



ES Modifier IT-tool for formulators

NVvA

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- 2) Introduction of the ES Modifier
- 3) Demonstration with an example
- 4) Agenda 2010

Producent

E-SDS

E-SDS

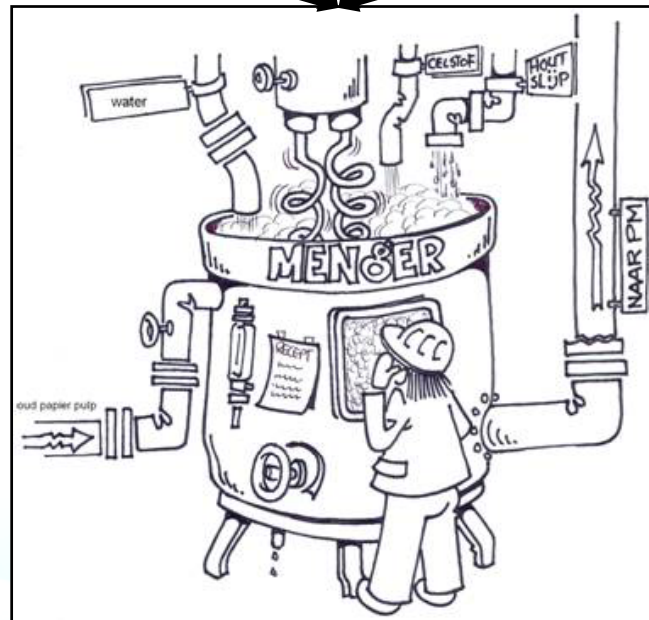
E-SDS

E-SDS

E-SDS

E-SDS

Formuleerder



Eindgebruiker

E-SDS

Background

- Issue of ES for preparations was discussed as being a key issue early in the guidance development
- Modifying/ scaling of Exposure Scenarios (ES) was identified as a must early in the discussions (Arona network)

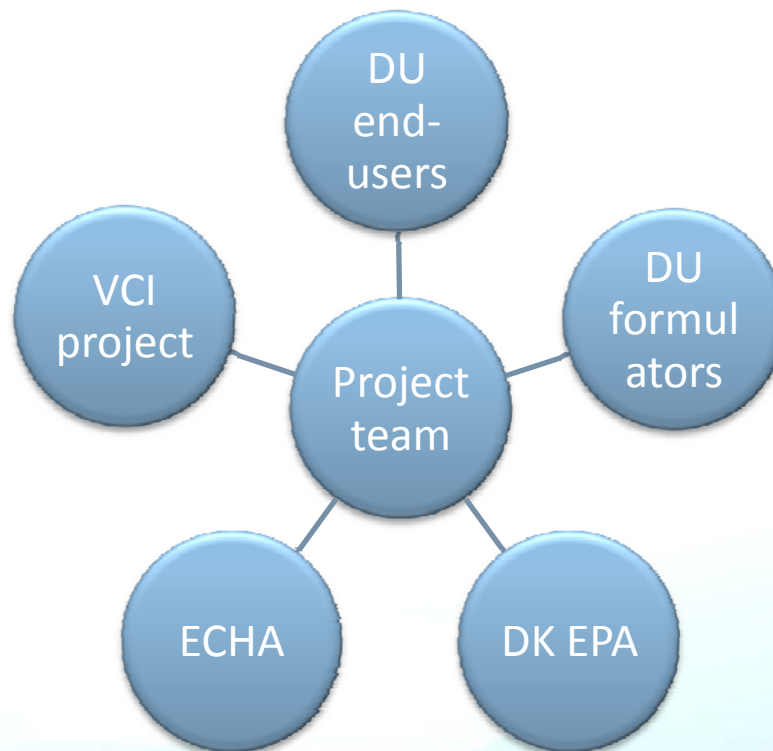
ES Modifier – Objectives

- Development of a user friendly IT tool to support
 - end users in checking and modifying suppliers ES to fit own conditions
 - formulators in preparing ES for preparations
 - Support preparation of DU CSR

Assumptions:

- Simplicity is a pre-condition for success among end users
- However, flexibility is needed from a formulators perspective

Project organisation



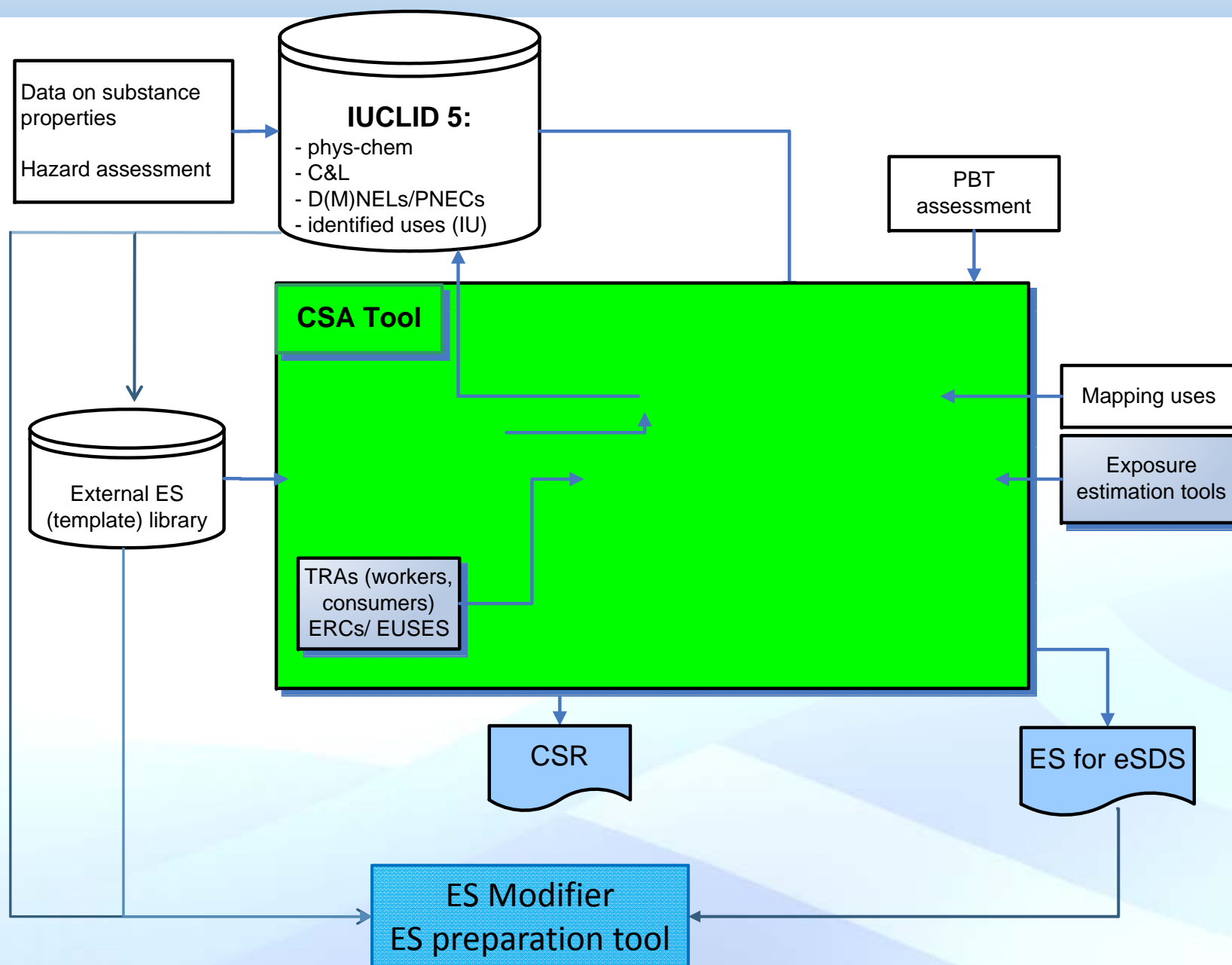
Project team

Confederation of Danish Industry

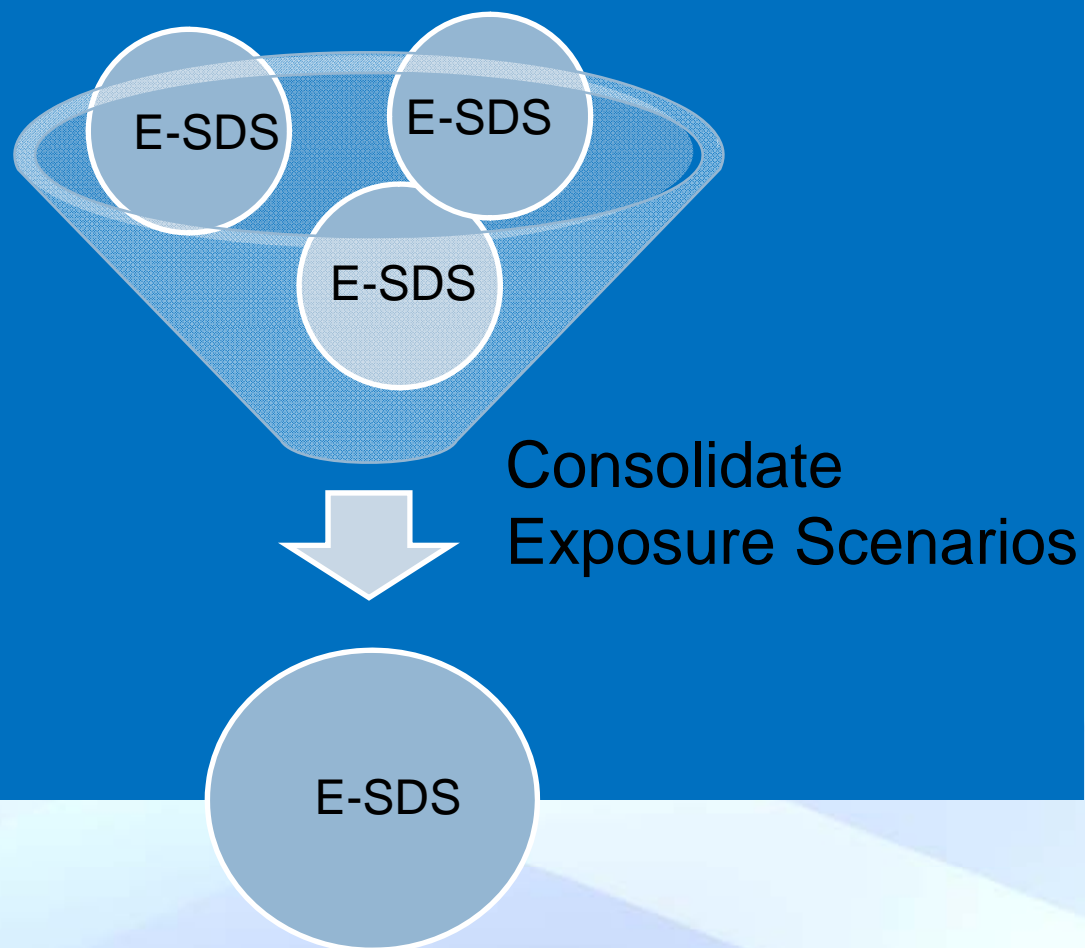
DHI
(DHI Shanghai – programming)

TNO

CSA and the role ES Modifier



ES Modifier



Consolidate exposure scenarios

- For each exposure route identify the lead substance (critical component)
 - DPD+ = Dangerous Preparation Directive + considering volatility
 - Must not be applied for Carc1, Carc2, Mut1, Mut2, Rep1, Rep2, respiratory sensitizers, and PBT/vPvB substances
- For each exposure route extract the OC/RMM for the lead substance from the ES (if available). If not check the SDS.
- Combine all OC/RMMs for the various exposure routes

Some basic features of ES Modifier

- Stand alone application
- Flexible inter-phase to IUCLID and CHESAR via XML
- Integrate exposure models in line with guidance

Default :

- ECETOC TRA and EUSES

Other models (will be) included:

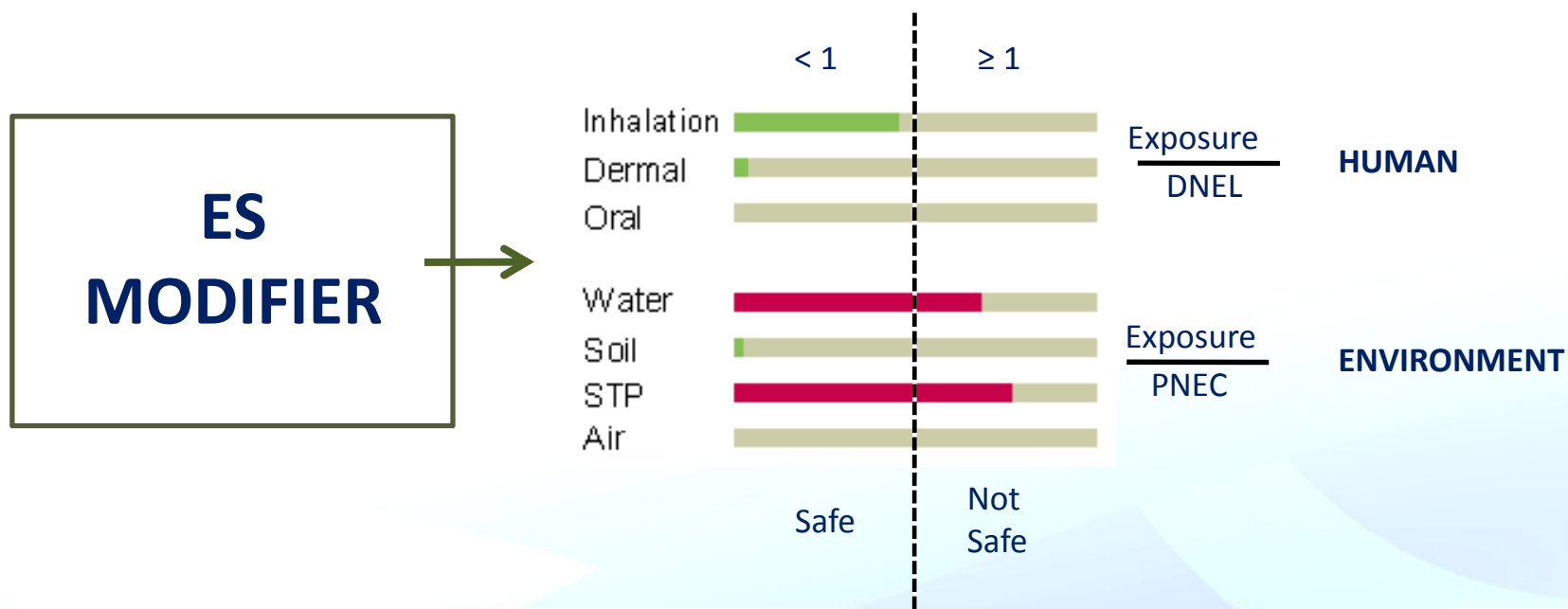
- Stoffenmanager; RISKOFDERM; COSHH-BAUA ; ART

- Inter-phase with ERM/ SDS systems?

Key OUTPUT: Calculation of RCR

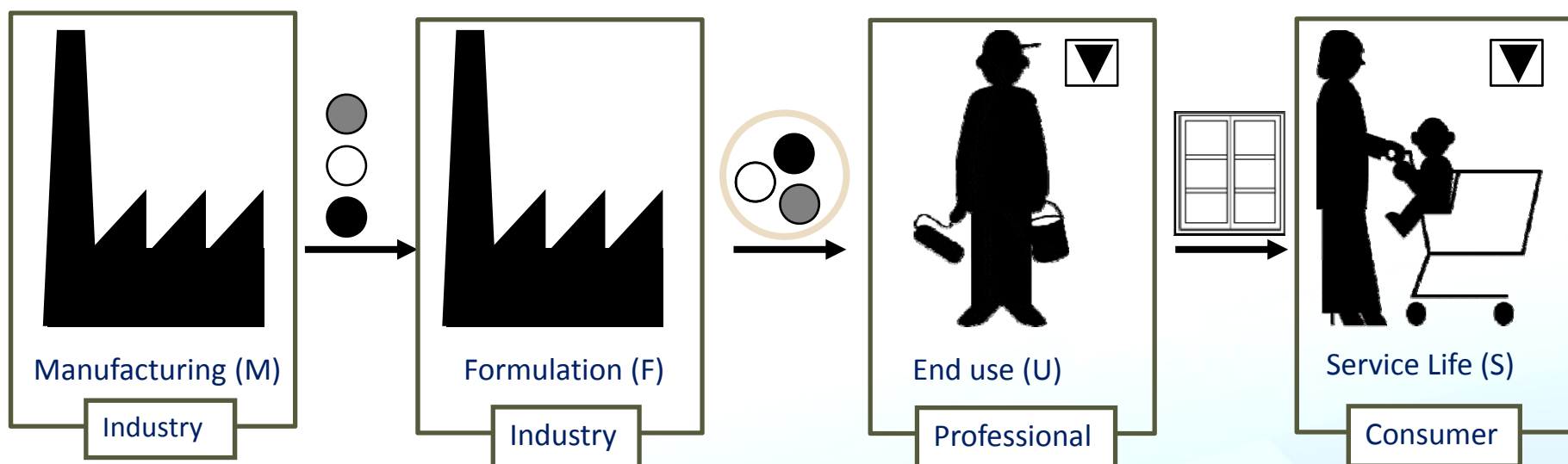


Risk Characterisation Ratio



Headlines for a USE

1. Lifecycle stage



2. User group

Industry
Professional
Consumer

3. Descriptors of use (SU, PC, PROC, AC)

How to use ES-modifier

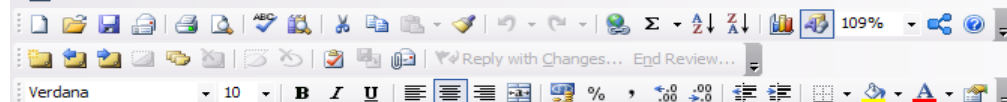
1. Choose lifecycle stage (and user group)
2. Insert substance data (directly/plug-in)
3. Describe overall use according to DoU
4. Choose models
(Default models are Ecetoc TRA and EUSES)
5. Describe specific details of use
6. Make calculations and observe RCR results












Microsoft Excel - ES-modifier - Prototype 2.0.xls

File Edit View Insert Format Tools Data Window Help

Type a question for help



	A	B	C	D	E	F	G
1							
2	CAS NUMBER	USE SECTOR	PRODUCT CATEGORY	PROCESS CATEGORY	ARTICLE CATEGORY		
3	HOME	<p>Welcome to ES-modifier</p> <p>On this sheet you get a very brief introduction to ES-modifier. Do you need more information? You can find a more detailed manual via the menu point MANUAL.</p> <p>With the menu point: LOAD STUDY, you can open studies which are filled in before. The menu point SAVE STUDY enables you to save your work.</p> <p>With the current version of ES-modifier, you can work on substance level. However, you have the possibility to enter substance data for up to 30 substances via the menu point SUBSTANCE DATA. You can do this either manually or by importing data. You should then select the substance to be used in the calculations via the drop-down list on the upper left corner.</p> <p>Besides substance data, you also need to specify:</p> <ul style="list-style-type: none"> "Life cycle stages (LCS)" - by clicking on one of the icons on the upper banner. For the LCS "End-use" and "Service life" you also need to specify the user group: industry, professional or consumer. The selected LCS and user group are then marked as white icons. "Descriptors of Use" (DoU): Sector of Use (SU), Product Category (PC), Process Category (PROC), Article Category (AC). For more details on these categories, contact the manual. More detailed use data - you do this via the menu point USE DATA. <p>As a default, ES-modifier applies the ECETOC model for the human exposure calculations and EUSES for the environmental exposure calculations. Do you want to apply another model? Please go to the menu point MODEL DATA. If you want to adjust some of the default settings, you can do this via the menu point USE DATA.</p> <p>Calculation results are specified on 3 levels:</p> <ul style="list-style-type: none"> RCR - thermometer shown on the lower left corner. The RCR is the "Risk Characterization Ratio". If the RCR is below 1 then safe use can be assumed. Details of the RCR can be found via the menu point RCR DETAILS A report showing detailed input and output data 					
4	LOAD STUDY						
5	SAVE STUDY						
6	SUBSTANCE DATA						
7	PHYS.-CHEM. DATA						
8	HAZARD DATA						
9	MIXTURE DATA						
10	MODEL DATA						
11	USE DATA						
12	RCR DETAILS						
13	RESULTS - PRODUCT LEVEL						
14	REPORT						
15	   						
16	Inhalation						
17	Dermal						
18	Oral						
19	Water						
20	Soil						
21	STP						
22	Air						
23	RCR						
24	LCS						
25	Use categories -						
26	Select substance -						
27	Substance phys.-chem. data -						
28	Substance tox data -						
29	Model data -						
30	Use data -						
31	Calculation						

	A	B	C	D	E	F	G
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20	Soil						
21	STP						
22	Air						
23	LCS - Use categories - Select substance - Substance phys.-chem. data - Substance tox data - Model data - Use data - Calculation						

Navigation: Welcome Main

		MANUFACTURE	FORMULATION	END USE	SERVICE LIFE
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	A	B	C	D	E	F	G
		MANUFACTURE	FORMULATION	END USE	SERVICE LIFE		
1	CAS NUMBER	USE SECTOR	PRODUCT CATEGORY	PROCESS CATEGORY	ARTICLE CATEGORY		
2	HOME	<div> <div>SU1 Manufacture of bulk, large scale chemicals (including petroleum products)</div> <div>SU2 Manufacture of fine chemicals</div> <div>SU3 Manufacture of basic metals</div> <div>SU4 Chemical formulation and packaging</div> <div>SU5 Manufacture of other non-metallic mineral products e.g. plasters, cement</div> <div>SU6 Industrial Manufacturing (all)</div> <div>SU7 Manufacture of food products</div> <div>SU8 Manufacture of textiles, leather, fur</div> </div>					
3	LOAD STUDY						
4	SAVE STUDY						
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7	HAZARD DATA						
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19	Water						
20	Soil						
21	STP						
22	Air						

can find a

int SAVE

LCS - Use categories - Select substance - Substance phys.-chem. data - Substance tox data - Model data - Use data - Calculation

	CAS NUMBER	USE SECTOR	PRODUCT CATEGORY	PROCESS CATEGORY	ARTICLE CATEGORY
1					
2	HOME				
3	LOAD STUDY				
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Calculation results are specified on 3 levels:

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- Details of the RCR can be found via the menu point RCR DETAILS
- A report showing detailed input and output data

LCS - Use categories - Select substance - Substance phys.-chem. data - Substance tox data - Model data - Use data - Calculation

Welcome Main

	A	B	C	D	E	F	G	H	I	J	K
											
	CAS NUMBER		USE SECTOR		PRODUCT CATEGORY		PROCESS CATEGORY		ARTICLE CATEGORY		
1											
2	HOME		Page 1 of 6 *: Required input 1 2 3 4 5 6								
3	LOAD STUDY		CAS-RN * 106-88-7 9003-36-5 6809-97-2 2855-13-2 100-51-6								
4	SAVE STUDY		Name 1,2-epoxybutan Bisphenol F Epo Monoglycidyleth Isophorone diar Benzyl alcohol								
5	SUBSTANCE DATA		logKow * 0,68 7,58 5,50 1,90 1,10 -								
6	PHYS.-CHEM. DATA		Vapour pressure * 24000,0 1,6E-12 1,4E-05 33,0 13,0 Pa								
7	HAZARD DATA		Water solubility * 95000,0 0,00010 0,14 15000,0 43000,0 mg/L								
8	MIXTURE DATA		Biodegradability (1-6) * 1 6 6 6 1 -								
9	MODEL DATA		Molar mass * 72,0 552,0 256,0 170,0 108,0 g/mol								
10	USE DATA		Melting point * -150,0 10,0 -15,2 oC								
11	RCR DETAILS		Boiling point 63,3 648,0 314,0 247,0 205,0 oC								
12	RESULTS - PRODUCT LEVEL		Halflife in air 8,80 0,080 0,33 0,19 1,94 days								
13	REPORT		Photolytic halflife 100000,0 100000,0 100000,0 100000,0 100000,0 days								
14			Hydrolytic halflife 100000,0 100000,0 100000,0 100000,0 100000,0 days								
15	RCR		Chemical type (1-19) * 3 1 1 1 1 -								
16	Inhalation		PEC, regional, water * 0,10 0,010 0,010 0,010 0,010 ug/L								
17	Dermal		PEC, regional, soil * 0,010 0,010 0,010 0,010 0,010 mg/kg ww								
18	Oral		Content (manufacture) * 100,0 100,0 100,0 100,0 100,0 wt%								
19	Water		Content (formulation) * 10,0 10,8 4,80 7,70 7,40 wt%								
20	Soil		Content (end-use) * 10,0 10,8 4,80 7,70 7,40 wt%								
21	STP		Content (service life) wt%								
22	Air										
23	LCS - Use categories - Select substance - Substance phys.-chem. data - Substance tox data - Model data - Use data - Calculation										

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
			MANUFACTURE		FORMULATION		END USE		SERVICE LIFE						
1	106-88-7		USE SECTOR		PRODUCT CATEGORY		PROCESS CATEGORY		ARTICLE CATEGORY						
2	HOME		Substance cas		Adhesive A										
3	LOAD STUDY		106-88-7		10,0										
4	SAVE STUDY		9003-36-5		10,8										
5	SUBSTANCE DATA		6809-97-2		4,80										
6	PHYS.-CHEM. DATA		2855-13-2		7,70										
7	HAZARD DATA		100-51-6		7,40										
8			69-72-7		1,00										
9			1477-55-0		2,00										
10	MIXTURE DATA														
11	MODEL DATA														
12	USE DATA														
13	RCR DETAILS														
14	RESULTS - PRODUCT LEVEL														
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34	LCS - Use categories - Select substance - Substance phys.-chem. data - Substance tox data - Model data - Use data - Calculation														
35															










Import data



RCR

Inhalation
Dermal
Oral
Water
Soil
STP
Air

	A	B	C	D	E	F	G	H	I	J	K
			MANUFACTURE		FORMULATION		END USE		SERVICE LIFE		
1	CAS NUMBER		USE SECTOR		PRODUCT CATEGORY		PROCESS CATEGORY		ARTICLE CATEGORY		
2	CAS-RN		Name								
3	106-88-7		1,2-epoxybutane								
4	9003-36-5		Bisphenol F Epoxy Resin								
5	6809-97-2		Monoglycidylether, C12-14 alcohols								
6	2855-13-2		Isophorone diamine								
7	100-51-6		Benzyl alcohol								
8	69-72-7		Salicylic acid								
9	1477-55-0		m-phenylenebis(methylamine)								
10	MIXTURE DATA										
11	MODEL DATA										
12	USE DATA										
13	RCR DETAILS										
14	RESULTS - PRODUCT LEVEL										
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	A	B	C	D	E	F	G	H		
			 MANUFACTURE		 FORMULATION		 END USE		 SERVICE LIFE	
1	106-88-7		USE SECTOR	PRODUCT CATEGORY	PROCESS CATEGORY	ARTICLE CATEGORY				
2	HOME									
3	LOAD STUDY									
4	SAVE STUDY									
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9	MODEL DATA									
10	USE DATA									
11	RCR DETAILS									
12	RESULTS - PRODUCT LEVEL									
13	REPORT									
14	   									
15	RCR									
16	Inhalation		Exposure route:	Inhalation						
17	Dermal		Target:	Worker						
18	Oral		Selected model	ECETOC						
19	Water		Category	ECETOC STOFFENMANAGER COSHH-BAUA						
20	Soil		Exposure route:	ECETOC						
21	STP		Target:	ECETOC						
22	Air		Model	ECETOC						
23			Category	Not specified						
			Exposure route:	Oral						
			Target:	Worker						
			Model	ECETOC						
			Category	Not specified						
			Target:	Environment						
			Exposure route:	Environment						
			Model	EUSES (env.)						
			ERC Category	14						
			<div>Release data</div>							
22	LCS - Use categories - Select substance - Substance phys.-chem. data - Substance tox data - Model data - Use data - Calculation									
23										

	A	B	C	D	E	F	G	H	I	J	
			MANUFACTURE		FORMULATION		END USE		SERVICE LIFE		
1	106-88-7		SU16		PC1		PROC9		ARTICLE CATEGORY		
2	HOME		*: Required input								
3	LOAD STUDY		Human health exposure assessment								
4	SAVE STUDY		Risk Management Measures								
5	SUBSTANCE DATA		Physical state of product *				Daily cleaning				
6	HAZARD DATA		Dustiness (if solid product)				Regular maintenance				
7	MIXTURE DATA		Application duration *				Ventilation				
8	MODEL DATA		# of similar operations				PPE - dermal				
9	USE DATA		Product amount (per time)				PPE - inhalation				
10	RCR DETAILS		Where				LEV *				
11	RESULTS - PRODUCT LEVEL		How				Containment				
12	REPORT		Area				Segregation				
13	Update calculations		Room volume				RMM - environment				
14	RCR		Temperature								
15			Distance from source								
16	Inhalation										
17	Dermal										
18	Oral										
19	Water										
20	Soil										
21	STP										
22	Air										
23	LCS - Use categories - Select substance - Substance phys.-chem. data - Substance tox data - Model data - Use data - Calculation										
Welcome Main											

	106-88-7	SU4	PC1	PROC7	ARTICLE CATEGORY
1					
2	HOME	*: Required input			
3	LOAD STUDY	Human health exposure assessment			
4	SAVE STUDY	Physical state of product *		Risk Management Measures	
5	SUBSTANCE DATA	Dustiness (if solid product)		Daily cleaning	Yes
6	HAZARD DATA	Application duration *		Regular maintenance	Yes
7	MIXTURE DATA	# of similar operations		Ventilation	No general ventilation
8	MODEL DATA	Product amount (per time)		PPE - dermal	None
9	USE DATA	Where		PPE - inhalation	None
10	RCR DETAILS	How		LEV *	No
11	RESULTS - PRODUCT LEVEL	Area		Containment	No enclosure of source
12	REPORT	Room volume		Segregation	The worker does not work in a
13		Temperature		RMM - environment	None
14		Distance from source			
15	RCR				
16	Inhalation				
17	Dermal				
18	Oral				
19	Water				
20	Soil				
21	STP				
22	Air				
		Environmental exposure assessment			
		Production days per year *		d/y	
		Annual tonnage *		kg/y	

LC50 Use categories - Select substance - Substance phys.-chem. data - Substance tox data - Model data - Use data - Calculation

Substance: A chemical element in its natural state or obtained by a manufacturing process. It may include additives necessary to preserve stability and impurities from the manufacturing process

FORMULATION

END USE

SERVICE LIFE

PC1

PROC7

ARTICLE CATEGORY

HOME

LOAD STUDY

SAVE STUDY

SUBSTANCE DATA
PHYS.-CHEM. DATA

HAZARD DATA

MIXTURE DATA

MODEL DATA

USE DATA

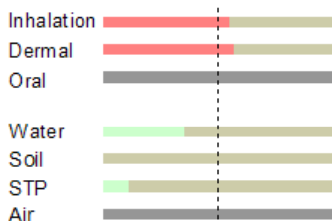
RCR DETAILS

RESULTS - PRODUCT LEVEL

REPORT



RCR



Human health exposure assessment

Physical state of product * Liquid, viscosity like water

Dustiness (if solid product)

Application duration * 8,00 hr

of similar operations 1,00 /d

Product amount (per time) kg

Where

How

Area 100,0 m2

Room volume 100,00 m3

Temperature 25,0 oC

Distance from source

Risk Management Measures

Daily cleaning Yes

Regular maintenance Yes

Ventilation No general ventilation

PPE - dermal None

PPE - inhalation None

LEV * No

Containment No enclosure of source

Segregation The worker does not work in a

RMM - environment None

Environmental exposure assessment

Production days per year * 220,0 d/y

Annual tonnage * 10000,0 kg/y

LCS - Use categories - Select substance - Substance phys.-chem. data - Substance tox data - Model data - Use data - Calculation



Adhesive A

SU4

PC1

PROC7

ARTICLE CATEGORY

HOME

LOAD STUDY

SAVE STUDY

SUBSTANCE DATA

PHYS.-CHEM. DATA

HAZARD DATA

MIXTURE DATA

MODEL DATA

USE DATA

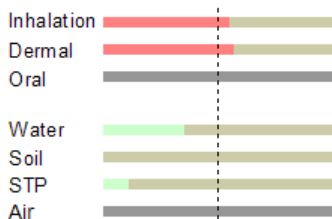
RCR DETAILS

RESULTS - PRODUCT LEVEL

REPORT



RCR



Product level calculations

Product:

Adhesive A

Exposure route

Inhalation

Dermal

Oral

Eye

Environment

Sum of RCR (crit. subst.)

2,00

1,93

-

-

0,26

Substance

Calculated LSI for substances in product for the various exposure routes

1,2-epoxybutane

2400,0

0,10

0,10

0,0050

0,0040

Bisphenol F Epoxy Resin

0,0E+00

0,11

0,0E+00

0,0054

0,0E+00

Monoglycidylether, C12-14 alcohols

0,0E+00

0,048

0,0E+00

0,0024

0,019

Isophorone diamine

0,0E+00

0,077

0,0031

0,0E+00

0,0031

Benzyl alcohol

0,038

0,0E+00

0,0030

0,0E+00

0,0E+00

Salicylic acid

2,2E-05

0,010

0,00040

0,0020

0,0E+00

m-phenylenebis(methylamine)

0,0E+00

0,0040

0,0E+00

0,0E+00

0,0E+00

LCS - Use categories - Select substance - Substance phys.-chem. data - Substance tox data - Model data - Use data - Calculation

Welcome Main

File Rediger Vis Indsæt Formater Funktioner Data Vindue Hjælp

A B C D E F G

106-88-7 SU10 PC1 PROC4 ARTICLE CATEGORY

HOME
LOAD STUDY
SAVE STUDY
SUBSTANCE DATA
PHYS.-CHEM. DATA
TOX DATA
MIXTURE DATA
MODEL DATA
USE DATA
RCR DETAILS
REPORT
MANUAL
CLOSE DOWN

RCR

Inhalation
Dermal
Oral
Water
Soil
STP
Air

Exposure route:
Target:
Selected model
Category

Inhalation
Worker
ECETOC
Use in a batch or other process (including related process stages e.g. filtration, drying) where or

Exposure route:
Target:
Model
Category

Dermal
Worker
ECETOC
Use in a batch or other process (including related process stages e.g. filtration, drying) where or

Exposure route:
Target:
Model
Category

Oral
Worker
Not relevant/not implemented
Not relevant

Target:
Exposure route:
Model
ERC Category

Environment
Environment
EUSES (env.)
2

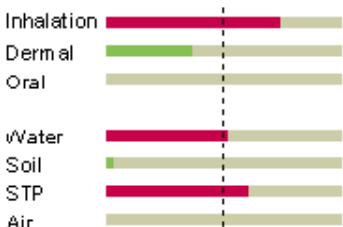
Release data

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DA 98% 19:17

ARTICLE CATEGORY

RCR



ERC Category

Not defined

Close and save

2

Release data

ARTICLE CATEGORY

Air

ERC Category

Close and save

Release data

File Rediger Vis Indsæt Formater Funktioner Data Vindue Hjælp

A B C D E F G

106-88-7 SU10 PC1 PROC4 ARTICLE CATEGORY

HOME
LOAD STUDY
SAVE STUDY
SUBSTANCE DATA
PHYS.-CHEM. DATA
TOX DATA
MIXTURE DATA
MODEL DATA
USE DATA
RCR DETAILS
REPORT
MANUAL
CLOSE DOWN

RCR

Inhalation
Dermal
Oral
Water
Soil
STP
Air

Exposure route:
Target:
Selected model
Category
Use in a batch or other process (including related process stages e.g. filtration, drying) where or

Exposure route:
Target:
Model
Category
Use in a batch or other process (including related process stages e.g. filtration, drying) where or

Exposure route:
Target:
Model
Category
Not relevant

Target:
Exposure route:
Model
ERC Category

Inhalation
Worker
ECETOC
Dermal
Worker
ECETOC
Oral
Worker
Not relevant/not implemented
Environment
Environment
EUSES (env.)
2

Release data

Calculation completed

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Report Exposure Scenario



Chemical

A

Section 1

Exposure scenario title

Title

MyUse

Life Cycle Stage

Formulation

Use Descriptors

SU

SU3

PC

PC1

PROC

PROC 5, PROC 8a, PROC 9

ERC

ERC 2

Activities covered

activity 1, Activity 2, Activity 3

Section 2

Operational conditions and risk management measures

Section 2.1

Operational conditions and risk management measures (human)

Name of contributing scenario (activity)	activity 1	Activity 2	Activity 3
Further details		Manually drawing off or pouring of a product	Manually drawing off or pouring of a product
Process category	PROC 5	PROC 8a	PROC 9
Model: inhalation	ECETOC	StoffenManager	StoffenManager
Model: dermal	ECETOC	ECETOC	ECETOC
Model Oral			
Temperature (oC)	25	25	25
Physical state	Liquid	Liquid	Liquid

Agenda 2010

- ES modifier available via
<http://es-modifier.dhigroup.com/>
- Further development of the software tool:
ready in september 2010
 - Integration of DPD+
 - Consolidate Exposure Scenarios
 - Report of Exposure Scenarios for formulations
- Cooperation with relevant stakeholders a.o.
Down stream Users (organisations), CEFIC,
ECHA