriate adjustment factor to obtain the toxicity-based TEEL, i.e., Human data are divided by the "human only" factors for LC_{lo}, LD_{lo}, and TC_{lo}, rat data are divided by the "rat-only" factors for LC_{50}, LD_{50}, and TD_{lo}. All other human-equivalent toxicity concentration are divided by the "all data" factors.

"t-s" Worksheet

This worksheet calculates estimated TEEL-2 and TEEL-3 values from the human-equivalent concentrations derived from the listed toxicity and lethality parameters.

A	B	C	D	E	F	G	H	I	J
		LD 50				LC 50			
No.	Chemical	HLC50eq	Spec	TEEL-3 estimate		HLC50eq	Spec	TEEL-3 estimate	
		mg/m^3		mg/m^3	Orig. units	mg/m^3		mg/m^3	Orig. units
1	ERPGs	6.83E+1	r	3.41E+1	1.57E+1	9.87E+3	r	9.87E+1	4.55E+1
2	Tox data only	8.14E+2	r	4.07E+2	4.07E+2	2.27E+3	r	2.27E+1	2.27E+1
3	HT-3, tox data	7.00E+2	r	3.50E+2	8.55E+1	9.55E+4	r	9.55E+2	2.33E+2
4	No HTs, LC_{50}					9.91E+4	r	9.91E+2	9.91E+2
5	HT-2, some tox					1.03E+4	r	1.03E+2	1.03E+2

Column

A = Input!A4

B = Bring(Input!B4)

C = Bring(Tcalcs!G4)

D = Bring(Input!AH4)

E = First_Num(IF(D4="r",C4/2,C4/2))

F = First_Num(IF(LEFT(Input!F4,1)="m",E4,E4/'H-Ts min'!$C4))

G = Bring(Tcalcs!V4)

H = Bring(Input!AT4)

I = First_Num(IF(H4="r",G4/100,G4/100))

J = First_Num(IF(LEFT(Input!F4,1)="m",I4,I4/'H-Ts min'!$C4))

"t-s" Worksheet (continued)

A	B	K	L	M	N	O	P	Q	R
No.	Chemical	LD lo				LC lo			
		HLCloeq	Spec	TEEL-3 estimate		HLCloeq	Spec	TEEL-3 estimate	
		mg/m^3		mg/m^3	Orig. units	mg/m^3		mg/m^3	Orig. units
1	ERPGs	1.76E+3	chd	1.76E+3	8.13E+2	2.00E+3	hmn	4.00E+1	1.84E+1
2	Tox data only	2.10E+3	r	2.10E+3	2.10E+3				
3	HT-3, tox data	1.58E+3	r	1.58E+3	3.85E+2	5.93E+4	rb	5.93E+2	1.45E+2
4	No HTs, LC_{50}								
5	HT-2, some tox	1.75E+2	mu	1.75E+2	1.75E+2				

Column

A = Input!A4

B = Bring(Input!B4)

K = Bring(Tcalcs!L4)

L = Bring(Input!AK4)

M = First_Num(IF(Human(L4),K4/1,K4/1))

N = First_Num(IF(LEFT(Input!F4,1)="m",M4,M4/'H-Ts min'!$C4))

O = Bring(Tcalcs!Z4)

P = Bring(Input!AX4)

Q = First_Num(IF(Human(P4),O4/50,O4/100))

R = First_Num(IF(LEFT(Input!F4,1)="m",Q4,Q4/'H-Ts min'!$C4))

"t-s" Worksheet (continued)

A	B	S	T	U	V	W	X	Y	Z
No.	Chemical	TD lo				TC lo			
		HLCloeq	Spec	TEEL-2 estimate		HLCloeq	Spec	TEEL-2 estimate	
		mg/m^3		mg/m^3	Orig. units	mg/m^3		mg/m^3	Orig. units
1	ERPGs	5.69E+1	r	5.69E+1	2.62E+1	4.01E+1	hmn	4.01E+0	1.85E+0
2	Tox data only					2.12E+1	hmn	2.12E+0	2.12E+0
3	HT-3, tox data	1.73E+2	r	1.73E+2	4.24E+1	2.05E+2	hmn	2.05E+1	5.00E+0
4	No HTs, LC_{50}								
5	HT-2, some tox								

Column

A = Input!A4

B = Bring(Input!B4)

S = Bring(Tcalcs!R4)

T = Bring(Input!AN4)

U = First_Num(IF(OR(T4="r"),S4/1,S4/1.5))

V = First_Num(IF(LEFT(Input!F4,1)="m",U4,U4/'H-Ts min'!$C4))

W = Bring(Tcalcs!AD4)

X = IF(W4="","",Bring(Input!BB4))

Y = First_Num(IF(Human(X4),W4/10,W4/15))

Z = First_Num(IF(LEFT(Input!F4,1)="m",Y4,Y4/'H-Ts min'!$C4))

"Proc t-Ts" Worksheet

This worksheet selects TEEL-2 and TEEL-3 values from the "H-Ts" and "t-Ts" worksheets, using hierarchy-based values if available, followed by toxicity-based values in the order presentd unless a human (including men, woman, children and infants) toxicity parameter is available.

A	B	C	D	E	F	G	H	I	J	K	L	M
No.	Chemical	Units of Original Limits	Toxicity-derived TEEL-2s				Toxicity-derived TEEL-3s					
			Hierarchy TEEL-2	TClo	TDlo	TEEL-2	Hierarchy TEEL-3	LC50	LClo	LD50	LDlo	TEEL-3
1	ERPGs	ppm	3.50E+1	-1.85E+0	2.62E+1	3.50E+1	7.50E+1	4.55E+1	-1.84E+1	1.57E+1	-8.13E+2	7.50E+1
2	Tox data only	mg/m^3	2.12E+0		2.27E+1		4.07E+2	2.10E+3	2.27E+1			
3	HT-3, tox data	ppm	5.00E+0	3.00E+2	2.33E+2	1.45E+2	8.55E+1	3.85E+2	3.00E+2			
4	No HTs, LC_{50}	mg/m^3						9.91E+2				9.91E+2
5	HT-2, some	mg/m^3	1.00E+0			1.00E+0		1.03E+2			1.75E+2	1.03E+2

Column

A = Input!A4

B = Bring(Input!B4)

C = Bring(Input!F4)

D = Bring('H-Ts'!I4)

E = IF(OR('t-Ts'!X4="hmn",'t-Ts'!X4="wmn",'t-Ts'!X4="chd"),-1*Bring('t-Ts'!Z4),Bring('t-Ts'!Z4))

F = IF(OR('t-Ts'!T4="hmn",'t-Ts'!T4="wmn",'t-Ts'!T4="chd"),-1*Bring('t-Ts'!V4),Bring('t-Ts'!V4))

G = IF(MIN(E4:F4)<0,First_Num(D4,First_Human(E4:F4)),First_Num(D4:F4))

H = Bring('H-Ts'!J4)

I = IF(OR('t-Ts'!H4="hmn",'t-Ts'!H4="wmn",'t-Ts'!H4="chd"),-1*Bring('t-Ts'!J4),Bring('t-Ts'!J4))

J = IF(OR('t-Ts'!P4="hmn",'t-Ts'!P4="wmn",'t-Ts'!P4="chd"),-1*Bring('t-Ts'!R4),Bring('t-Ts'!R4))

K = IF(OR('t-Ts'!D4="hmn",'t-Ts'!D4="wmn",'t-Ts'!D4="chd"),-1*Bring('t-Ts'!F4),Bring('t-Ts'!F4))

L = IF(OR('t-Ts'!L4="hmn",'t-Ts'!L4="wmn",'t-Ts'!L4="chd"),-1*Bring('t-Ts'!N4),Bring('t-Ts'!N4))

M = IF(MIN(I4:L4)<0,First_Num(H4,First_Human(I4:L4)),First_Num(H4:L4))

"ProcTs" Worksheet

This worksheet selects TEEL-2 and TEEL-3 values from the "Proc t-Ts" worksheet, TEEL-0 and TEEL-1 values from the "H-Ts min" worksheet. This ensures that hierarchy-based TEELs are used if available, followed by toxicity-based values for TEEL-2 and TEEL-3. Values are rounded down to factors or multiples of ten of 1.0, 1.25, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 5.0, 6.0, and 7.5, unless the value is within 5% of the next higher number (e.g., 290 will be rounded up to 300, rather than down to 250). In the absence of either, TEELs are estimated using the mean ratios of existing ERPGs.

A	B	C	D	E	F	G
No.	Chemical	Calculated TEELs (unadjusted)				Units of original limits
		TEEL-0	TEEL-1	TEEL-2	TEEL-3	
1	ERPGs	2	10	35	75	ppm
2	Tox data only	1	3	3	20	mg/m3
3	HT-3, tox data	15	15	15	300	ppm
4	No HTs, LC_{50}	7.5	25	200	1000	mg/m3
5	HT-2, some tox	0.05	0.15	1	100	mg/m3

Column

A = Input!A4

B = Bring(Input!B4)

C = Max_Num(First_Num('H-Ts'!$G4,chem_round(First_Num('Proc t-Ts'!$G4/(T0_1*T1_2),'Proc t-Ts'!$M4/(T0_1*T1_2*T2_3),'H-Ts'!$H4/T0_1),'H-Ts'!$H4)),'H-Ts min'!D4)

D = Max_Num(First_Num('H-Ts'!$H4,chem_round(First_Num('Proc t-Ts'!$G4/T1_2,'Proc t-Ts'!$M4/(T1_2*T2_3),'H-Ts'!$I4/T1_2,'H-Ts'!$G4),'H-Ts'!$I4)),'H-Ts min'!E4)

E = Max_Num(First_Num('H-Ts'!I4,chem_round(First_Num('Proc t-Ts'!G4,'Proc t-Ts'!M4/T2_3),'H-Ts'!J4)),'H-Ts min'!F4)

F = Max_Num(First_Num('H-Ts'!J4,chem_round(First_Num('Proc t-Ts'!$M4,'Proc t-Ts'!$G4*T2_3),1E+299)),'H-Ts min'!G4)

G = Bring(Input!F4)

"Rec TEELs" Worksheet

This worksheet reduces all values with mg/m^3 units to a maximum of 500 mg/m^3, and ensures that $T_0 \leq T_1 \leq T_2 \leq T_3$

A	B	C	D	E	F	G	H
No.	Chemical	CAS Number	Recommended Temporary Emergency Exposure Limits				Units of original limits
			TEEL-0	TEEL-1	TEEL-2	TEEL-3	
1	ERPGs	00107-13-1	2	10	35	75	ppm
2	Tox data only	00105-60-2	1	3	3	20	mg/m3
3	HT-3, tox data	00140-88-5	15	15	15	300	ppm
4	No HTs, LC_{50}	28182-81-2	7.5	20	200	500	mg/m3
5	HT-2, some tox	01310-65-2	0.05	0.15	1	100	mg/m3

Column

A = Input!A4

B = Bring(Input!B4)

C = Bring(Input!C4)

D = MgLimit(MIN_Num(ProcTs!C4:$F4),H4)

E = MgLimit(MIN_Num(ProcTs!D4:$F4),H4)

F = MgLimit(MIN_Num(ProcTs!E4:F4),H4)

G = MgLimit(First_Num(ProcTs!F4),H4)

H = Bring(Input!F4)

Appendix 4: Macros used in Excel Workbook Calculations

1 *Function to Pick the First Number In List*

```
Function First_Num(Num1 As Variant, Optional Num2 As Variant, _
   Optional Num3 As Variant, Optional Num4 As Variant, _
   Optional Num5 As Variant, Optional Num6 As Variant, _
   Optional Num7 As Variant, Optional Num8 As Variant, _
   Optional Num9 As Variant, Optional Num10 As Variant, _
   Optional Num11 As Variant, Optional Num12 As Variant, _
   Optional Num13 As Variant, Optional Num14 As Variant, _
   Optional Num15 As Variant, Optional Num16 As Variant, _
   Optional Num17 As Variant, Optional Num18 As Variant, _
   Optional Num19 As Variant, Optional Num20 As Variant _
   ) As Variant

   Starts at Num1. Note: all num's may be ranges.
     Returns Null if no number or "0" value found.

   First_Num = ""

   First_Num = Num_Range(Num1)
   If (Not (First_Num = "") Or IsMissing(Num2)) Then Exit Function
   First_Num = Num_Range(Num2)
   If (Not (First_Num = "") Or IsMissing(Num3)) Then Exit Function
   First_Num = Num_Range(Num3)
   If (Not (First_Num = "") Or IsMissing(Num4)) Then Exit Function
   First_Num = Num_Range(Num4)
   If (Not (First_Num = "") Or IsMissing(Num5)) Then Exit Function
   First_Num = Num_Range(Num5)
   If (Not (First_Num = "") Or IsMissing(Num6)) Then Exit Function
   First_Num = Num_Range(Num6)
   If (Not (First_Num = "") Or IsMissing(Num7)) Then Exit Function
   First_Num = Num_Range(Num7)
   If (Not (First_Num = "") Or IsMissing(Num8)) Then Exit Function
   First_Num = Num_Range(Num8)
   If (Not (First_Num = "") Or IsMissing(Num9)) Then Exit Function
   First_Num = Num_Range(Num9)
   If (Not (First_Num = "") Or IsMissing(Num10)) Then Exit Function
   First_Num = Num_Range(Num10)
   If (Not (First_Num = "") Or IsMissing(Num11)) Then Exit Function
   First_Num = Num_Range(Num11)
   If (Not (First_Num = "") Or IsMissing(Num12)) Then Exit Function
   First_Num = Num_Range(Num12)
   If (Not (First_Num = "") Or IsMissing(Num13)) Then Exit Function
   First_Num = Num_Range(Num13)
   If (Not (First_Num = "") Or IsMissing(Num14)) Then Exit Function
   First_Num = Num_Range(Num14)
   If (IsMissing(Num15)) Then Exit Function
   First_Num = Num_Range(Num15)
   If (Not (First_Num = "") Or IsMissing(Num16)) Then Exit Function
   First_Num = Num_Range(Num16)
```

```
   If (Not (First_Num = "") Or IsMissing(Num17)) Then Exit Function
   First_Num = Num_Range(Num17)
   If (Not (First_Num = "") Or IsMissing(Num18)) Then Exit Function
   First_Num = Num_Range(Num18)
   If (Not (First_Num = "") Or IsMissing(Num19)) Then Exit Function
   First_Num = Num_Range(Num19)
   If (Not (First_Num = "") Or IsMissing(Num20)) Then Exit Function
   First_Num = Num_Range(Num20)

End Function
```

2 Function to use another cells "value" even if null

```
Function Bring(Num1 As Variant) As Variant
   Starts at Num1
      Returns False if no number or "0" value found.
  Temp = holds temporary first word

   temp = ""
   If (Not IsMissing(Num1)) Then
      If (IsNumeric(Num1)) Then
        If (Num1 <> 0) Then temp = Num1
      Else
         temp = Num1
      End If
   End If

   Bring = temp

End Function
```

3 Function to Find Minimum of Numbers Ignoring Non-Numeric and Empty or 0 Cells

```
Function Min_Num(Num1 As Variant, Optional Num2 As Variant, _
   Optional Num3 As Variant, Optional Num4 As Variant, _
   Optional Num5 As Variant, Optional Num6 As Variant, _
   Optional Num7 As Variant, Optional Num8 As Variant, _
   Optional Num9 As Variant, Optional Num10 As Variant, _
   Optional Num11 As Variant, Optional Num12 As Variant, _
   Optional Num13 As Variant, Optional Num14 As Variant, _
   Optional Num15 As Variant, Optional Num16 As Variant, _
   Optional Num17 As Variant, Optional Num18 As Variant, _
   Optional Num19 As Variant, Optional Num20 As Variant _
   ) As Variant

   Starts at Num1 and assumes all are numbers >= 0, and at least one number is present
      Returns an "1E+300" if no number found.
   MINT - Temporary Minimum

Dim MINT As Double
   MINT = 1E+300
```

Begin Testing Each Variable

```
  MINT = Application.Min(Extreme_Range(Num1, False), MINT)
  If (IsMissing(Num2)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num2, False), MINT)
  If (IsMissing(Num3)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num3, False), MINT)
  If (IsMissing(Num4)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num4, False), MINT)
  If (IsMissing(Num5)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num5, False), MINT)
  If (IsMissing(Num6)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num6, False), MINT)
  If (IsMissing(Num7)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num7, False), MINT)
  If (IsMissing(Num8)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num8, False), MINT)
  If (IsMissing(Num9)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num9, False), MINT)
  If (IsMissing(Num10)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num10, False), MINT)
  If (IsMissing(Num11)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num11, False), MINT)
  If (IsMissing(Num12)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num12, False), MINT)
  If (IsMissing(Num13)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num13, False), MINT)
  If (IsMissing(Num14)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num14, False), MINT)
  If (IsMissing(Num15)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num15, False), MINT)
  If (IsMissing(Num16)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num16, False), MINT)
  If (IsMissing(Num17)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num17, False), MINT)
  If (IsMissing(Num18)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num18, False), MINT)
  If (IsMissing(Num19)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num19, False), MINT)
  If (IsMissing(Num20)) Then GoTo 10
  MINT = Application.Min(Extreme_Range(Num20, False), MINT)
10 Min_Num = MINT
  If (MINT = 1E+300) Then Min_Num = ""
End Function '
```

4 Function to Find Maximum of Numbers Ignoring Non-Numeric and Empty or 0 Cells

```
Function Max_Num(Num1 As Variant, Optional Num2 As Variant, _
  Optional Num3 As Variant, Optional Num4 As Variant, _
  Optional Num5 As Variant, Optional Num6 As Variant, _
  Optional Num7 As Variant, Optional Num8 As Variant, _
  Optional Num9 As Variant, Optional Num10 As Variant, _
  Optional Num11 As Variant, Optional Num12 As Variant, _
```

```
Optional Num13 As Variant, Optional Num14 As Variant, _
Optional Num15 As Variant, Optional Num16 As Variant, _
Optional Num17 As Variant, Optional Num18 As Variant, _
Optional Num19 As Variant, Optional Num20 As Variant _
) As Variant
```

Starts at Num1 and assumes all are numbers >= 0, and at least one number is present
Returns an "0" if no number found. MAXT - Temporary Minimum

```
Dim MAXT As Double
MAXT = 0
```

Begin Testing Each Variable

```
MAXT = Application.Max(Extreme_Range(Num1, True), MAXT)
If (IsMissing(Num2)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num2, True), MAXT)
If (IsMissing(Num3)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num3, True), MAXT)
If (IsMissing(Num4)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num4, True), MAXT)
If (IsMissing(Num5)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num5, True), MAXT)
If (IsMissing(Num6)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num6, True), MAXT)
If (IsMissing(Num7)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num7, True), MAXT)
If (IsMissing(Num8)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num8, True), MAXT)
If (IsMissing(Num9)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num9, True), MAXT)
If (IsMissing(Num10)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num10, True), MAXT)
If (IsMissing(Num11)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num11, True), MAXT)
If (IsMissing(Num12)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num12, True), MAXT)
If (IsMissing(Num13)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num13, True), MAXT)
If (IsMissing(Num14)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num14, True), MAXT)
If (IsMissing(Num15)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num15, True), MAXT)
If (IsMissing(Num16)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num16, True), MAXT)
If (IsMissing(Num17)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num17, True), MAXT)
If (IsMissing(Num18)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num18, True), MAXT)
If (IsMissing(Num19)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num19, True), MAXT)
If (IsMissing(Num20)) Then GoTo 10
MAXT = Application.Max(Extreme_Range(Num20, True), MAXT)
```

```
10 Max_Num = MAXT
   If (MAXT = 0) Then Max_Num = ""

End Function
```

5 Checks a Given Range to see if it contains a number

```
Function Num_Range(MyRange As Variant) As Variant

   Check Range for Numbers
     Return Null if no numbers

  Cell is temporary Value
   Dim Cell As Variant

   Num_Range = ""

   If (Not (VarType(MyRange) = 8204)) Then
      If (IsNumeric(MyRange)) Then
        If (Not IsEmpty(MyRange)) Then
          If (Not (MyRange = 0)) Then
             Num_Range = MyRange
          End If
        End If
      End If
   Else
      For Each Cell In MyRange

         If (IsNumeric(Cell)) Then
            If (Not IsEmpty(Cell)) Then
              If (Not (Cell = 0)) Then
                Num_Range = Cell
                Exit For
              End If
            End If
         End If

      Next Cell
   End If
End Function
```

6 Checks a Given Range to the minimum number ignoring non-numeric and empty cells

```
Function Extreme_Range(MyRange As Variant, Big As Boolean) As Variant

   Check Range for Minimum or maximum (if Big True) Number
     Return 1E+300 for min or 0 for max if no numbers

  Cell is temporary Value
  Dim Cell As Variant

  If (Big) Then
```

```
    Extreme_Range = 0
  Else
    Extreme_Range = 1E+300
  End If

  If (Not (VarType(MyRange) = 8204)) Then
    If (IsNumeric(MyRange) And Not IsEmpty(MyRange)) Then Extreme_Range = MyRange
  Else
    For Each Cell In MyRange

      If (IsNumeric(Cell) And Not IsEmpty(Cell)) Then
        If (Big) Then
          Extreme_Range = Application.Max(Extreme_Range, Cell)
        Else
          Extreme_Range = Application.Min(Extreme_Range, Cell)
          End If
      End If

    Next Cell
  End If

End Function
```

7 Function to Pick the First Human Based Value in List

```
Function First_Human(MyRange As Variant) As Variant

  'MyRange must be a range or cell reference, not a number.   Returns only human based values.
    'If NO human values found, returns first number or "" if no numbers present.
  'MyRange is the range containing all present arguments
  'Treats Negative Numbers as ""

  First_Human = ""
  If (Not (VarType(MyRange) = 8204)) Then
    If (IsNumeric(MyRange) And Not IsEmpty(MyRange)) Then _
          First_Human = Abs(MyRange)
  Else

    For Each Cell In MyRange
      If (IsNumeric(Cell) And Not IsEmpty(Cell)) Then
        If (Cell > 0) Then
          Cell = ""
        Else
          First_Human = Abs(Cell)
          Exit Function
        End If
      End If

    Next Cell

  End If
End Function
```

8 *Function to Return TRUE If species Is Human*

```
Function Human(Species As Variant) As Boolean

  Species is the species source for given data.
  Returns FALSE except for "hmn", "wmn", or "chd"

  Select Case Species
    Case "hmn", "wmn", "chd"
      Human = True
    Case Else
      Human = False
  End Select

End Function
```

9 *Function to Limit Num to 500 If Units are mg/cm3*

```
Function MgLimit(num As Variant, units As Variant) As Variant

  num is the to be limited to 500 if in mg units
  units - units of num.  Either "mg/cm3" or "ppm"

  If (Left(units, 1) = "m" And IsNumeric(num)) Then
    MgLimit = Application.Min(num, 500)
  Else
    MgLimit = num
  End If

End Function
```

10 *Chemical Procedure Rounding Function*

```
Function Chem_Round(num As Variant, HTnum As Variant) As Variant

    'Scheme used for each decade:

   1  - <1.25  = 1.0
   1.25 - <1.5  = 1.25
   1.25 - <2    = 1.5
   2  - <2.5   = 2.0
   2.5 - <3.0   = 2.5
   3  - <3.5   = 3.0
   3.5 - <4     = 3.5
   4  - <5     = 4.0
   5  - <6     = 5.0
   6  - <7.5   = 6.0
   7.5 -       = 7.5

   Htnum is next higher Hierarchial TEEL Value (must not exceed)
   num is the Proc TEELs value
   lnum base 10 log of the number
```

sign indicates the sign of the log10 of the number 0- positive or 1 - negativeioninum integer portion of log of number
dec decimal portion of log (or 1 - decimal portion if negative)
tnum number between 0 and 10 based on decimal portion of log, then used to store final answer
xPer if a number is within xPer of next higher number it is rounded up. All others are rounded down.

```
Dim lnum As Double, dec As Double, tnum As Double, xPer As Double
Dim inum As Integer, sign As Integer

  Rounding up percentage

xPer = 5#

  If (IsNumeric(num)) Then

  lnum = Log10(num * (1 + xPer / 100))
  sign = 0
  If (lnum < 0) Then sign = 1
  inum = Fix(lnum)
  dec = lnum - inum + sign
  tnum = 10 ^ dec
  Select Case tnum
    Case 1 To 1.24999999999
      tnum = 1
    Case 1.2499999999 To 1.499999999
      tnum = 1.25
    Case 1.4999999999 To 1.99999999
      tnum = 1.5
    Case 1.99999999 To 2.4999999999
      tnum = 2
    Case 2.4999999999 To 2.999999999
      tnum = 2.5
    Case 2.999999999 To 3.4999999999
      tnum = 3
    Case 3.4999999999 To 3.999999999
      tnum = 3.5
    Case 3.999999999 To 4.999999999
      tnum = 4
    Case 4.999999999 To 5.999999999
      tnum = 5
    Case 5.999999999 To 7.4999999999
      tnum = 6
    Case Else
      tnum = 7.5
  End Select
  dec = Log10(tnum) - sign
  tnum = 10 ^ (inum + dec)
  Chem_Round = Application.Min(tnum, HTnum)
Else
  Chem_Round = num
End If

End Function
```

```
Static Function Log10(X)
   Log10 = Log(X) / Log(10#)
End Function
```