A.I.S.E.

REACH Exposure Assessment Consumer Tool

(REACT)

USER MANUAL

December 2009

1. INTRODUCTION

The A.I.S.E. REACT Consumer Tool allows quantitative estimation of systemic consumer exposures to substances that are present in preparations used by consumers. The tool calculates substance exposure via inhalation, dermal, and oral routes separately and also provides a summation of all the relevant exposure routes. The tool can also calculate Risk Characterization Ratios (RCR) for the different exposure routes separately and for the overall exposure. RCRs are only calculated provided that substance specific hazard data values (e.g., DNELs) are entered in the User Input worksheet by the user. The tool does not provide hazard data values and these need to be defined by the user.

This User Manual provides guidance for working with the A.I.S.E. REACT Consumer Tool.

2. GETTING STARTED

The tool contains eight worksheets, each of which can be navigated via the tabs at the bottom of the tool. Table 1 below summarises these worksheets and explains the information provided within each sheet.

Table 1. Worksheets contained in the A.I.S.E. REACT Consumer Tool

Worksheet Name	Content
User Input	User-specific entries are entered and products are selected to generate exposure estimates and risk characterization ratios (RCR).
Results	Displays exposure estimates and RCRs for product categories and subcategories.
Dermal	Displays dermal exposure estimates and RCRs for the product subcategories and shows the algorithms and parameters used to calculate them.
Inhalation	Displays inhalation exposure estimates and RCRs for the product subcategories and shows the algorithms and parameters used to calculate them.
Oral	Displays oral exposure estimates and RCRs for the product subcategories and shows the algorithms and parameters used to calculate them.
Def_AISE H&P2009a	Shows the A.I.S.E./HERA 2009 Table of Habits and Practices for consumer products in Western Europe. From this table, the default exposure parameters were retrieved.
Def_AISE H&P2009b	Lists additional data required to estimate adult exposure to air freshener ingredients. From this table, defaults for air freshener consumer exposure calculation were retrieved.
Def_TRA2009	Lists subpopulations specific (child, adult) default parameters used to estimate exposure. This is the same list as used in the ECETOC TRA Consumer Tool.

By default, upon opening, the "User Input" worksheet is shown because it is where all User-required entries are made. This worksheet contains colour-coded cells that identify inputs necessary for running the tool. Yellow cells are for information that must be entered before the tool can generate results. Blue cells are optional – they allow you to record substance specifics (substance name, CAS#, data source of reference values) and to record any comments you may have. Changes can be made only in the yellow and blue cells. All other cells are locked to protect equations from being unintentionally deleted and to prevent Users from over-riding default parameters set in the tool.

3. USING THE TOOL

Exposure estimates and RCRs can be calculated for a product category or for individual product subcategories. When a product category is selected, the product giving worst case exposure within this category will be displayed.

All User-required entries outlined below (step 1 to 4) need to be made in the "User Input" worksheet.

STEP1
In the "Assessment Identification" table, fill in the substance name and CAS#. You can also record the date and any comments you may have.

ASSESSMENT IDENTIFICATION			
Substance name			
CAS number			
Date			
Version			
Comments			

STEP2
In the "Hazard Data values" table, enter reference value(s) for the substance being evaluated (for example, an oral DNEL). Note that the units are fixed as mg/kg/day.
A reference value is only needed for the route(s) (dermal, oral, inhalation) that are relevant to the selected product categories / subcategories.

HAZARD DATA VALUES			
Reference value in mg/kg/day		Data source:	
Dermal	1		
Oral			
Inhalation	0.01		

STEP3
For dermal exposure, select and enter data in the table "Ingredient Specific Parameter Values (only for dermal exposure calculations)". This table only has to be filled in when dermal exposure is relevant for the selected product categories / subcategories. Using the drop down, the User can then fill cell E21 by selecting either Kp or F4 for the direct skin contact calculation. For cell E22, the User can indicate the availability of Sdep for the indirect skin contact calculation by selecting either yes or no. Numerical values can be entered in cells E23 and E25 depending on the previous choices. A value for F4 in cell E24 is always needed for indirect skin contact calculation. If a value for F4 is not specified by the User, a default conservative value of 1 (= 100%) will be used.

INGREDIENT SPECIFIC PARAMETER VALUES (ONLY FOR DERMAL EXPOSURE CALCULATIONS)	
	Select:
For direct skin contact: Is exposure based on permeation coefficient (Kp) or weight fraction absorbed through skin (F4)?	F4
For indirect skin contact: Is amount of substance deposited on frabric (Sdep) available or not?	no
Permeation coefficient, Kp (cm.hour-1)	
Weight fraction absorbed through skin, F4 (-) (mandatory for indirect skin contact calculation)*	1
Amount of substance deposited on fabric, Sdep (mg.cm-2)	

STEP4
In the "Exposure Assessment" table, select the product categories/subcategories for which an exposure estimate and an RCR are needed.

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For relevant product categories, put a "√"in column C for the respective product category in column D. Enter F1 and F7, if relevant, in column F and G.
For relevant product subcategories, put a "√" in column C for the respective product subcategory in column E. Again, enter F1 and F7, if relevant, in column F and G.
If no value for F7 is entered, a default conservative value of 1 (=100 %) will be used.

Explanation of F1 and F7:
The value F1 in column F is termed "ingredient fraction by weight" meaning a value of ≤1 can be entered.
The value F7 in column G is termed "fraction respirable particles" and again is expressed as a fraction where 1.0 = 100%.

EXPOSURE ASSESSMENT				
		Exposure route(s):	All	Inhalation
Select Use (more than one is possible)	AISE Product Category	AISE Product Subcategory	F1 Ingredient fraction by weight (-)	F7 Fraction respirable particles (-)*
	LAUNDRY REGULAR (AISE C1, PC35)	LAUNDRY REGULAR		-
		Powder		-
		Liquid		-
☑	LAUNDRY COMPACT (AISE C2, PC35)	LAUNDRY COMPACT	0.1	-
		Powder		-
		Liquid/gel		-
		Tablet		-
	FABRIC CONDITIONERS (AISE C3, PC35)	FABRIC CONDITIONERS		-
		Liquid Regular		-
		Liquid Concentrate		-
	LAUNDRY ADDITIVES (AISE C4, PC35)	LAUNDRY ADDITIVES		-
		Powder Bleach		-
		Liquid Bleach (ml)		-
		Tablet		-
	HAND DISHWASHING (AISE C5, PC35)	HAND DISHWASHING		-
☑		Liquid Regular (a)	0.15	-
		Liquid Concentrate (a)		-
	MACHINE DISHWASHING (AISE C6, PC35)	MACHINE DISHWASHING		-
		Powder		-
		Liquid		-
		Tablet		-
	SURFACE CLEANERS (AISE C7, PC35)	SURFACE CLEANERS		
		Liquid (a)		-
		Powder (a)		-
		Gel (neat)		-
☑		Spray (neat)	0.05	0.5
	TOILET CLEANERS (AISE C8, PC35) (**)	TOILET CLEANERS	-	-
		Powder	-	-

4. VIEWING RESULTS

The second work sheet or tab is named "Results". Once the User Input sheet has been completed, click on the Results tab to view the results of exposure estimates and RCRs for both product categories and subcategories (see two results tables below).
Rows for the product categories/subcategories selected in the User Input worksheet are highlighted in green. Risk characterization ratios exceeding 1 are displayed in red.
If no reference value or other ingredient specific parameter value has been entered when those values are needed, the error message "no data" will be displayed, prompting the User to enter the necessary values in the User Input worksheet.

The total exposure in column G is the sum of the dermal, oral, and inhalation exposure. The overall RCR in column K is the total exposure divided by the worst-case relevant reference value entered in the User Input worksheet.

OUTPUT BY PRODUCT CATEGORY

AISE Product Category	Dermal exposure	Inhalation exposure	Oral exposure	Total exposure	Dermal RCR	Inhalation RCR	Oral RCR	Overall RCR
	mg/kg/day	mg/kg/day	mg/kg/day	mg/kg/day	-	-	-	-
LAUNDRY REGULAR (AISE C1, PC35)								
LAUNDRY COMPACT (AISE C2, PC35)	7.63E+00	-	-	7.63E+00	7.63E+00	-	-	7.63E+00
FABRIC CONDITIONERS (AISE C3, PC35)								
LAUNDRY ADDITIVES (AISE C4, PC35)								
HAND DISHWASHING (AISE C5, PC35)								
MACHINE DISHWASHING (AISE C6, PC35)								
SURFACE CLEANERS (AISE C7, PC35)								
TOILET CLEANERS (AISE C8, PC35)								
LAUNDRY AIDS (AISE C12, PC35)								
INSECTICIDES AND REPELLANTS (**)								
REPELLANTS (**)								
WATER SOFTENERS (AISE C9, PC35) (**)								
FURNITURE, FLOOR & LEATHER CARE								
WIPES (AISE C15, PC35)								
DRAIN PRODUCTS (AISE C13, PC35) (**)								
AIR FRESHENERS AEROSOL (AISE C17, PC3)								
AIR FRESHENERS NON-AEROSOL (AISE C18, PC3)								
OVEN CLEANERS (AISE C10, PC35) (**)								
CARPET CLEANERS (AISE C11, PC35) (**)								
DESCALERS (AISE C14, PC35) (**)								

OUTPUT BY PRODUCT SUBCATEGORY

AISE Product Category	AISE Product Subcategory	Dermal exposure	Inhalation exposure	Oral exposure	Total exposure	Dermal RCR	Inhalation RCR	Oral RCR	Overall RCR
		mg/kg/day	mg/kg/day	mg/kg/day	mg/kg/day	-	-	-	-
LAUNDRY REGULAR (AISE C1, PC35)	LAUNDRY REGULAR								
	Powder								
	Liquid								
LAUNDRY COMPACT (AISE C2, PC35)	LAUNDRY COMPACT								
	Powder								
	Liquid/gel								
	Tablet								
FABRIC CONDITIONERS (AISE C3, PC35)	FABRIC CONDITIONERS								
	Liquid Regular								
	Liquid Concentrate								
LAUNDRY ADDITIVES (AISE C4, PC35)	LAUNDRY ADDITIVES								
	Powder Bleach								
	Liquid Bleach (ml)								
	Tablet								
HAND DISHWASHING (AISE C5, PC35)	HAND DISHWASHING								
	Liquid Regular (a)	1.56E-01	-	7.43E-04	1.57E-01	1.56E-01	-	no data	no data
	Liquid Concentrate (a)								
MACHINE DISHWASHING (AISE C6, PC35)	MACHINE DISHWASHING								
	Powder								
	Liquid								
	Tablet								
SURFACE CLEANERS (AISE C7, PC35)	SURFACE CLEANERS								
	Liquid (a)								
	Powder (a)								
	Gel (neat)								
	Spray (neat)	7.15E+00	3.01E-02	-	7.18E+00	7.15E+00	3.01E+00	-	7.18E+02

To view the algorithms and parameters used to calculate the route-specific exposure estimates, select either the "Dermal, Inhalation, or Oral" tab. Again, the product categories/subcategories selected in the User Input worksheet are highlighted in green.

DERMAL

Product category (from AISE H&P table)	Exposures, dermal, SYSTEMIC only	Algorithms	F1 - Ingredient fraction by weight	C - Concentration in wash solution	Kp - Permeation coefficient	t - Duration of exposure	Sder - Dermal surface area	n - Product use frequency
			fraction	mg/cm³	cm/hour	hours	cm²	tasks/day
LAUNDRY REGULAR (AISE C1, PC35)								
Powder	Direct skin contact handwash laundry	Expsys = F1 x C x Kp x t x Sder x n / BW	no data	10	no data	0.167	2082.5	2.6
	Direct skin contact pretreatment laundry	Expsys = F1 x C x Kp x t x Sder x n / BW	no data	600	no data	0.167	857.5	0.50
	Indirect skin contact clothes wearing	Expsys = F1 x (M x (F'/W) x FD x FL) x Sder x F2 x F3 x F4 / BW	no data	-	-	-	14315	-
	Total dermal exposure							
Liquid	Direct skin contact handwash laundry	Expsys = F1 x C x Kp x t x Sder x n / BW	no data	10	no data	0.167	2082.5	1.4
	Direct skin contact pretreatment laundry	Expsys = F1 x C x Kp x t x Sder x n / BW	no data	1000	no data	0.167	857.5	0.5
	Indirect skin contact clothes wearing	Expsys = F1 x (M x (F'/W) x FD x FL) x Sder x F2 x F3 x F4 / BW	no data	-	-	-	14315	-
	Total dermal exposure							
LAUNDRY COMPACT (AISE C2, PC35)								

INHALATION

Product category (from AISE H&P table)	Exposures, inhalation, SYSTEMIC only	Algorithms	F1 - Ingredient fraction by weight	C' - Total mass sprayed per use	C" - Room volume	Qinh - Breathing inhalation rate	T - Duration of exposure	n - Product use frequency	F7 - Fraction of respirable particles
			fraction	mg/task	m³	m³/h	hours	tasks/day	fraction
SURFACE CLEANERS (AISE C7, PC35)									
Spray (neat)	Inhalation during spraying	Exp_{sys} = (F1 x (C'/C") x Qinh x T x n x F7 x F8 x F9) / BW	no data	30000	15	1.08	0.167	1	1
LAUNDRY AIDS (AISE C12, PC35)									
Ironing Aids - Spray	Inhalation during spraying	Exp_{sys} = (F1 x (C'/C") x Qinh x T x n x F7 x F8 x F9) / BW	no data	20000	20	1.08	1	0.71	1
FURNITURE, FLOOR & LEATHER CARE MAINTENANCE PRODUCTS (AISE C20, PC31)									
Spray	Inhalation during spraying	Exp_{sys} = (F1 x (C'/C") x Qinh x T x n x F7 x F8 x F9) / BW	no data	60000	58	1.08	1	0.43	1
AIR FRESHENERS AEROSOL (AISE C17, PC3)									
Aerosol i) aqueous	Inhalation during use	Exp_{sys} = (Q$_{inh}$ * T * TWA BAMA) / BW	no data	8400	2.5	0.54	0.25	1	-
Aerosol i) non-queous	Inhalation during use	Exp_{sys} = (Q$_{inh}$ * T * TWA BAMA) / BW	no data	5400	2.5	0.54	0.25	1	-
AIR FRESHENERS NON-AEROSOL (AISE C18, PC3)									
Perfume in/on solid substrate	Inhalation during use	Exp_{sys} = (Q$_{inh}$ * T * TWA BAMA) / BW	no data	1.74	2.5	0.54	0.25	1	-
Diffusers (heated + electrical)	Inhalation during use	Exp_{sys} = (Q$_{inh}$ * T * TWA BAMA) / BW	no data	0.72	58	0.54	4	1	-

ORAL

Product category (from AISE H&P table)	Exposures, oral, SYSTEMIC only	Algorithms	F1 - Ingredient fraction by weight	C - Concentration in product	Ta - Amount of water left on dishes after rinsing	Sa - area of dishes in daily contact with food	BW - Body weight	Exposure	Unit	Risk Characterization Ratio
			fraction	mg/ml	ml/cm²	cm²	kg	mg/kg/day	mg/kg/day	-
HAND DISHWASHING (AISE C5, PC35)										
Liquid Regular (a)	Oral - Indirect exposure residues	Exp_{sys} = F1 x C x Ta x Sa / BW	no data	1	5.50E-05	5400	60		mg/kg/day	
Liquid Concentrate (a)	Oral - Indirect exposure residues	Exp_{sys} = F1 x C x Ta x Sa / BW	no data	1	5.50E-05	5400	60		mg/kg/day	
MACHINE DISHWASHING (AISE C6, PC35)										
Powder	Oral - Indirect exposure residues	Exp_{sys} = F1 x C x Ta x Sa / BW	no data	1	5.50E-05	5400	60		mg/kg/day	
Liquid	Oral - Indirect exposure residues	Exp_{sys} = F1 x C x Ta x Sa / BW	no data	1	5.50E-05	5400	60		mg/kg/day	
Tablet	Oral - Indirect exposure residues	Exp_{sys} = F1 x C x Ta x Sa / BW	no data	1	5.50E-05	5400	60		mg/kg/day	

5. VIEWING DEFAULT PARAMETERS

Default parameters used in the exposure estimate calculations are listed in the "Def_AISE H&P2009a", the "Def_AISE H&P2009b", and the "Def_TRA2009" worksheets. These worksheets are for information only and are therefore protected and cannot be changed by the User. Data that can be overridden can be done only in the User Input worksheet.

6. SOME ADDITIONAL INFORMATION

a. Exposure Calculation for Air Fresheners
Calculation of air concentrations for inhalation exposure to Air Fresheners is performed using the (British Aerosols Manufacturers Association) BAMA Indoor Air Model © BAMA 2008
[http://www.bama.co.uk/regulatory]

b. Use of Permeation Coefficient (Kp) or Weight Fraction Absorbed Through Skin (F4) and Derivation of Dermal RCRs

When deriving a dermal RCR, care needs to be taken that a dermal exposure calculation in which the dermal absorption has been factored in (either using Kp or F4) is compared to a "systemic" hazard data value. It must not be compared to an external dose hazard data value obtained from a dermal toxicity study (a study where the animals were dosed by the dermal route).