

Case 1 DPD+

The purpose of this case is to get some experience in using the DPD+ methodology. You can find the [guidance document for the DPD+-methodology on this platform](http://elearn.moodle2.dk/mod/resource/view.php?id=259) (<http://elearn.moodle2.dk/mod/resource/view.php?id=259>).

Q 1)

Use the Guidance document for the DPD+-methodology to identify the concentration limits for classification. Mark the below classification which cannot be handled by the DPD+-methodology and where expert judgement is required:

Xn;R22	Mut 2; R46	R42
Xi;R38	R52/53	R43
Carc 1;R45	N;R51/53	Rep 2;R60
T+;R28	R67	C;R35

Q 2)

Please tick the critical substance(s) in relation to dermal exposure (by only using the general classification concentration limits):

Mixture A)

80 % 2-Methylpyridine

Classification: R10 Xn;R20/21/22 Xi;R36/37; LSI=80/25=3.2

15 % 2,3-Dinitrophenol

Classification: T;R23/24/25 R33 N;R51/53; LSI=15/3=5

5 % Hexachlorocyclopentadiene

Classification: Xn;R22 T;R24 Tx;R26 C;R34 N;R50/53; LSI=3/5=0.6

Mixture B)

68 % Propylencarbonate

Classification: Xi;R36; LSI:-

30 % Morpholine

Classification: R10 Xn;R20/21/22 C;R34; LSI=30/5=6

2 % Sodium fluoracetate

Classification: Tx;R26/27/28 N;R50; LSI=2/0,1=20

Mixture C)

34 % o-Xylene

Classification: R10 Xn;R20/21 Xi;R38; LSI=34/25=1.36

33 % p-Xylene

Classification: R10 Xn;R20/21 Xi;R38; LSI=33/25=1.32

33 % m-Xylene

Classification: R10 Xn;R20/21 Xi;R38; LSI=33/25=1.32

The substances do also have also the same mode of action so it will correct to consider the total concentration of xylenes ...

Q 3)

Sæt X ud for det/de kritiske stof(fer) i forhold til eksponering ved indånding (ignorér her evt. stofs specifikke koncentrationsgrænser og brug de generelle):

Mixture A)

89 % n-Propyl Alcohol

Classification: F;R11 Xi;R41 **R67**

Vapor pressure: 15 Torr;

LSI= $15 \cdot 89 / 25 = 53,4$

10 % Acetonitrile

Classification: F;R11 Xn;R**20**/21/22 Xi;R36

Vapor pressure: 89 Torr

LSI= $10 \cdot 89 / 25 = 35,6$

1 % Methanol

Classification: F;R11 T;R**23**/24/25-**39**/23/24/25

Vapor pressure: 97 Torr

LSI= $1 \cdot 97 / 1 = 97$

Mixture B)

45 % o-Xylene

Classification: R10 Xn;R**20**/21 Xi;R38

Vapor pressure: 6,2 Torr

LSI= $45 \cdot 6,2 / 25 = 11,2$

45 % Pyridine

Classification: F;R11 Xn;R**20**/21/22

Vapor pressure: 18 Torr

LSI= $45 \cdot 18 / 25 = 32,4$

10 % Cyclohexane

Classification: F;R11 Xn;R65 Xi;R38 **R67** N;R50/53

Vapor pressure: 78 Torr

LSI= $10 \cdot 78 / 25 = 31,2$

Case 2 Preparation of exposure scenario for a cleaning agent

The composition of a professional cleaning agent “Multizymes” is as shown in the below table.

Table 0.1 Composition of Multizymes

CAS-RN	REACH	Name	Concentration in product (wt%)
532-32-1	01-2119460683-35-xxxx	Sodium benzoate	0.5
67-63-1	00-2119455854-00-xxxx	2-propanol	12.5
9000-90-2	01-2119938627-26-xxxx	Amylase	2
9014-01-1	01-2119480434-38-xxxx	Subtilisin	4

All substances are REACH registered and the formulator has received exposure scenarios for all substances.

The formulator wants to make a flexible, consolidated exposure scenario for the product. Therefore, he also wants to include several PROCs covering the same activity, as he knows that his customers do not handle the product in the precise same way.

The formulator has received exposure scenarios for all substances in his product – both covering his own use and his customers use.

Table 0.2 gives an overview of the customer uses of the product.

Table 0.3 gives an overview of the information of the received ES.

Table 0.4 gives an overview of the substance data.

Exercise 1: Prepare a flexible, consolidated ES (manually) for the end-use, assuming that no scaling can be used.

a) Identify the critical components for each exposure route

Below table shows the calculated LSI. From these calculations, the critical substances are identified:

- Environment: Subtilisin
- Dermal: Subtilisin
- Inhalation (dust, aerosols): Subtilisin
- Inhalation (vapor): propanol
- Eye: propanol
- Oral: not considered as no consumer use.

Substance	W_i	Exposure route	R-phrase	GR_i	LSI	Remark
Subtilisin	4	Inhalation (A,D)	R42	1	4	Include expert judgement
		Inhalation (A,D)	R37	20	0.2	
		Inhalation (V)	R42	1	4E-4	
		Inhalation (V)	R37	20	2E-5	
		Dermal	R38	20	0.2	
		Environment	R50	0.25	16	
		Eye	R36	20	0.2	
Propanol	12.5	Inhalation (A,D)	R67	25	0.5	
		Inhalation (V)	R67	25	3025	
		Dermal			-	
		Environment			-	
		Eye	R36	20	0.625	
Amylase	4	Inhalation (A,D)	R42	1	2	Include expert judgement
		Inhalation (V)			2E-4	
		Dermal			-	
		Environment			-	
		Eye			-	
Benzoic acid sodium	0.5	Inhalation			-	
		Dermal			-	
		Environment			-	
		Eye	R36	20	0.025	

b) for each exposure route, collect the relevant operational conditions (OP) and relevant Risk Management Measures (RMMs) from the ES for the critical components

See below table

Activity	Process category	Inhalation (critical substance propanol (vapor), subtilisin (aerosols))				Respiratory Protection	Dermal (critical substance: subtilisin) Gloves	Eye (critical substance propanol) Goggles	Environment (critical component: subtilisin) Amount per year
		Aerosols	Inhalation (propanol (vapor))	LEV					
Transfer of industrial detergent, maintenance or disinfectant (charging/discharging) to a dedicated cleaning equipment	PROC8a	No	>4 hr/d	No	No	Yes	Yes	The amount of subtilisin should not exceed 10 kg per year – this corresponds to 2500 kg product per year	
Transfer of industrial detergent, maintenance or disinfectant (charging/discharging) to a dedicated cleaning equipment	PROC8b	No	>4 hr/d	No	No	Yes	Yes		
Dilution of cleaning agent	PROC5	No	>4 hr/d	No	No	Yes	No		
Using a diluted industrial cleaning solution in a closed cleaning equipment	PROC1	No	>4 hr/d	No	No	No	No		
Using a diluted industrial cleaning solution in a semi closed cleaning equipment	PROC2	No	>4 hr/d	No	No	Yes	No		
Using the diluted product in a dedicated equipment; opportunity for exposure arises	PROC4	No	>4 hr/d	No	No	Yes	No		
Spraying of cleaning product.	PROC11	Yes	<15 min/d	No	Half-mask	Yes	Yes		
Brushing an industrial cleaning solution	PROC10	No	>4 hr/d	No	No	Yes	Yes		
Brushing a diluted cleaning or product (after spraying)	PROC10	No	>4 hr/d	No	No	Yes	Yes		
Treatment of articles by dipping or pouring with product	PROC13	No	>4 hr/d	No	No	Yes	Yes		
Quality control of products	PROC15	No	>4 hr/d	No	No	Yes	Yes		

c) select the most conservative RMMs and OPs (from above) and prepare the final list of RMMs and OPs

No conflict between the RMMs and OPs so the upper table shows the consolidated ES.

Exercise 2: Prepare a flexible, consolidated ES (using ES-Creator) for the end-use, assuming that scaling using the exposure models is allowed. *Note that the substances and their properties already are defined in ES-Creator.*

See file: Exercise_2_solution.pdf

Table 0.2 End use of Multizymes

Life cycle stage DoU	Process categories	Amount	Conc. (%)	Duration per day (min)	Outdoor	Indoor with LEV	Indoor without LEV	Respiratory Protection	Eye protection (goggles)	Protection of hands (gloves)
End use PC35	Activity	<2000 kg/year	Concentration of product							
ERC 4	Transfer of industrial detergent, maintenance or disinfectant (charging/discharging) to a dedicated cleaning equipment (machine/vessel)	PROC8a	100	60	No	No	Yes	No	Yes	Yes
SU 20	Transfer of industrial detergent, maintenance or disinfectant (charging/discharging) to a not-dedicated cleaning equipment (bucket or similar)	PROC8b	100	60	No	No	Yes	No	Yes	Yes
	Dilution of cleaning agent	PROC5	10	15	No	No	Yes	No	Yes	Yes
	Using a diluted industrial cleaning solution in a closed cleaning equipment	PROC1	10	480	No	No	Yes	No	No	No
	Using a diluted industrial cleaning solution in a semi closed cleaning equipment	PROC2	10	480	No	No	Yes	No	No	No
	Using the diluted product in a dedicated equipment; opportunity for exposure arises	PROC4	10	480	No	No	Yes	No	No	No
	Pressure spraying of a diluted industrial cleaning product.	PROC 11	10	480	No	No	Yes	Yes	Yes	Yes
	Brushing an industrial cleaning solution	PROC10	100	480	No	No	Yes	No	Yes	Yes
	Brushing a diluted cleaning or product (after spraying)	PROC10	10	480	No	No	Yes	No	Yes	Yes
	Treatment of articles by dipping or pouring with product	PROC13	100	220	No	Yes	No	No	Yes	Yes
	Quality control of products	PROC15	100	60	No	No	Yes	No	Yes	Yes

Table 0.3 Overview of received ES for the ingredients. Life cycle stage: End-use. SU: SU 20. ERC: ERC 4. PC: PC35

Activity	ERC	sodium benzoate	Yearly amount						Yearly amount					Yearly amount				
			2-propanol						Amylase					Subtilisin				
Activity	Process category	sodium benzoate	Max conc. Of substance (wt%)	Max duration	LEV	Respiratory Protection	Gloves	Goggles	Max conc. Of substance (wt%)	Max duration	LEV	Respiratory Protection	Gloves	Max conc. Of substance (wt%)	Max duration	LEV	Respiratory Protection	Gloves
Industrial end-use as cleaning agents	ERC 4	-	<10,000 kg/year						<500 kg/year					<10 kg/year				
Transfer of industrial detergent, maintenance or disinfectant (charging/discharging) to a dedicated cleaning equipment	PROC8a	-	100	>4 hr/d	No	No	No	Yes	5	>4 hr/d	No	No	Yes	5	>4 hr/d	No	No	Yes
Transfer of industrial detergent, maintenance or disinfectant (charging/discharging) to a dedicated cleaning equipment	PROC8b	-	100	>4 hr/d	No	No	No	Yes	5	>4 hr/d	No	No	Yes	5	>4 hr/d	No	No	Yes
Dilution of cleaning agent	PROC5		100	>4 hr/d	No	No	No	No	5	>4 hr/d	No	No	Yes	5	>4 hr/d	No	No	Yes
Using a diluted industrial cleaning solution in a closed cleaning equipment	PROC1	-	100	>4 hr/d	No	No	No	No	5	>4 hr/d	No	No	No	5	>4 hr/d	No	No	No
Using a diluted industrial cleaning solution in a semi closed cleaning equipment	PROC2	-	100	>4 hr/d	No	No	No	No	5	>4 hr/d	No	No	Yes	5	>4 hr/d	No	No	Yes
Using the diluted product in a dedicated equipment; opportunity for exposure arises	PROC4	-	100	>4 hr/d	No	No	No	No	5	>4 hr/d	No	No	Yes	5	>4 hr/d	No	No	Yes
Spraying of cleaning product.	PROC11	-	100	>4 hr/d	No	No	No	Yes	5	<15 min/d	No	Half-mask	Yes	5	<15 min/d	No	Half-mask	Yes

Activity	ERC	sodium benzoate	Yearly amount						Yearly amount					Yearly amount				
			2-propanol						Amylase					Subtilisin				
Industrial end-use as cleaning agents	ERC 4	-	<10,000 kg/year						<500 kg/year					<10 kg/year				
Activity	Process category	sodium benzoate	Max conc. Of substance (wt%)	Max duration	LEV	Respiratory Protection	Gloves	Goggles	Max conc. Of substance (wt%)	Max duration	LEV	Respiratory Protection	Gloves	Max conc. Of substance (wt%)	Max duration	LEV	Respiratory Protection	Gloves
Brushing an industrial cleaning solution	PROC10	-	100	>4 hr/d	No	No	No	Yes	5	>4 hr/d	No	No	Yes	5	>4 hr/d	No	No	Yes
Brushing a <u>diluted</u> cleaning or product (after spraying)	PROC10	-	100	>4 hr/d	No	No	No	Yes	5	>4 hr/d	No	No	Yes	5	>4 hr/d	No	No	Yes
Treatment of articles by dipping or pouring with product	PROC13	-	100	>4 hr/d	No	No	No	Yes	5	>4 hr/d	Yes	No	Yes	5	>4 hr/d	Yes	No	Yes
Quality control of products	PROC15	-	100	>4 hr/d	No	No	No	Yes	5	<4 hr/d	Yes	No	Yes	5	<4 hr/d	Yes	No	Yes

Table 0.4 Overview of substance data.

CAS_RN	EINECS	Name	logKow	Physical state	Psat (Pa)	Psat_temp (°C)	Sw (mg/L)	Sw_temp (°C)	Biodegradability	Mw	Melting_point (°C)	Boiling_point (°C)	EU_Classification	CLP_Classification
532-32-1	208-534-8	Benzoic acid, sodium salt	1.88	Slightly dusty solid	4.90E-07	25	556000	25	RB	144.1	436	450	Xi; R36	Eye Irrit. 2A H319
67-63-0	200-661-7	propan-2-ol	0.05	Liquid	6050	25	1000000	25	RB	60.1	-89.5	82.3	F; R11 Xi; R36	Flam. Liquid 2 H225; Eye Irrit. 2 H319; STOT Single Exp. 3 H336
9000-90-2	232-565-6	Amylase, α -	-2.95	Slightly dusty solid	1.00E-20	25	1000000	25	RB	1000	50	500	R42	Resp. Sens. 1 H334
9001-62-1	232-619-9	Lipase, triacylglycerol	-3.1	Slightly dusty solid	1.00E-20	25	1000000	25	RB	1000	50	500	R42	Resp. Sens. 1 H334
9014-01-1	232-752-2	Subtilisin	-3.1	Slightly dusty solid	1.00E-20	25	1000000	25	RB	1000	50	500	Xn; R22 Xi; R36/37/38 R42 N; R50	Acute Tox. 4 H302; Skin Irrit. 2 H315; Eye Irrit. 2 H319; Resp. Sens. 1 H334; Aquatic Acute 1 H400

RB: Readily biodegradable