
Conceptual evaluation of Tier 1 models

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25.03.2014

Conceptual evaluation ↔ Tier 1 model

Concepts for exposure modelling, for example:

- Cherrie et al., 1996,
- Schneider et al., 1999,
- Tielemans et al., 2008.

Tier 1 models

- do not have to fulfil all details included in these publications
(ECHA guidance R14)

Outline

Evaluated Tools

- (EASE v.2)
- ECETOC TRA v.2 / v.3
- MEASE v.1.02.01
- EMKG-EXPO-TOOL
- Stoffenmanager v.4.5
- RISKOFDERM v. 2.1

Evaluation - Results

- Transparency
- Algorithm and Parameters
- Applicability matrix
- Usemap
- Application under REACh
- Summary/ Conclusion

ECETOC TRA – the worker part

v.2 (2009), v.3 (2012)

■ **Routes**

- Inhalation
- Dermal

■ **Background information**

- User guidance
- Model reports (TR107 & 114)
- Information in the tool

Physical-chemical properties - minimum input for Human Health and Environmental Assessment

Molecular weight
Vapour pressure (Pa OR hPa)
Water solubility
Partition coefficient octanol-water (- OR Log(Kow))
Biodegradability test result
Chemical class for Koc-QSAR
Koc (L.kg⁻¹) OR Log(Koc)
Partition coefficient $k_{\text{soil/water}}$
Partition coefficient $k_{\text{sediment/water}}$
Partition coefficient to suspended solids

	123 g.mol ⁻¹
	1.00E-03 Pa
	mg.L ⁻¹
	Kow
	Koc
	L.kg ⁻¹
	L.kg ⁻¹
	L.kg ⁻¹

Additional physico-chemical parameter input for refined environmental assessment (TIER 2)

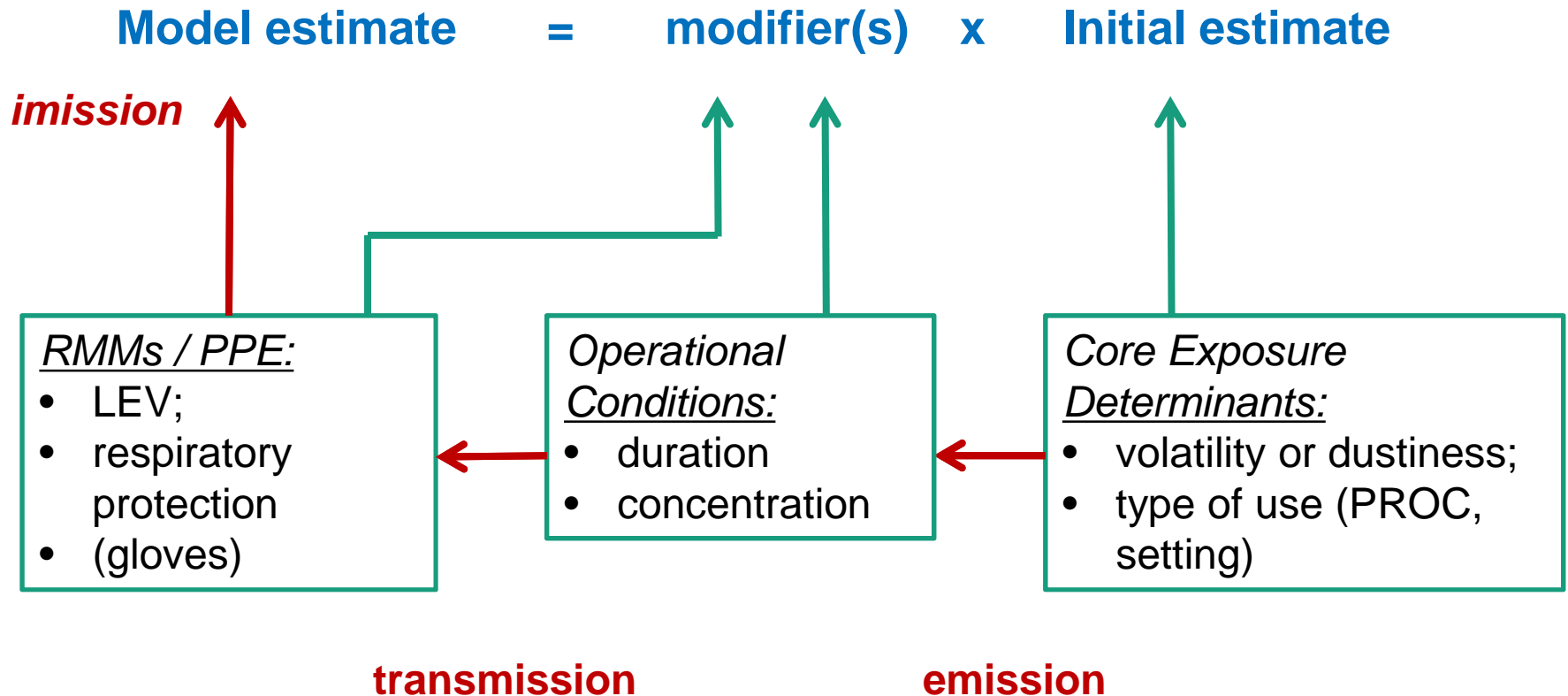
Human Health Assessment - Workers

Scenario name

Process Category
(PROC)
PROC 5
PROC 5

Type of setting
(PROC 7 and
Industrial, P
always profes
professional
professional

ECETOC TRA: Algorithm



MEASE - “The metals’ EASE”

v.1.02.01 by EBRC on behalf of EUROMETAUX (2010)

Routes:

- Inhalation
- Dermal

Background information

- MEASE glossary
- HERAG fact sheet
- Fransman et al., 2008

MEASE 1.02.01 Exposure Assessment Tool For Metals And Inorganic Substances		© 2009, 2010 EBRC Consulting GmbH D. Vetter Hannover, Germany	
Substance characteristics		Model parameters	Exposure modifier
Molecular weight (g/mol)			(using default of 24.45 g/mol)
Melting point (°C)			---
Vapour pressure (Pa)	20000		20000 Pa
Physical form	Liquid		High fugacity (vapour pressure based)
Content in preparation (including alloys)	> 25%		100%
Operational conditions (OC)		Model parameters	Exposure modifier
Process category	7 - Industrial spraying		---
Process temperature (°C)			---
Scale of operation	Industrial use		Industrial use
Duration of exposure (minutes)	> 240 minutes		100%
OCs used for dermal exposure assessment		Model parameters	Exposure modifier
Pattern of use	Closed system without breaches		Low dermal exposure potential
Pattern of exposure control	Non-direct handling		Low dermal exposure potential
Contact level	None		Low dermal exposure potential
Risk management measures (RMM)		Model parameters	Exposure modifier
Implemented RMMs	No RMMs		100%
RMM efficiency based on	Median estimate		(as reflected in reduction factor above)
Respiratory protective equipment (RPE)	No RPE		100%
Use of gloves	No gloves		100%
Exposure estimate			Exposure estimate
Dermal exposure estimate			0.5 µg/cm ² /day
Exposed skin area			480 cm ²
Total dermal loading			0.24 mg/day
Inhalation exposure estimate			500 mg/m³

MEASE: Algorithm

Refinement of EASE and ECETOC TRA v.2

Inhalation

- based on ECETOC algorithm
- partly refined - data for metals
- „massive objects“, „aqueous solutions“
- additional RMMs

Core Exposure Determinants

- volatility or dustiness
- type of use (PROC, setting)

Operational conditions

- duration
- concentration

RMMs / PPE

- LEV
- respiratory protection
- gloves

Model estimate = Initial estimate x modifier(s)

Dermal

- based on EASE logic tree
- refined - data for metals
- new modifiers

Core Exposure Determinants

- pattern of use
- pattern of exposure control
- contact level
- except gaseous substances
- PROC → skin area

EMKG-EXPO-TOOL

by BAuA, Part of EMKG concept (=“Einfaches Maßnahmenkonzept Gefahrstoffe”, “Easy to use workplace control scheme for hazardous substances”)



Route

- Inhalation

Background information

- the EMKG concept (BAuA)
- COSHH related publications
- help function within tool

EMKG - Exposure assessment part for liquids

Definition of volatility bands ?				Alternative input of boiling point [°C] and operating temperature [°C] ?	
Band	At normal temperature (~20°C)	Operating temp. (o.t.)	Vapour pressure (kPa at o.t.)	input b.p.	input o.t.
Low	boiling point above 150°C	b.p. $\geq 5 \times \text{o.t.} + 50$	< 0.5		
Medium	boiling point between 50 and 150°C	other cases	0.5 - 25		
High	boiling point below 50°C	b.p. $\leq 2 \times \text{o.t.} + 10$	> 25		

Scale of use bands ?	
Band	Description
Small	millilitres up to 1 litre for liquids
Medium	litres (batch sizes between 1 and 1000 litres for liquids)
Large	cubic metres (batch sizes of greater than 1 m ³ for liquids)

Short term exposure ?	
Activity < 15 min. during a full 8 h shift?	
Yes	No

Applications on surfaces > 1m ² ?	
e.g. painting, applying adhesives etc. and more than 1 litre product used per shift!	
Yes	No

Control strategies ?		
Control Approach	Type	Description
1	General ventilation	Good general ventilation and good work practice
2	Engineering control	Local exhaust ventilation (e.g. single point extract, partial enclosure, not complete containment) and good work practice
3	Containment	Enclosed, but small breaches may be acceptable. Good Work practice.

Exposure potential bands (EP)			
Solids – EP band	Use band	Volatility band	Description
1	Small	Low	Millilitres of low volatility liquid
2	Small	Medium or High	Millilitres of medium / high volatility liquid, litres / cubic metres of low volatility liquid
	Medium or Large	Low	Cubic metres of low volatility liquid
3	Large	Medium	Cubic metres of medium volatility liquid, litres of medium / high volatility liquid
	Medium	Medium or High	Cubic metres of high volatility liquid
4	Large	High	Cubic metres of high volatility liquid

Predicted exposure ranges: Liquids				
Control Approach	Predicted exposure level for vapour, ppm			
	Solids EP Band 1 (mL of low VP liquid)	Solids EP Band 2 (mL of med./high VP liquid or L / m ³ of low VP liquid)	Solids EP Band 3 (m ³ of med. VP liquid or L of med. / high VP liquid)	Solids EP Band 4 (m ³ of high VP liquid)
1	< 5	5 - 50	50 - 500	> 500
2	< 0.5	0.5 - 5	5 - 50	5 - 500
3	< 0.05	0.05 - 0.5	0.5 - 5	0.5 - 5

EMKG-EXPO-TOOL: Algorithm

- **Exposure is determined by two principles**

1. exposure potential of the substance

- the scale of use (amount of substance per event)
- volatility (boiling point, process temperature, vapour pressure); dustiness

2. control approach

- → control guidance sheets!

→ **set of logic criteria**

(almost identical to COSHH essentials)

Stoffenmanager - REACH part

v.4.5 by TNO, Arbo unie, Ernst & Young

■ *Route*

- Inhalation

■ *Background information*

- Schinkel et al. (2010)
- Tielemans et al. (2008)
- Marquart et al. (2008)
- help function within tool

Risk assessment inhalation

+ explanation

Name:	: 400acetone 100% every day
Location:	: test
Product:	: 400Acetone 100%
Dilution:	: 100
Task:	: Handling of liquids at high pressure resulting in substantial generation of mist or spray/haze

↓ Step 1 of 4

Name the exposure assessment: *

Select a location: *

Is the substance a solid or a liquid? *
 Solid Liquid

Select a product *

If you dilute the product with water, please give the percentage product in the solution
 % (100% is undiluted)

Characterize your task: *

Select an item
Handling of liquids in tightly closed containers
Handling negligible amounts of product
Handling of liquids where only small amounts of product may be released

Stoffenmanager : Algorithm

based on Tielemans et al., 2008

- **mixed effect regression model**

$$[(\varepsilon_i \cdot h \cdot \eta_{lc} \cdot d_{gv,NE}) + (\varepsilon_i \cdot h \cdot \eta_{lc} \cdot d_{gv,FF}) + (\varepsilon_i \cdot a)] \cdot \eta_{PPE}$$

near field emission

far field emission

passive emission

C_t : total concentration score

- **fitting procedure with measured exposure values**

- most scores assigned on logarithmic scale
- $\text{Ln}(Y_{ij}) = X_{ij} = \beta_0 + \beta_1 \cdot \text{Ln}(C_T) + \delta_i + \varepsilon_{ij}$

RISKOFDERM

within the RISKOFDERM project (2006)

- **Route**

- **Dermal**

- hands and body

- **Background information**

- **User guidance**

- **Warren et al., 2006**

- **Help function in the tool**

Filling, mixing or loading (DEO unit 1)		
You can move the input messages with the input fields by dragging and dropping		
Question	Answer	Additional explanation
What is the quality of the ventilation related to the task done?	Normal or good ventilation	Good (mechanical) ventilation and/or proper local exhaust ventilation
What is the frequency of (skin) contact with the contaminant?	More than rare contact	It happens on average once or more per scenario
What kind of (skin) contact with the contaminant occurs?	Light contact	Touching of contaminated surfaces and/or limited deposition of dust or aerosols
What type of product is handled?	Low or moderately dusty solid	A low or moderately dusty solid either does not produce clearly visible dust in the air, or the dust can be seen only briefly
Are significant amounts of aerosols or splashes generated in the task?	No	Task does not lead to substantial interaction between product and air, nor to dropping of product on a hard surface
What is the level of automation of the task done by the worker?	Manual task	The task is largely done manually with substantial interaction between worker and package, contaminated installation or product

6 different Dermal Exposure Operation units (DEO)

RISKOFDERM - Algorithm

Generic form of linear mixed effect model:

$$Y_{i,j} = \alpha_0 + \alpha_1 I_{1,ij} + \alpha_2 I_{2,ij} + \dots + \beta_i + \Sigma_{ij}$$

j^{th} log-transformed
measurement
on the i^{th} worker

mean log-
transformed
potential dermal
exposure for the
DEO

α_n - **fixed effects**
(**determinants** of exposure,
e.g. ventilation)

I_n presence/absence (1/0)

β_i : random effect for the i^{th} worker

Σ_{ij} : random error associated with the j^{th} measurement on the i^{th} individual

Algorithms and exposure determinants

- **different types of algorithms**
 - logic tree \leftrightarrow initial concentration + modifiers \leftrightarrow linear mixed effects models
- **internal validation**
 - fitting procedures to measured data \leftrightarrow expert judgement
- **varying number of determinants and level of detail \rightarrow different scopes, e.g.**
 - RISKOFDERM covers body exposure
 - MEASE, Stoffenmanager offer more RMM options
 - only ECETOC TRA, MEASE offer gloves

Applicability matrix

1/2

Applicability	EMKG-EXPO-TOOL	Stoffen-manager v.4.5	ECETOC TRA v2	ECETOC TRA v3	MEASE	RISKOFDERM
Route	Inh.	Inh.	Inh.+derm.	Inh.+derm.	Inh.+derm.	Derm.
Covered physical state	solid liquid	solid liquid	solid liquid = volatile	solid liquid = volatile	solid liquid gaseous	solid liquid
Beyond Scope	Dusts by abrasive techniques, open spray, gases, pesticides, fumes, wood dusts, CMR substances	Fibres, gases or hot working techniques (welding, soldering); abrasion and impact of solid objects not recommended	Fibres, liquid aerosols or emissions from hot processes (e.g. fumes). Solids in liquids. Caution recommended for CMRs	Fibres, liquid aerosols or emissions from hot processes (e.g. fumes). Solids in liquids. Caution recommended for CMRs	Organic substances & some restrictions concerning special combinations of PROC/ physical properties	Sometimes restrictions due to original data set (e.g. "only on manual tasks for powders") fumes not covered

Applicability matrix

2/2

Applicability	EMKG-EXPO-TOOL	Stoffen-manager v.4.5	ECETOC TRA v.2	ECETOC TRA v.3	MEASE	RISKOFDERM
Type of enterprises	SME	industrial & professional	industrial & professional	industrial & professional	industrial & professional	industrial & professional
Use categories process or task based	task	task	process	process (+ „peak exposure“)	process	task
Farfield factors	partly included via cgs	same task by other workers	Not included	Not included	Not included	Not included
Other information		only model which covers stone / wood dust				only model which covers body exposure



Not all situations are applicable for all models!

Application under REACh

- **ECHA guidance R14**
recommends all tools evaluated in the eteam project
- **PROC system**
MEASE, Stoffenmanager v.5, ETETOC TRA v.2/3
- **RCR calculation**
only ECETOC TRA
- **CSR compatible output format or export files**
none of the tools
- **Implementation into Chesar**

ECETOC TRA	same algorithm
Stoffenmanager v.5	import files
all tools	label the exposure estimation - tool used

Conclusion

- Scope & Limitations
 - exposure route, use, applicability domain
- Level of Detail
 - Stoffenmanager[®], MEASE, RISKOFDERM → at the border to higher tiers
- „BEST“ tool
 - depends on situation & user

Thank you very much for your attention!



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