ECHA
EUROPEAN CHEMICALS AGENCY

REPORT ENES5 break-out sessions

BREAK-OUT SESSION G	CCA (Critical Component Approach)
Presenter - SME	Onno Jongerius
Moderator	Steven Van de Broeck
Rapporteur	Cécile Rousseau

cefic
Fecc
DUCC
Downstream Users of Chemicals Co-ordination group
EUROMETAUX
EUROPEAN ASSOCIATION OF METALS
concawe

Exposure Scenario processing for mixtures

Critical Component Approach (CCA)

Brussels, ENES5 meeting 21&22 November 2013: Breakout session G

Jongerius consult BV

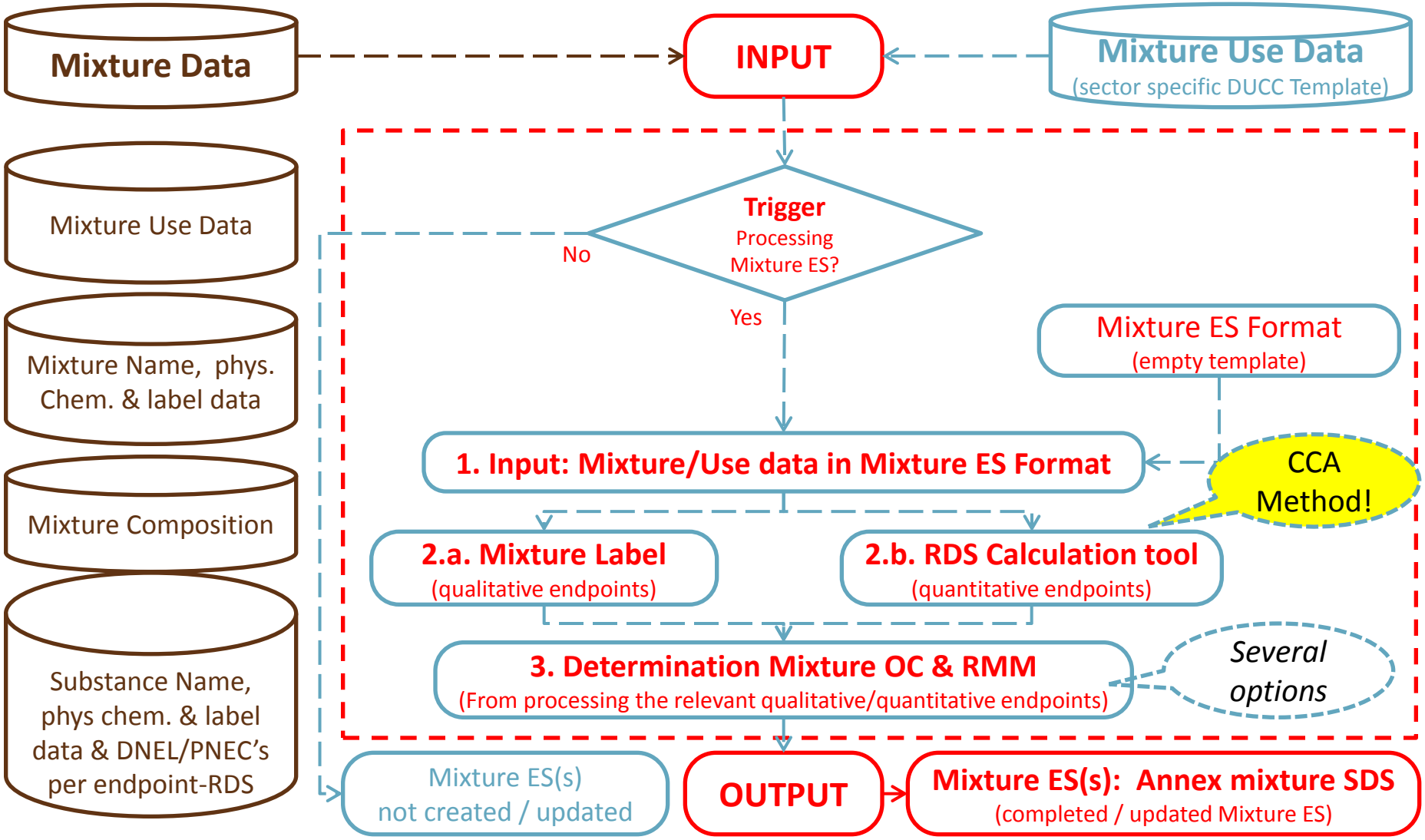
Onno Jongerius

Caesar Consult

Joost van Rooij

Outline Generic Mixture Exposure Scenario approach (GMES)

Stepwise process to complete the Mixture ES format "top-down"



Critical Component Approach (CCA)

The main principles of the CCA method

- The **CCA method,** as proposed by Jongerius Consult & Caesar Consult, determines the so-called **critical components**

- Possible **critical components** are identified based on DNEL-/PNEC-values for the following endpoints:
  - Inhalation: short / long term & local / systemic
  - Dermal: short / long term & local / systemic
  - Oral: short / long term - systemic
  - Aquatic environment

- For each endpoint a **Risk Determining Substance (RDS) score** is calculated. The highest RDS score determines the critical component per endpoint.

$$\text{RDS-score}_{\textit{inhalation endpoints}} = Vp * C_i / DNEL_i$$

$$\text{RDS-score}_{\textit{other health endpoints}} = C_i / DNEL_i$$

$$\text{RDS-score}_{\textit{environmental endpoints}} = C_i / PNEC_i$$

Vp = Vapour Pressure (hPa, at 20/25°C)

C_i = Concentration of substance (i) in mixture (%)

DNEL or PNEC$_i$ = relevant DNEL or PNEC of substance (i)

ENES5: Test Mixture M1 - industrial use in rigid foams

Determination RDS via CCA Calculation Tool

ENES5: Test Mixture M1 - industrial use in rigid foams										
Mixture classification DPD+	**Component**	**Conc in mixture (%)**	**REACH registered substance**	**VP (Pa) 20C**	**Worker DNEL, inhal, syst, longterm (mg/m^3)**	**Worker DNEL , dermal, syst, longterm (mg/kg/day)**	**PNEC (mg/l)**	**Classification DSD**	**Classification CLP**	**SDS available**
not classified	A	60,00	yes	< 0,01	98	13,9	0,2	not classified	not classified	SDS
	B	16,00	yes	1,00E-06	3,9	7	0,02	not classified	Eye.Corr/Irr.2 H319	Ext-SDS
	C	10,00	no	< 0,01	---	---	---	R22	Acut.Tox.4 H302	SDS
	water	11,50	no	2,30E+03	---	---	---	not classified	not classified	no
	D	1,20	yes	4,00E+02	35	EBW	0,002	R10, R22, R23, R24, R34	H226, Acut.Tox.3 H301, Acut.Tox.3 H311, Skin.Corr.1B H314, Acut.Tox.3 H331	Ext-SDS
	E	0,70	yes	3,00E+01	0,529	0,15	0,0549	R22, R24, R34	Acut.Tox.4 H302, Acut.Tox.3 H311, Skin.Corr.1B H314	Ext-SDS
	F	0,57	yes	7,50E-02	0,31	0,2	0,084	R34, R52/53	Acut.Tox.5 H303, Acut.Tox.5 H313, Skin.Corr.1B H314, Skin.Sens.1B H317, Aquat.Chron.3 H412	no
	G	0,03	yes	9,10E+01	14,6 (local)	---	4,40E-04	Rep.Cat3 R62, R53	H226, Rep.Tox.Cat2 H361, Aquat.Chron.4 H413	no

CCA Tool - ENES5 M1

CCA Calculation tool - Demo

(draft beta version)

Calculation RDS-Score - ENES 5: Test Mixture M1 - industrial use in rigid foams

Mixture	**Breakdown**	**Substance details**					**DNEL Worker**				**PNEC**	
Product	Substance name	Substance Hazard Statements	Substance in product (%)	Cut-off value %	Vapour presure (hPa)	VP temp (°C)	**4. INHALATION - Long term - Systemic**		**8. DERMAL- long term - Systemic**		**I. ENVIRONMENT - Aquatic - Fresh water**	
							DNEL	RDS-Score	DNEL	RDS-Score	PNEC	RDS-score
							mg/m3		mg/kg bw/d		mg/l	
Test Mixture M1	A		60,00%		1,00E-04	20	98	non hazardous	13,9	non hazardous	0,2	non hazardous
	B	H319	16,00%	1,0%	1,00E-08	20	3,9	0,000	7,0	0,023	0,02	**8,0**
	C	H302	10,00%	1,0%	1,00E-04	20		no DNEL		no DNEL		no PNEC
	water		11,50%		2,30E+01	20		non hazardous		non hazardous		non hazardous
	D	H226, H301, H311, H314, H331	1,20%	0,1%	4,00E+00	20	35	0,001		no DNEL	0,002	6,0
	E	H302, H311, H314	0,70%	0,1%	3,00E-01	20	0,529	**0,004**	0,2	**0,047**	0,0549	0,13
	F	H303, H313, H314, H317, H412	0,57%	1,0%	7,50E-04	20	0,31	below cut off	0,2	below cut off	0,084	below cut off
	G	H226, H361, H413	0,03%	1,0%	9,10E-01	20		below cut off		below cut off	4,40E-04	below cut off

ENES5 Example “Sanitary Cleaner” (AISE)

Stepwise process to complete the Mixture ES format “top-down”(2)

Mixture Use Data (sector specific DUCC Template(s))

Mixture Use Data

1. Input: Mixture/Use data in Mixture ES Format

2.a. Mixture Label (qualitative endpoints)

3. Determination Mixture OC & RMM (From processing the relevant qualitative/ quantitative endpoints)

2.b. RDS Calculation tool (quantitative endpoints)

Mixture name

ES Title & mixture use

Mixture label

Qualitative Endpoints

Mixture uses: contributing scenarios (CS)

Mixture OC /RMM per CS

Mixture uses: ERC / SPERC

Mixture OC /RMM Env.

Result CCA Method

RDS per Quant. Endp.

MIXTURE EXPOSURE SCENARIO FORMAT (WORKER)

Name of mixture	<Product specific mixture name>		
Section 1 – Title of Exposure Scenario (ES)			Sector code (ES)
Title	<DUCC Template: "Short ES Title">		<DUCC Template: "Code (DU)">
Processes and activities covered	Contributing Scenario (CS)	Sector cod…	
	<DUCC Template: "Short description of process or activity 1">	<DUCC Temp…	
	<DUCC Template: "Short description of process or activity 2">	<DUCC Templa…	
	<DUCC Template: "Short description of process or activity 3"> -> Etc.	<DUCC Template: "…	<DUCC Template: "PROC at No 3">
Sector of use	<DUCC Template: "Full description of the SU">	-	<DUCC Template: "SU">
Environmental release category	<DUCC Template: "Full description of the ERC / SPERC">	<DUCC Template: "SPERC">	<DUCC Template: "ERC">

Section 2 - Conditions of use affecting exposure

Characteristics of mixture - general		Irritation / corrosion	Sensitization	Acute toxicity	Carcinogenicity / mutagenicity
		Qualitative endpoints relevant for chemical safety assessment			
Physical state of mixture (at 20°C and 101.3 kPa)	liquid		No	No	No
Classification of undiluted mixture: R-Phrases	<R-Phrases of Mixture>				
Classification of undiluted mixture: H-Phrases	<H-Phrases of Mixture>				

2.1 Control of workers exposure

Operational conditions	
Temperature of process	Ambient (unless stated differently)
Frequency/duration of use	8-hours/day - 5 workdays/week (unless stated differently)
Indoor or outdoor	indoor (unless stated differently)

Contributing Scenario (task / activity)	% of mixture in handled product?	Risk Management Measures (RMM)
<DUCC Template: "Short description of process or activity 1">		…RMMs processed for each relevant health endpoint (qualitative via mixture label a…
<DUCC Template: "Short description of process or activity 2">		…RMMs processed for each relevant health endpoint (qualitative via mixture label and qua…
<DUCC Template: "Short description of process or activity 3"> -> Etc.	<Mixture %>	<RMMs determined for the specific CS as compilation of the RMMs processed for each relevant health endpoint (qualitative via mixture label and quantitative … RDS)>

2.2 Control of environmental exposure

Environmental release category	typical (sp)ERC value		Environmental control measures
<DUCC Template: "Full description of the ERC / SPERC">	Fraction used at main source	<(sp)ERC: "Fraction used at main source">	<RMMs determined for the (spe)ERC based … the quantitative endpoint(s) per RDS>
		…ssion days per year">	
		…icipal STP">	
		…ase fraction to air">	
		…ase fraction to waste water">	
	Release fraction to soil	<(sp)ERC: "Release fraction to soil">	
	River flow rate for dilution	flow rate for … m³/day	
	Type of *on site* Risk Management measures	<(sp)ERC: "Type of on site Risk Management measures">	
	Efficiency of *on site* Risk Management Measures	<(sp)ERC: "Efficiency of on site Risk Management Measures">	

Section 3 - Exposure estimation and reference to its source

Quantitative endpoints relevant for chemical safety assessment - Risk Determining Substances (RDS) via Critical Component Approach (CCA)

Endpoint			Risk Determining Substance	EC number	% in mixture	Limit value (DNEL-worker / PNEC)		Physical / chemical factors relevant for RDS selection / chemical … assessment		
Inhalation	short term	local	<RDS name from CCA Calculation>	< See CCA>	< See CCA>	<RDS-value>	ppm	Vapour pressure (hPa)	<RDS-value>	Fugacity …
		systemic	<RDS name from CCA Calculation>	< See CCA>	< See CCA>	<RDS-value>	ppm	Vapour pressure (hPa)	<RDS-value>	Fuga…
	long term	local	<RDS name from CCA Calculation>	< See CCA>	< See CCA>	<RDS-value>	ppm	Vapour pressure (hPa)	<RDS-value>	
		systemic	<RDS name from CCA Calculation>	< See CCA>	< See CCA>	<RDS-value>	ppm	Vapour pressure (hPa)	<RDS-value>	
Dermal	short term	local	<RDS name from CCA Calculation>	< See CCA>	< See CCA>	<RDS-value>	mg/cm²	Not applicable		
		systemic	<RDS name from CCA Calculation>	< See CCA>	< See CCA>	<RDS-value>	mg/kg bw			
	long term	local	<RDS name from CCA Calculation>	< See CCA>	< See CCA>	<RDS-value>	mg/cm²			
		systemic	<RDS name from CCA Calculation>	< See CCA>	< See CCA>	<RDS-value>	mg/kg bw			
Environment	aquatic	fresh water	<RDS name from CCA Calculation>	< See CCA>	< See CCA>	<RDS-value>	mg/L	Vapour pressure (hPa)	<RDS-value>	
			<RDS name from CCA Calculation>	< See CCA>	< See CCA>	<RDS-value>		Degradability		N…

3.1 Worker - Chemical Safety Assessment based on the characteristics of mixture and the risk determing substance(s)

[general statement referring to the Chemical Safety Assessment method used and explaining that when RMMs/OCs instructions are implemented all qualitative and quantitative health hazards are controlled (Risk Characterization Ratios (RCRs) are below 1)].

3.2 Environment - Chemical Safety Assessment based on risk determing substance in mixture

[general statement referring to the Chemical Safety Assessment method and explaining that when RMMs/OCs instructions are implemented all environmental hazards are controlled (RCRs are below 1]

Section 4 - Guidance to Downstream User to evaluate if he works inside boundaries set by the ES

Further information on the assumptions contained in this Exposure Scenario can be found/obtained from: <www.company.com> and/or <www.sector.org>. Scaling can be done using the exposure estimation tool originally used. Expert advice may be needed.

ENES5 Example “Sanitary Cleaner” (AISE)

Output: Mixture ES “Sanitary Cleaner”

Name of mixture	Sanitary Cleaner (test formulation ENES5)

Section 1 – Title of Exposure Scenario (ES)			Sector code - ES
Title	Professional Use of General surface cleaning products		AISE-P305
Processes and activities covered	Contributing Scenario (CS)	Sector code - CS	Use descriptor code
	Transfer of professional cleaning or maintenance product (charging/discharging) to a cleaning equipment (machine/vessel/bucket)	AISE_CSP01	PROC8a
	Brushing a diluted professional cleaning solution, desinfectant or maintenance product	AISE_CSP08	PROC10
	Brushing a concentrated professional cleaning or maintenance product.	AISE_CSP10	PROC10
Sector of use	Professional uses: Public domain (administration, education, entertainment, services, craftsmen)	-	SU22
Environmental release category	AISE 16 - Wide Dispersive Use in 'Down the Drain' cleaning and maintenance products (Consumers and Professionals)	AISE SPERC 8a.1.a.v1	ERC8a

Section 2 - Conditions of use affecting exposure

Characteristics of mixture - general		**Qualitative endpoints relevant for chemical safety assessment**			
		Irritation / corrosion	**Sensitization**	**Acute toxicity**	**Carcinogenicity / mutagenicity**
Physical state of mixture (at 20°C and 101.3 kPa)	liquid	Skin and eye corrosive	No	No	No
Classification of undiluted mixture: R-Phrases	R34				
Classification of undiluted mixture: H-Phrases	H314				

2.1 Control of workers exposure

Operational conditions

Temperature of process	Ambient (unless stated differently)
Frequency/duration of use	8-hours/day - 5 workdays/week (unless stated differently)
Indoor or outdoor	indoor (unless stated differently)

Contributing Scenario (task / activity)	**% of mixture in handled product?**	**Risk Management Measures (RMM)**
Transfer of professional cleaning or maintenance product (charging/discharging) to a cleaning equipment (machine/vessel/bucket)	100%	Use suitable eye protection and gloves.
Brushing a diluted professional cleaning solution, desinfectant or maintenance product	<10%	If diluted less then 100 times (% of mixture >1%): use suitable eye protection and gloves.
Brushing a concentrated professional cleaning or maintenance product.	100%	Use suitable eye protection and gloves.

2.2 Control of environmental exposure

Environmental release category	**typical (sp)ERC value**		**Environmental control measures**
AISE 16 - Wide Dispersive Use in 'Down the Drain' cleaning and maintenance products (Consumers and Professionals)	Fraction used at main source	0,00075	[Prevent leaks and prevent soil / water pollution caused by leaks. Dispose of waste product or used containers according to local regulations.]
	Emission days per year	365	
	Municipal STP	yes	
	Release fraction to air	0	
	Release fraction to waste water	1	
	Release fraction to soil	0	
	River flow rate for dilution	18000 m^3/day	
	Type of *on site* Risk Management measures	-	
	Effectivity of on site risk management Measures	-	

ECHA
EUROPEAN CHEMICALS AGENCY

Minimum required information

- DNEL/PNEC
- uses
- classification of the substances
- composition of the mixture
- good quality ES for top down approach
- expertise

cefic

Fecc

Downstream Users of Chemicals Co-ordination group

EUROMETAUX
EUROPEAN ASSOCIATION OF METALS

concawe

ECHA
EUROPEAN CHEMICALS AGENCY

Main points discussed

- Focus mainly on CCA but also how it could be processed in mixture exposure scenario format
- Demonstration of the method on real examples
- Discussion about what was covered in the SDS vs exposure scenario's (eg: gloves)

cefic
Fecc
Downstream Users of Chemicals Co-ordination group
EUROMETAUX
EUROPEAN ASSOCIATION OF METALS
concawe

ECHA
EUROPEAN CHEMICALS AGENCY

General Pros

- reduces the number of substances to process
- similar process steps as DPD+
- Identification of the RDS is fully automated
- built on PNEC/DNEL as hazard identifiers
- Avoid jump of classification
- good starting point to deal with mixtures and good option on the way of automation of MES
- bottom up approach easier to apply
- the approach covers qualitative and quantitative endpoints

cefic
Fecc
DUCC
Downstream Users of Chemicals Co-ordination group
EUROMETAUX
EUROPEAN ASSOCIATION OF METALS
concawe

General Cons

- this approach can be an overshoot for “easy” mixtures
- not all environmental endpoints covered (eg: soil)
- DNEL/PNEC values not always available

Downstream Users of Chemicals Co-ordination group

ECHA
EUROPEAN CHEMICALS AGENCY

Applicability domain / limitations

- Covers all health endpoints and freshwater
- Applicability to solids in liquids and as such is still in question
- Cannot proceed substances with no DNEL/PNEC that do not contribute to classification (eg: PBT, exposure based waived DNEL)

cefic
Fecc
DUCC
Downstream Users of Chemicals Co-ordination group
EUROMETAUX
EUROPEAN ASSOCIATION OF METALS
concawe

ECHA
EUROPEAN CHEMICALS AGENCY

Practical issues in application / work-around

- How to deal with several substances some of them having DNELs and others none for the same endpoint?
- What to do if several DNELs are available (reliability of DNELs found in the CSRs / other sources)?
- General remark about these methods is the comparison of the outcomes of these methods

cefic
Fecc
DUCC
Downstream Users of Chemicals Co-ordination group
EUROMETAUX
EUROPEAN ASSOCIATION OF METALS
concawe

Minimum required training

- The first step (CCA) can be fully automated : does not need too much training
- The following steps need expert judgement

ECHA
EUROPEAN CHEMICALS AGENCY

Time required to develop the Safe use information

- The first step (CCA) can be fully automated : does not take a long time
- The following steps need more expert judgement and can then take longer

cefic
Fecc
Downstream Users of Chemicals Co-ordination group
EUROMETAUX
EUROPEAN ASSOCIATION OF METALS
concawe

ECHA
EUROPEAN CHEMICALS AGENCY

Required actions to develop the method to operational status

- Need to make the assumptions of the method more explicit and justified
- Improve the environmental analysis
- Make it adapted to ESCOM XML
- The whole output picture should not be provided to the end user

cefic

Fecc

DUCC
Downstream Users of Chemicals Co-ordination group

EUROMETAUX
EUROPEAN ASSOCIATION OF METALS

concawe

General Conclusions and recommendations from the group

- These methods have to be extensively tested
- Maybe consider the possibility of a hybrid method to pick the best things from the different methods

ECHA
EUROPEAN CHEMICALS AGENCY

Proposed follow-up action	Who should take the lead
Testing	
Comparison exercises	
Justification	

cefic
Fecc
DUCC
Downstream Users of Chemicals Co-ordination group
EUROMETAUX
EUROPEAN ASSOCIATION OF METALS
concawe

ECHA
EUROPEAN CHEMICALS AGENCY

Thank you for your attention

cefic

Fecc

DUCC
Downstream Users of Chemicals Co-ordination group

EUROMETAUX
EUROPEAN ASSOCIATION OF METALS

concawe