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APPENDIX A: **Questionnaire for the expert judgment study**

Questionnaire on chemical process route selection based on assessment of inherent environmental hazard, occupational health and safety

Dear Expert,

    I am doing a research to assess chemical process routes based on their hazards on the environment, occupational health and safety. For this research, I am in the process of gathering data on expert opinion from several experts. Therefore I would appreciate if you could fill the questionnaire overleaf as a support for my research.

Thank you,

Sureshinie Warnasooriya

(Researcher)

Please fill the following:

Name of the Expert:

Designation:

Expertise area:

Date:

Questionnaire

1. Chemical plants under normal daily operational conditions release chemical pollutants into aquatic, atmospheric and terrestrial environments. These emissions cause environmental impacts. Based on your opinion please state whether aquatic environmental impacts or terrestrial environmental impacts or atmospheric environmental impacts are relatively more important.

   Allocate;

   > 3 - most important environment
   > 2 - intermediately important environment
   > 1 - least important environment

Environment	Value
Aquatic	
Atmospheric	
Terrestrial	

2. Environment, safety and occupational health can be damaged due to daily operations and resulting emissions in chemical process plants. According to your opinion, allocate marks (out of 100) for these three damage categories.

   In your opinion:

   - Whether damages to environment are more important compared to damages to health during occupational activities.
   - Whether damages to environment are more important compared to damages due to safety aspects.
   - Whether damages to health during occupational activities are more important compared to damages due to safety aspects.

   Please give more marks to the more important damage category based on your opinion.

Damage category	Marks
Environment	
Occupational health	
Safety	
Total	**100**

: **Database of pre-calculated fugitive emission rates for process module stream developed in the estimation of fugitive emissions**

Process Module (fugitive emission rate, kg/h)												
Stream	Service	Absorber	Stripper		Flash	LEX	Ion exch	CSTR	PFR	Distillation		Total Comp
			Normal	Vacuum						Normal	Vacuum	
Feed 1	G/V	0.024	0.117	0	0.057		0.052	0.102	0.059	0.044	0	0.454
	LL		0.098	0	0.053	0.048	0.044	0.082	0.127	0.036	0	
	HL		0.060	0	0.046	0.025	0.029	0.044	0.082	0.021	0	
Feed 2	G/V							0.110	0.063			
	LL	0.113					0.235	0.088	0.052			
	HL	0.063					0.125	0.046	0.029			
Outlet 2/3	G/V	0.109	0.002		0.021		0.123		0.163	0.025	0	
	LL	0.464	0.225			0.055	0.100	0.560	0.271	0.405	0.239	
	HL	0.324	0.127			0.036	0.054	0.378	0.156	0.254	0.137	
	G&LL mix								0.498			
	G&HL mix								0.380			
Outlet 3/4	G/V											
	LL	0.236	0.159	0	0.301	0.097				0.217	0.139	
	HL	0.134	0.094	0	0.165	0.059				0.137	0.082	
G:gas, V:vapour, LL: light liquid, HL: heavy liquid, mix: mixture, LEX: liquid-liquid extractor, ion exch: ion exchanger, and comp: compressor												

source: (Hassim et al., 2010)

Explanation on fluid streams: G/V - Gas/Vapour stream
LL   - liquid stream mainly contains chemicals with atmospheric vapour pressure > 0.3 kPa
HL   - other than gas and light liquid services

APPENDIX C: Pre-calculated area estimates of standard process modules

Process Module	Process floor area of the module (m²)
Absorber	82
Liquid Extractor	48
Stripper	147
Flash evaporator	72
Distillation	129
Ion Exchanger	28
PFR	108
CSTR	95

(Source: Hassim et al., 2010)

APPENDIX D — Expert judgment results for relative importance of safety parameters

Expert judgment results used in this work was taken from Lawrence, (1996), in his study on 'assessing inherent safety' to find the importance of safety parameters. Eight experts have been selected and they were asked to indicate the importance of various parameters used to assess process routes on safety. According to their indications "5" means a parameter that is very important and "1" means it is not important. They were also asked to indicate "Essential" considering whether the parameter is essential for assessing inherent safety according to their opinion. The total score for each parameter represents its importance. The fourth expert has not responded and therefore no results are indicated in the table (Lawrance, 1996).

Table D.1 Expert judgment results used in determining CRSI (considering the results of Lawrence's (1996) study)
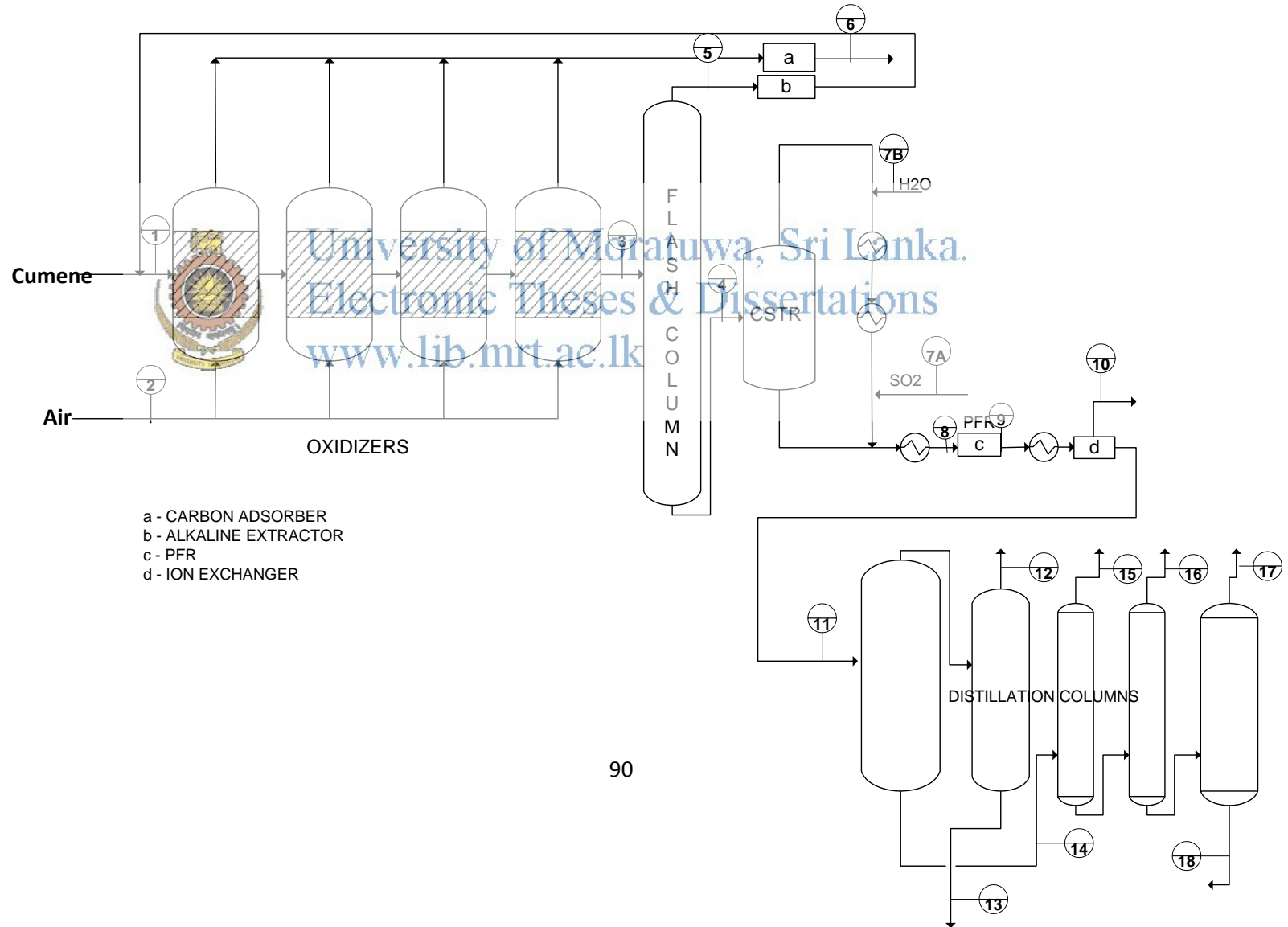
Parameter	Expert								Total
	1	2	3	4	5	6	7	8	
Inventory	5	5	5		5	5	5	5	35
Reactivity	5	5	2		5	5	3	5	30
Temperature	3	2	5		5	5	3	5	28
Pressure	3	3	5		3	5	3	3	25
Flammability	4	5	5		-	5	4	2	25
Explosiveness	5	5	5		-	-	4	3	22

NOTE: Expert judgment results for Reactivity parameter considered in this work are the same as those results given for Chemical stability in Lawrence's study (1996).
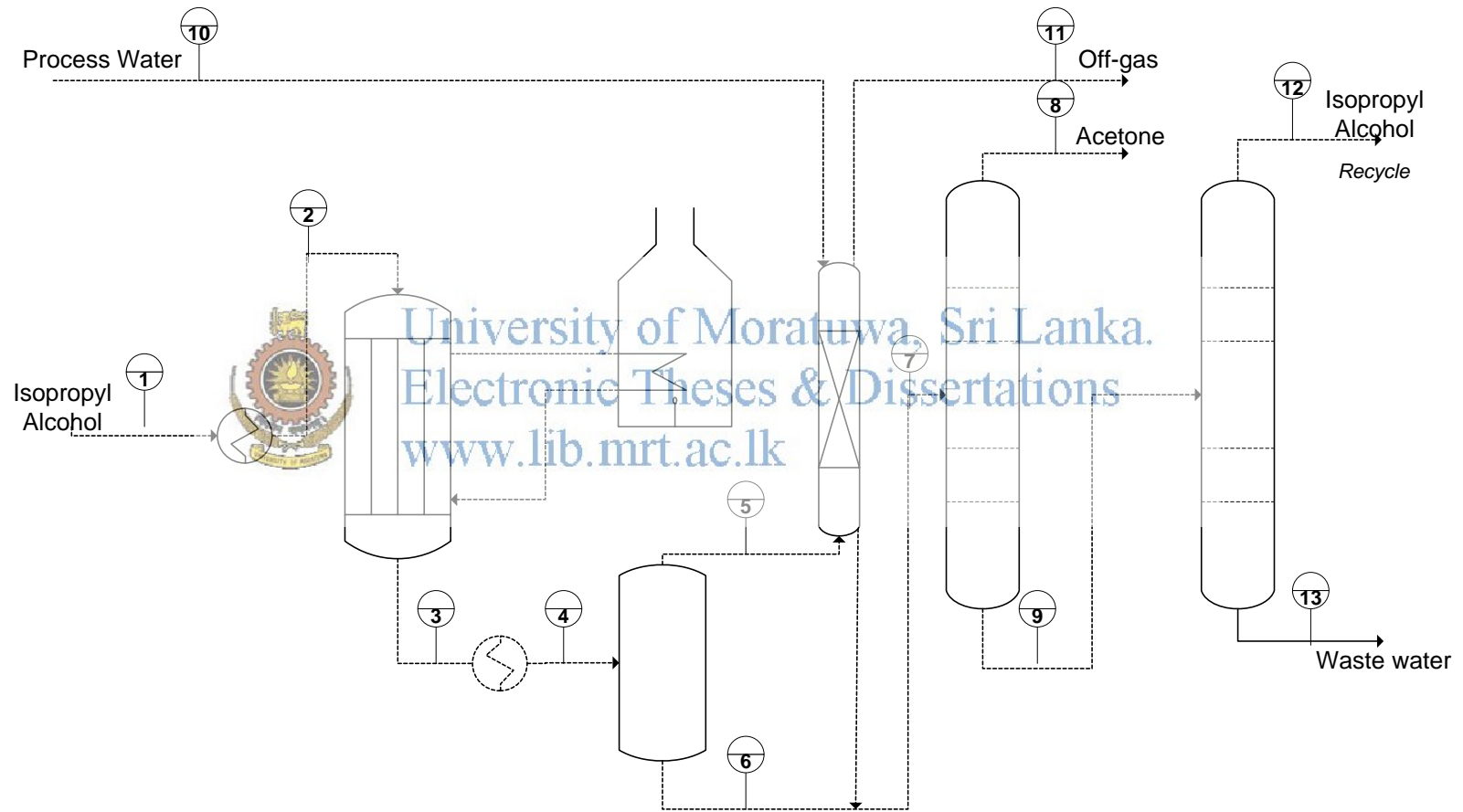
G.1   PFD for Cumene oxidation route (R1)

Cumene

Air

OXIDIZERS

FLASH COLUMN

CSTR

H2O

SO2

PFR

a - CARBON ADSORBER
b - ALKALINE EXTRACTOR
c - PFR
d - ION EXCHANGER

DISTILLATION COLUMNS

G.2   PFD for 2-Propanol dehydrogenation route (R2)

G.3   PFD for Propene direct oxidation route (R3)
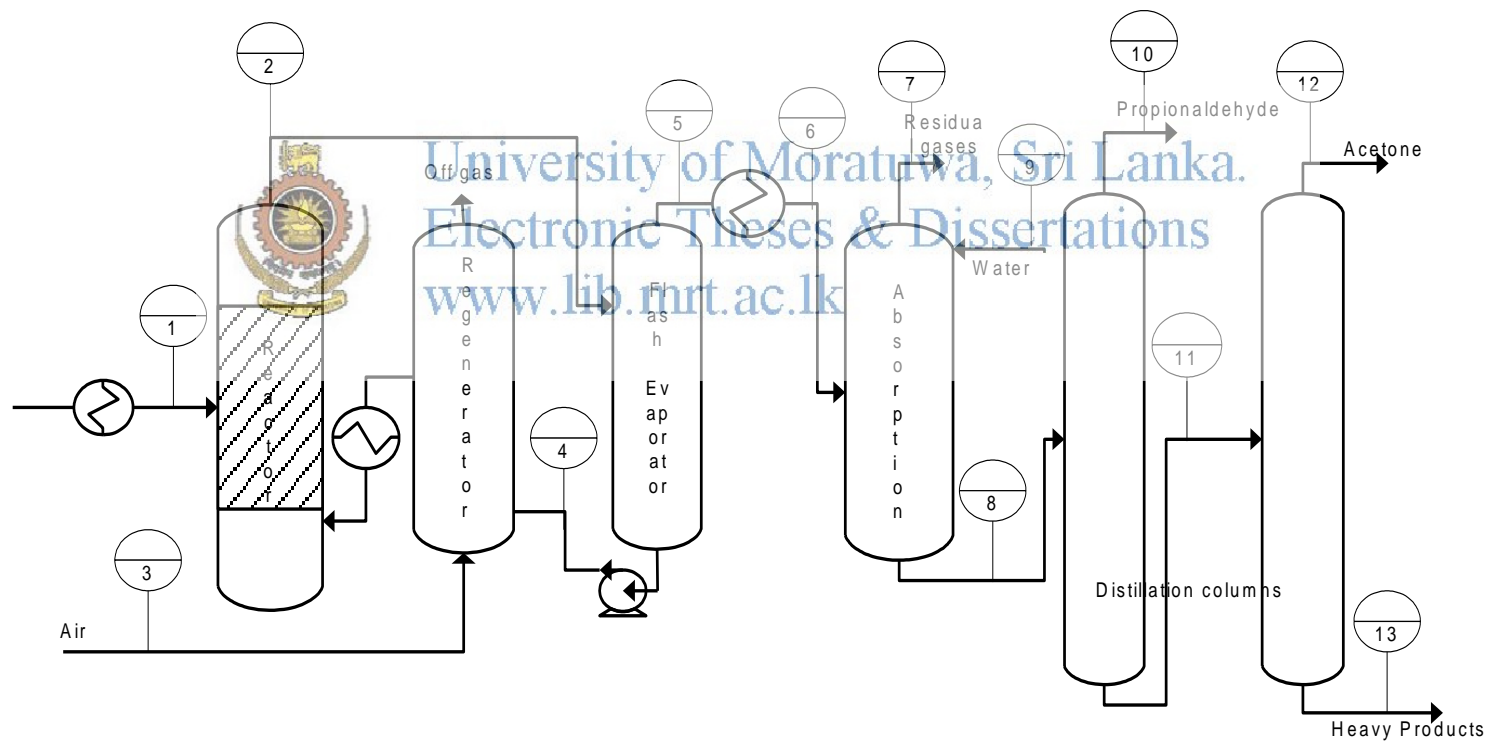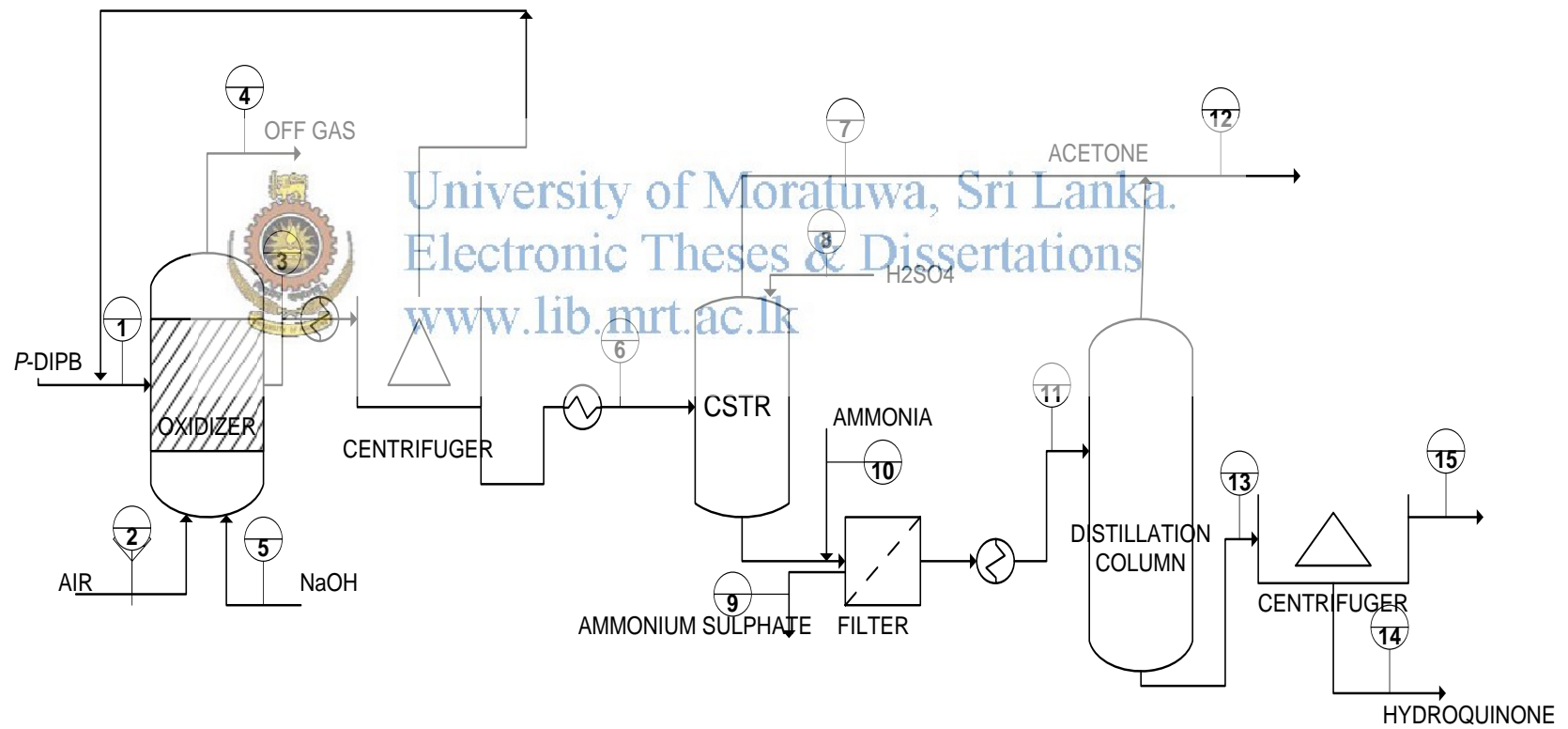
APPENDIX F　　　　　　　**Total chemical inventory present**

in Acetone manufacturing routes

Route	Chemical	Total Inventory in the plant (t)
R1	Cumene	582.58
	Cumene Hydroperoxide	63.39
	Dimethylphenylmethanol	2.55
	Acetophenone	3.67
	Dicumylperoxide	2.34
	Acetone	42.85
	Phenol	93.36
	α-Methylstyrene	2.24
	Sulfur Dioxide	0.01
R2	IPA	22.26
	Acetone	33.00
	Hydrogen	0.98
	Propene	1.45
R3	Propene	14.59
	Acetone	34.55
	Propanal	1.26
	Dichloroacetone	0.78
	HCl	0.25
R4	Acetone	17.76
	Hydroquinone	18.17
	p-DIPB	159.11
	p-DIPB-DHP	92.01
	C-HPO	32.86
	A-HPO	6.60
	NH_4SO_4	1.11
	NaOH	1.24
	Sodium formate	1.08

APPENDIX G Chemical inventory emitted to the environment and Predicted Environmental Concentrations of chemicals in the environment

Route	Chemical	Chemical Inventory emitted to the environment (mol/h)	Predicted Environmental Concentration (PEC)		
			Water (molm^{-3})	Atmosphere (molm^{-3})	Soil (molm^{-3})
R1	Cumene	117706.04	0.0025	0.0011	0.1414
	Cumene Hydroperoxide	8247.21	0.1400	0.0001	0.2488
	Dimethylphenylmethanol	0	0	0	0
	Acetophenone	9538.85	0.2974	0.0001	0.1391
	Dicumylperoxide	0	0	0	0
	Acetone	34876.43	1.3877	0.0046	0.0098
	Phenol	3577.07	0.1582	0	0.0561
	α-Methylstyrene	587.87	0	0	0.0001
	Sulfur Dioxide	0	0	0	0
R2	IPA	1146.45	0.0459	0	0.0006
	Acetone	1622.26	0.0660	0.0002	0.0005
	Hydrogen	324452.84	0.0001	7.8031	0
	Propene	22927.07	0	0	0
R3	Propene	3455.17	0	0	0
	Acetone	2128.12	0.0866	0.0003	0.0006
	Propanal	1368.25	0.0014	0	0.0001
	Dichloroacetone	3426.62	0.1992	0.0005	0.0039
	HCl	0	0	0	0
R4	Acetone	7247.22	0	0	0
	Hydroquinone	165.04	0.0122	0	0.0006
	p-DIPB	53685.90	0.0002	0.0003	0.1602
	p-DIPB-DHP	17829.69	3.1450	0	8.0822
	C-HPO	58416.35	0.6743	0.0006	0.7392
	A-HPO	12699.21	-	-	-
	NH$_4$SO$_4$	5610.28	0.0666	0.0113	0.0025
	NaOH	2539.34	0.4693	0	0.0091
	Sodium formate	12699.21	0.5445	0	0

- No data

STEP 1:   Calculation of Predicted Environmental Concentration (PEC)

PEC calculation is shown here for a total direct emission rate of 117704.06 mol/h Cumene, determined based on material balance calculations for Cumene oxidation route.

Step 1.a: **Calculation of fugacity capacity constant, Z (mol/ (m³.Pa) values**

Table H.1: Fugacity capacity values

Compartment	Z definition (Mackay, 2001)	For Cumene in cumene oxidation route
Air	$Z_A = 1/RT$	$Z_A = 0.0004$ R = 8.314 (gas constant -Pa m³/mol K) T =298.15 (absolute temperature -K)
Water	$Z_W = 1/H = C^S/P^S = Z_A/K_{AW}$	$Z_W = 0.0009$ H – Henry's law constant (Pa m³/mol) C^S =0.51 (Solubility in water - mol/m³) P^S =599.95 (vapor pressure -Pa) K_{AW} – Air-Water partition coefficient
Soils	$Z_S = L K_{OC} Z_W (\rho_S/1000)$ $K_{OC} = 0.41 K_{OW}$ $K_{OW} = 4570.88$	$Z_S = 0.0506$ K_{OC} – Organic carbon-Water Partition coefficient L = 0.02 (mass fraction organic carbon) K_{OW} – Octanol-Water Partition coefficient $\rho_S = 1500$ (density of soil - kg/m³)
Sediment (Bottom , Suspended)	$Z_S = L K_{OC} Z_W (\rho_S/1000)$ $K_{OC} = 0.41 K_{OW}$ $K_{OW} = 4570.88$	$Z_S = 0.1012$ K_{OC} – Organic carbon-Water Partition coefficient L = 0.04 (mass fraction organic carbon) K_{OW} – Octanol-Water Partition coefficient $\rho_S = 1500$ (density of sediment - kg/m³)
Biota	$Z_B = L K_{LW} Z_W (\rho_B/1000)$ $K_{LW} = K_{OW}$ $K_{OW} = 4570.88$	$Z_B = 0.1975$ K_{OC} – Organic carbon-Water Partition coefficient L = 0.048 (mass fraction organic carbon) K_{OW} – Octanol-Water Partition coefficient $P_B = 1000$ (density of sediment - kg/m³)

Step 1.b: **Calculation of fugacity, f (Pa) values**

Fugacity level II model is used for emissions from a plant due to daily operating conditions with the assumption that no advective emission inflow or outflow in the selected environment. Direct emission rate is obtained according to the material balance and process flow diagram. It is assumed that reactions of emissions follow simple first order kinetics.

$f = I/\Sigma D_T$

f - Fugacity (Pa)

I – Total input rate (mol/h) = Advective input rate + Direct input rate

$D_T = D_R + D_A$; D_R - D reaction, D_A - D advection, $D_R = VZk$

V – Volume (m^3)

Z - Fugacity capacity constant

k – Rate constant (1/h) = 0.693/t

t – Residence time (h)

Table H.2: ΣD_T determination for level II fugacity model

Compartment	Z	t	k	V	D_T
Air	0.0004	39.5	0.0175	6.00E+09	42106.33
Water	0.0009	360	0.0019	7.00E+09	12.13
Soil	0.0506	720	0.0010	4.50E+04	2.19
Sediment	0.1012	3240	0.0002	2.10E+09	0.45
				ΣD_T	**42121.10**

The steady state fugacity f, which is common for all compartments;

$f = I/\Sigma D_T$

I =   0 + 117706.04 mol/h

f =   117706.04/ 42121.10 =   **2.79** Pa

Step 1.c: Calculation of Predicted Environmental Concentration

$$PEC_i = Z_i f$$

Where;

PEC_i = PEC of ith compartment Z_i = Z for i^{th} compartment

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Table H.3: Predicted Environmental Concentration of environment compartments

Compartment	Z (Pa)	f (mol/Pa.m³)	PEC (mol/m³)
Air	0.0004	2.79	0.0011
Water	0.0009	2. 79	0.0025
Soil	0.0506	2. 79	0.1414
Sediment	0.1012	2. 79	0.2828

STEP 2: Calculation of ETHI

Step 2.a: Calculation of Chemical Water Hazard Index (CWHI)

For Cumene;

$$CWHI_i = \frac{PEC_{wi}}{ChV_i} = \mathbf{0.66}$$

$PEC_{wi} = 0.0025$ mol/m³
$ChV_i = 0.0038$ mol/m³ (ECOSAR value for Daphnid)

Step 2.b: Calculation of Chemical Terrestrial Hazard Index (CTHI)

For Cumene;

$$CTHI_i = \frac{\left[\dfrac{TDI_{wx}PEC_{wi}}{\rho_w} + \dfrac{TDI_{fx}PEC_{si}}{\rho_s}\right]}{oralChL_{xi}} \times M_i = \mathbf{0.01}$$

$PEC_{wi} = 0.0025$ mol/m³ $PEC_{si} = 0.1414$ mol/m³

$TDI_{wx} = 100$ mg/kg/day $TDI_{fx} = 50$ mg/kg/day

$\rho_w = 1500$ kg/m³ $\rho_s = 1000$ kg/m³

$oralChL_{xi} = 1400$ Rat oral mg/kg $M_i = 120.19 \times 10^{-3}$ kg/mol

Step 2.c: Calculation of Chemical Atmospheric Hazard Index (CAHI)

For Cumene;

$$CAHI_i = \frac{PEC_{ai}}{inhChL_i} = \mathbf{0.31}$$

PEC_{ai} = 0.0011 mol/m^3

$inhChL_i$ = 0.0036 mol/m^3 (Sub chronic inhalation toxicity for rats)

Step 2.d: Evaluation of RWHI, RTHI and RAHI for cumene oxidation route

$$RWHI = \sum_{i=1}^{n} CWHI_i = 17.48 = \qquad 1$$

$$RTHI = \sum_{i=1}^{n} CTHI_i = 0.23$$

$$RAHI = \sum_{i=1}^{n} CAHI_i = 2.42 = \qquad 1$$

Table H.4: CWHI, CTHI, CAHI for Cumene oxidation route

Chemical	CWHI	CTHI	CAHI
Cumene	0.66	0.01	0.31
Cumene HydroPeroxide	**4.02**	0.18	0.07
Dimethylphenylmethanol	NE	NE	NE
Acetophenone	**3.73**	0.01	0.31
Dicumylperoxide	NE	NE	NE
Acetone	0.66	0.01	0.11
Phenol	**8.41**	0.03	**1.59**
α-Methylstyrene	NE	NE	NE
Sulfur Dioxide	NE	NE	NE

NE: No Emission

Note:

In the situation where the RWHI, RTHI and RAHI exceed 1 it is considered as 1.

Environmental Toxicity Hazard Index (ETHI) for cumene oxidation route is calculated using the following equation.

ETHI = W_W * RWHI + W_A * RAHI + W_T * RTHI

Then substituting the W_W = 0.41, W_A = 0.34, W_T = 0.25 and RWHI, RTHI, RAHI

ETHI = 0.81

APPENDIX I   Process modules considered in OhHI evaluation

Table I.1:   For Cumene oxidation route

Process module	No. of modules
Plug flow reactor (PFR)	5
Flash evaporator	1
Absorber	1
Distillation unit	5
Ion exchanger	1
CSTR	1

Table I.2:   For IPA dehydrogenation route

Process module	No. of modules
Plug flow reactor (PFR)	1
Flash evaporator	1
Absorber	1
Distillation unit	2

Table I.3:   For Propene oxidation route

Process module	No. of modules
Plug flow reactor (PFR)	2
Flash evaporator	1
Absorber	1
Distillation unit	2

Table I.4:   For p-Diisopropylbenzene oxidation route

Process module	No. of modules
Plug flow reactor (PFR)	1
CSTR	1
Filter	1
Distillation unit	1
Centrifuge	2

Table I.5: Fugitive emission rates of chemicals present in Acetone manufacturing routes, workplace chemical concentration and chemical exposure limit values

Route	Chemical	Fugitive Emission Rate (kg/hr)	Workplace Chemical Concentration (mg/m³)	Chemical Exposure Limit(mg/m³)
R1	Cumene	1.15	0.308	245
	Cumene Hydroperoxide	0.64	0.1720	-
	Dimethylphenylmethanol	0.02	0.0065	10
	Acetophenone	.11	0.0281	49
	Dicumylperoxide	0.01	0.0030	-
	Acetone	1.41	0.376	2400
	Phenol	1.56	0.417	19
	α-Methylstyrene	0.43	0.116	240
	Sulfur Dioxide	0.11	0.029	13
R2	IPA	0.53	0.2302	980
	Acetone	1.13	0.4931	2400
	Hydrogen	0.07	0.0324	-
	Propene	0.11	0.0476	860
R3	Propene	0.12	0.0456	860
	Acetone	0.60	0.2391	2400
	Propanal	0.07	0.0266	48
	Dichloroacetone	0.03	0.0111	-
	HCl	0.13	0.0503	7
R4	Acetone	0.35	0.155	2400
	Hydroquinone	0.36	0.1597	2
	p-DIPB	0.23	0.1015	-
	p-DIPB-DHP	0.15	0.0647	-
	C-HPO	0.32	0.1427	10
	A-HPO	0.07	0.0287	-
	NH₄SO₄	0	0	10
	NaOH	0.03	0.0116	2
	Sodium formate	0.003	0.0013	9

- No data

APPENDIX J   **Example calculation for OhHI**

This example calculation was done for Cumene oxidation route.

STEP 1:   Quantification of Fugitive Emissions rate, FE_i

   Process modules present in the Cumene oxidation route were identified as Flash evaporator, Ion exchanger, CSTR, two PFRs and five distillation columns. Fugitive emission rate of each chemical present in the route was calculated by considering pre-calculated fugitive emission rates of process modules in appendix B and chemical composition of each flow according to the material balance.

   For cumene,   FE   = 1.15 kg/h

STEP 2:   Calculation of volumetric air flow rate, V

   According to the appendix C,

   Total floor area of process modules = 1380 m^2

   Following the procedure described is section 3.3,

   Volumetric air flow rate   = 3744553.81 m^3/h

STEP 3:   Workplace Chemical Concentration Calculation, WCC_i

   According to the equation 15,

   WCC= FE x 10^6/ V = 0.308 mg/m^3 for cumene

STEP 4:   Occupational health Hazard Index Calculation, OHI

   For cumene, CEL = 245 mg/m^3 (8-hrs PEL defined by OSHA)

   $$\frac{WCC}{CEL} = 0.0013$$

   According to the availability of data, contribution to OhHI by chemicals present in the Cumene oxidation route is shown in table J.I.

Table J.1: Contribution to OhHI by Chemicals in the Cumene oxidation route

Chemical	WCC_i / CEL_i
Cumene	0.0013
Cumene HydroPeroxide	-
Dimethylphenylmethanol	0.0006
Acetophenone	0.0006
Dicumylperoxide	-
Acetone	0.0002
Phenol	**0.0219**
α-Methylstyrene	0.0005
Sulfur Dioxide	0.0023

- denotes the chemicals for which data are not available on human exposure limits

From the equation (21),

$$OhHI = \sum_{i=1}^{n} \frac{WCC_i}{CEL_i}$$

Then OhHI for Cumene oxidation route is **0.0273**.

APPENDIX K   Example calculation for CRSI

Flammability, reactivity, explosiveness, inventory, temperature and pressure of the cumene oxidation route were scored as described in section 3.4.1. Calculation procedure for CRSI is presented below step by steps.

STEP 1:   Scoring inherent safety assessing parameters

Flammability and Reactivity of each chemical in the route were scored according to the NFPA ranks and explosiveness is scored by considering the difference in lower and upper explosive limits. Scores for chemical inventory were given according to the table 3.5 in chapter 3. Separate indices were calculated on these parameters by considering their relevant scores and are shown in table K.I.

Table K.1: Scores for Chemical Safety assessing parameters

| Chemical	Inventory		Flammability		Reactivity		Explosiveness	
	tonnes	InI	NFPA	FI	NFPA	RI	E	EI
Cumene	581.58	**1.0**	3	**0.75**	1	0.25	5.6	0.06
CHP	63.39	0.6	2	0.50	4	**1.00**	5.6	0.06
DMPM	2.55	0.2	2	0.50	0	0.00	-	-
AP	3.67	0.2	2	0.50	0	0.00	5.6	0.04
DCP	2.34	0.2	2	0.50	2	0.50	2.7	0.03
Acetone	42.85	0.6	3	**0.75**	0	0.00	10.2	**0.10**
Phenol	93.36	0.6	2	0.50	0	0.00	6.9	0.07
AMS	2.24	0.2	2	0.50	1	0.25	4.2	0.04
SO$_2$	0.01	0.0	0	0.00	-	0.00	0.00	-

Selected process safety assessing parameters Temperature and Pressure are assessed by reaction step wise. The Cumene oxidation route consists of two main reaction steps.

Reaction Step 1:
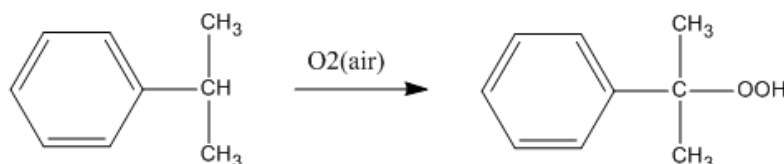
Reaction Step 2:
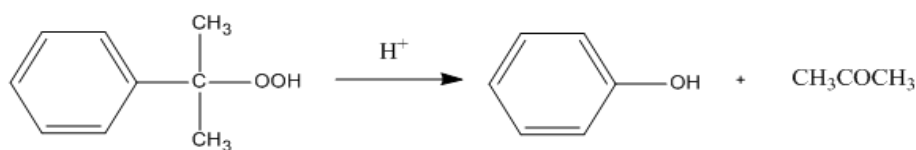
Process conditions for two reaction steps are as below.

Process Parameter	Reaction Step 1	Reaction Step 2
Temperature (^{0}C)	100	70
Pressure (atm)	1	0.987

Temperature Index (TI) and Pressure Index (PI) are calculated according to the tables 3.6 and 3.7 respectively. TI and PI values on two reaction steps of Cumene oxidation route are tabulated in table K.2.

Table K.2: Scores for Process Safety assessing parameters

	Reaction Step 1	Reaction Step 2
Temperature Index (TI)	**0.31**	0.20
Pressure Index (PI)	0.00	**0.06**

STEP 2: Chemical Safety Index & Process Safety Index Calculation

Maximums of inventory, flammability, reactivity and explosiveness indices of the route were combined according to the equation (25) to calculate Chemical Safety Index (CSI).

$$CSI = 0.21\max_{i=1..n}(InI_i) + 0.18\max_{i=1..n}(RI_i) + 0.15\max_{i=1..n}(FI_i) + 0.14\max_{i=1..n}(EI_i)$$

CSI = 0.21*1 + 0.18*1 + 0.15*0.75 + 0.14*0.10   = 0.52

Similar to the CSI, maximums of TI and PI are combined to calculate Process Safety Index (PSI) according to the equation (26).

$$PSI = 0.17\max_{j=1...m}(TI_j) + 0.15\max_{j=1...m}(PI_j)$$

PSI = 0.17*0.31 + 0.15*0.06   = 0.06

STEP 3: Calculation of CRSI

For Cumene oxidation route, CRSI is calculated according to the equation (27).

CRSI = 0.58