# **ORGANIC CHEMICAL INDUSTRY**

# **DOWNSTREAM UNITS**

# ORGANIC CHEMICAL INDUSTRY EXCEPT STEAM CRACKING, PVC PRODUCTION BY SUSPENSION PROCESS AND SPECIALITY ORGANIC CHEMICAL INDUSTRY

# SYNOPSIS SHEET

Prepared in the frame work of EGTEI

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## 1. Activity description and EGTEI contribution

In order to estimate costs of NMVOC emission reduction in the organic chemical industry, it was decided to split it into 4 sections and to consider an illustrative example for representing each of these sections [1]. The four sections are as follows:

- The steam cracking process with naphtha as feedstock and ethylene and propylene as products is considered as the illustrative example taken into account for representing all the production of lower olefins (ethylene, propylene, butanes and butadienes). Within the EC, there are 50 steam crackers and these are located on 39 sites [2].
- The PVC suspension process for representing a production of chemicals with sanitary impact.
- A process of the downstream chemistry for representing production of chemicals except the steam crackers, the PVC production and the speciality chemical industry. This production can be also representative of no sanitary impact unit.
- Production of pharmaceutical active ingredients representing the speciality chemical industry (production in batch processes and multipurpose plants).

In the three first activities NMVOC emissions are due to processes themselves, in the last one NMVOC emissions originate from solvent uses.

This synopsis sheet is related to down stream units only that is to say all types of organic chemical productions except the production of ethylene and propylene by the steam cracking process, the production of PVC by the suspension process and the speciality organic chemical industry. In fact this sector is assumed to address all continuous production of organic chemical compounds except PVC, ethylene and propylene productions.

This activity is consequently not represented by a production but by its NMVOC emissions. The representative activity unit used is the annual NMVOC emissions expressed in kt NMVOC/year.

NMVOC emissions result from:

- Diffuse emissions from storages of raw materials, storages of final products, loading and unloading operations and waste water treatment plants
- Fugitive emissions.

Diffuse emissions are not addressed in the background document. Only fugitive and stack emissions are addressed.

Organic chemical industry is addressed by the EC directive 96/61/EC of council of 1996, September 24<sup>th</sup> related to Integrated Pollution Prevention and Control (IPPC).

The methodology for this sector has been prepared on the basis of information provided by an expert group from UIC and CEFIC [4], [5].

This activity emits NMVOC. At a EU25 level for the year 2000 (according to the RAINS model: version CP\_CLE\_Aug04(Nov04)), NMVOC emissions were 178.8 kt representing 1.68% of total NMVOC emissions [10]. The resulting average emission factor is just lower than 1 t NMVOC /t NMVOC, indicating that reduction techniques are not commonly used in 2000 in the EC. These estimations could be modified in a near future due to information delivered by national experts during the bilateral consultations scheduled in 2005.

Organic chemical industry was considered as a unique sector in previous RAINS [9] version. EGTEI provides a first approach to tackle this complex sector by considering three sub activities (speciality chemical industry is not new and already considered in RAINS) in order to better represent costs and abatement scenarios. Data provided by EGTEI, emission factors, efficiencies and costs of reduction techniques are presently used in the new RAINS version for the modelling work carried in the scope of the CAFÉ programme and the revision of the Gothenburg Protocol and national emission ceiling directive.

Only one reference installation is considered.

Four primary measures based on different leak and detection and repair programmes (LDAR) are considered. In some Member states such programmes are mandatory.

EGTEI provides default emission factors (EF) with abatement efficiencies, investments, variable and fixed operating costs (OC) as well as unit costs expressed in €/t NMVOC abated and €/t NMVOC (as activity) for the four reduction measures.

Unit costs range from -127 to - 31 €/t NMVOC abated according to the reduction measure considered and from -14 to -44 €/t NMVOC (as activity). Negative costs indicate that savings are high and counter balance investments and operating costs.

National experts have to collect only one country specific parameter (wage costs) and one country and sector specific parameters (NMVOC recovered based on ethylene costs). These parameters can be very easily known through the chemical industry associations. National experts have also to provide the trend in activity level from 2000 to 2020 as well as the application and applicability rates of each abatement technique.

As the sector representation in RAINS [10] is presently based on the EGTEI proposal, it is recommended to national experts to complete ECODAT with country specific parameters which are not known from CIAM.

In the future however, any new technology which could be developed should be considered by EGTEI in the background document to continuously improve the sector representation and the EGTEI capacity to describe new technologies. It should be necessary to review the considered efficiencies regularly to update them and perhaps define an additional reduction technique if necessary.

#### 2. European regulation

Organic chemical industry is addressed by the EC Directive 96/61/EC of council of 1996, September 24<sup>th</sup> related to Integrated Pollution Prevention and Control (IPPC). No direct emission limit values are introduced in this Directive. Nevertheless permit emission limit values have to be based on BAT performances.

### 3. Methodology developed within EGTEI to represent the sector

### 3.1 Definition of the reference installation

From data collected by UIC at French level [4] and CEFIC at European level, a reference installation defined as unit emitting 230 t NMVOC per year has been taken into account. Stack NMVOC emissions are assumed to be negligible.

The boundaries of the reference installation taken into account for estimating costs of reduction measures, exclude diffuse emissions from storages and loading/unloading operations.

On average according to UIC, this installation has about 12000 potentially leaking points (valves, flanges, pumps, open ends...) of which 80% are accessible for control and repair. In the scope of this study, a simplified installation with 40 % valves and 60 % flanges is considered.

These assumptions are based on data collected by UIC at French level [5] and CEFIC at European level. The different VOC emission sources from different types of installations have been collected [5]. It has to be outlined that the measurement techniques used in Europe to estimate fugitive emissions from processes of the chemical industry are not yet well defined.

Emissions depend on the methodology used. The EPA 21 method [6] is used sometimes.

There are discrepancies between emissions declared in the past by industry and the emissions estimated now with EPA 21 method. The EPA 21 method presents several estimation techniques (emission factors, generic correlations for SOCMI (Synthetic Organic Chemical Manufacturing Industry). Each of these techniques gives different results and this can have consequences on the cost effectiveness of the LDAR programmes.

Fugitive emissions of the reference installation have been defined with the use of correlation equations provided by US EPA for SOCMI [6]. From a monitoring result expressed in ppm of NMVOC around a leaking point, the correlations give a quantity of VOC emitted in kg/year. It has to be kept in mind that the use of specific correlations which can be derived by industry for some processes gives lower emissions than the use of general SOCMI equations provided by EPA. The CEN [12] is presently

working on the redaction of a standard for the determination of NMVOC leaks from process equipment. The use of EPA correlations is recommended if user defined correlations are not available.

Reference Installation Code (RIC)	Description
01	Chemical unit – Reference VOC emissions 230 t VOC. Stack VOC emissions from the process assumed to be very low. Fugitive emissions: 12 000 potentially leaking points (valves, pumps, flanges, open ends); 9 600 accessible points. 40 % valves, 60 % flanges.

 Table 3.1.1:
 Definition of the reference installation

#### 3.2 Definition of emission abatement techniques

#### 3.2.1 Primary measures

Fugitive emissions can be reduced through a Leak Detection And Repair programme (LDAR) [6].

The LDAR technique consists in measuring the VOC concentration in the atmosphere around the potential leaking point, then selecting equipments leaking over a defined threshold value and finally operating a repair on those leaking items.

A LDAR programme is established according to the following principles:

- The definition of what constitutes a leak and fixation of corresponding thresholds,
- The fixation of the frequency of inspections,
- The listing and identification of components included,
- The procedures concerning repair of leaking components depending on the leak category.

Repair procedures related to leak category considered in primary measures are indicated in table 3.2.1.1.

4 LDAR programmes are considered for cost estimation. They differ from the leak thresholds considered and type of maintenance carried out.

Primary Measure Code PMC	Description		
00	No LDAR programme		
01	Establishment of the LDAR programme Inventory of all components and establishment of a database. First survey of all potential leak points of the plant (100 % of accessible points are considered and controlled), analysis of the first results of the survey. Tightening for points > 5 000 ppm Basic maintenance for 100 % points > 100 000 ppm during first shut down. Annual control between two shutdowns Intermediate campaign before shutdown: 20 % of accessible points are controlled each year (in five years all points are controlled). Tightening each year for 100 % controlled points > 5 000 ppm. Next Shutdown. Basic maintenance for 100 % measured points (during the 5 years) > 100 000 ppm.		

Table 3.2.1.1: Measures of reduction considered

02	Establishment of the LDAR programme				
	Inventory of all components and establishment of a database.				
	First survey of all potential leak points of the plant (100 % of accessible points are				
	considered and controlled), analysis of the first results of the survey.				
	Tightening for points > 1000 ppm.				
	Basic maintenance for points > 10 000 ppm during the first shut down.				
	Annual control between two shutdowns				
	Intermediate campaign before shutdown : 20 % of accessible points are				
	controlled each year (in five years all points are controlled).				
	Tightening each year for 100 % controlled points > 1 000 ppm.				
	Next Shutdown				
	Basic maintenance for 100 % measured points (during the 5 years) > 10 000				
	ppm.				
03	Establishment of the LDAR programme				
	Inventory of all components and establishment of a database.				
	First survey of all potential leak points of the plant (100 % of accessible points are				
	considered and controlled), analysis of the first results of the survey.				
	Tightening for points $> 1000$ ppm .				
	Basic maintenance for 100 % points > 5 000 ppm during the first shut down.				
	Annual control between two shutdowns				
	Intermediate campaign before shutdown : 20 % of accessible points are				
	controlled each year (in five years all points are controlled).				
	Tightening each year for 100 % measured points > 1 000 ppm.				
	Next Shutdown				
0.1	Basic maintenance for 100 % measured points (during the 5 years) > 5 000 ppm.				
04	Establishment of the LDAR programme				
	Inventory of all components and establishment of a database.				
	First survey of all potential leak points of the plant (100 % of accessible points are				
	considered and controlled), analysis of the first results of the survey.				
	Tightening for points > 1 000 ppm				
	Basic maintenance for flanges points >10 000 ppm during the first shut down.				
	Heavy maintenance for valves points > 10 000 ppm during the first shut down.				
	Annual control between two shutdowns				
	Intermediate campaign before shutdown: 20 % of accessible points are controlled				
	each year (in five years all points are controlled).				
	Tightening each year for points > 1 000 ppm.				
	Next Shutdown				
	Basic maintenance for 100 % measured (during the 5 years) > 10 000 ppm.				
	Heavy maintenance for 100 % measured (during the 5 years) > 10 000 ppm.				

### 3.2.2 Secondary measures

No secondary measure is taken into account.

## 4. Country specific data to be collected

Different types of country specific data have to be collected to give a clear picture of the situation in each Party. EGTEI proposes default values for these economical parameters which can be modified by the national expert if better data are available.

For down stream units, only one country and sector specific economic parameter and one country specific economic parameter are required. Activity and country specific economic parameter to define is the cost of ethylene assumed to represent the largest feedstock used and NMVOC recovered. They are presented in table 4.1 and 4.2 as the default costs proposed by EGTEL for this activity.

They are presented in table 4.	1 and 4.2 as the default	costs proposed by EGIEI for this activity.

Parameter	Default costs provided by EGTEI	Country specific cost	
Wages [€/h]	24.3	to be provided by national experts	

Table 4.1: Country specific economic parameter cost

Table 4.2. Activity and country specific economic parameter cost						
Parameter	Default cost provided by EGTEI	Country specific cost				
Ethylene €[net of taxes]/t	400	to be provided by national experts				

**Table 4.2:** Activity and country specific economic parameter cost

Information concerning activity levels from 2000 to 2020 as well as the description of the control strategy is also necessary (these data can be directly entered in ECODAT). A full definition of the work to be done by national experts is provided in the general EGTEI methodology [7].

The national expert can also modify the default unabated emission factor proposed by EGTEI to represent the reference situation of the coil coating for all Parties in a range of  $\pm$  10% with appropriate explanations.

 Table 4.2: Unabated emission factor [t NMVOC emitted / t NMVOC]

Default emission factor	Country specific emission factor		
1.0	To be provided by national experts		

**Remark:** For this activity, a simple method has been used in ECODAT to estimate costs. In fact for the time being to avoid complex computer programme, only default values can be used. For estimating countries specific costs the EXCEL sheet has to be used.

# 5. Default emission factors and cost data defined with the EGTEI methodology

Table 5.1 presents an overview of all data provided by the EGTEI methodology for the reference installation: default emission factors with abatement efficiencies, investments, variable and fixed operating costs as well as unit costs.

Table 5.1: Emission factors (EF),	abatement efficiencies,	investments,	operating costs (OC	C) for each
combination and unit costs				

RIC PMC SMC	NMVOC EF [t NMVOC/t NMVOC]	Abatement efficiency [%]	Investment [€]	Variable OC [€y]	Product recovery [€y]	Unit cost [∉t NMVOC abated]	Unit cost [ <del>€/</del> t NMVOC]
01 00 00	1	0	0	0	0	0	0
01 01 00	0,66	34	79 780	11 580	31 360	-127	-43.2
01 02 00	0,64	36	85 300	12 440	33 150	-123	-44.2
01 03 00	0,64	36	88 930	12 990	33 360	-113	-40.8
01 04 00	0,53	47	157 870	20 520	43 360	-31	-14.7

Negative annual costs means that LDAR programme cost is counter balanced by product saving.

It has to be kept in mind that NMVOC fugitive emissions depend on the method used for estimating them. EGTEI data are based on the use of EPA 21 method considering only generic correlations provided by EPA (the use of specific correlations could give lower emissions). The use of other types of estimation methods could give other costs.

### 6. Relevance of EGTEI information for integrated assessment modelling (IAM)

In the previous RAINS version [9], the sector ORG PROC represented the organic chemical industry as a whole. Storage of chemical products was considered under sector ORG\_STORE.

The module has been modified to take into account the EGTEI proposal. The organic chemical industry has been divided in three sub activities ("pharma" already represent the speciality organic chemistry). For down stream unit (under OTH\_ORG\_PR) the following reduction techniques are considered. Reduction measure definitions and their efficiencies are based on EGTEI proposals:

- OTH\_ORG -PR-LDARI: 34%
- OTH\_ORG -PR-LDARII: 36%
- OTH\_ORG -PR-LDARIII: 36%
- OTH\_ORG -PR-LDARIV: 47%

Data provided in EGTEI approach (emission factors) have been implemented in the new version of the RAINS model [10] for the modelling work carried out in the scope of the CAFÉ programme and the revision of the Gothenburg protocol. Costs are not yet available on the web site. According to information received from Z. Klimont, some other rules have been used to define investment costs for RAINS from EGTEI data for this activity (in order to remove labour costs from investments).

For this activity now, data provided by national experts through ECODAT can then be directly used by IIASA for introduction in the RAINS model.

## 7. Perspective for the future

The EGTEI proposal for the chemical industry representation in three sub sectors (steam cracking, PVC production by the suspension process and downstream units) and definitions of abatement techniques has been considered in the last update of RAINS [10].

NMVOC emissions mainly occur from leak on equipment. Monitoring of fugitive emissions is a very new activity. It should be interesting to update emission factors with results of monitoring which could be carried out in Europe mainly in countries where regulations have been implemented. It should be also necessary to update costs and for this, new experience in industry could be used.

#### 8. Bibliography

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- [10] Review of data used in RAINS-VOC model http://www.iiasa.ac.at/web-apps/tap/RainsWeb/
- [11] CITEPA. National reference centre for emissions inventories

## Example of data collection and use of EGTEI data – Case of France

# A. Country specific data collection and scenarios developed by the national expert

The French national expert has been able to complete ECODAT for downstream units with help of CITEPA [11] and consultation of the UIC [4].

All data have been prepared by the French national expert for the bilateral consultations member state – CIAM which ended in March 2004.

#### Country and sector specific economic parameters

For down stream units, only one country and sector specific economic parameter and one country specific economic parameter are required. There are presented in table A.1 and 4.2.

 Table A.1: Country specific economic parameter cost

Parameter	French specific cost
Wages [€/h]	23.4

#### Table A.2: Activity and country specific economic parameter cost

Parameter	Default cost provided by EGTEI	French specific cost
Ethylene €[net of taxes]/t	400	400

#### Activity level

The activity level from 2000 to 2020 is assumed to increase of 3 % per year.

Table A.3: Activit	ty levels on the reference	Installation	(kt NMVOC /	year)
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		0005	0010		0000
RIC	2000	2005	2010	2015	2020
01	40.7		10.1	04.0	
01	13.7	15.9	18.4	21.3	24.7
_	-		-	-	

#### **Emission factor**

The French emission factor used is equal to the default emission factor provided by EGTEI.

#### Table A.4: Unabated emission factor

Default unabated emission factor	French unabated emission factor			
[t NMVOC emitted /t NMVOC]	[t NMVOC/t NMVOC]			
1	1			

#### Current legislation control (CLE) scenario

In the current legislation control scenario (CLE), application rates of the different abatement techniques depend on regulation implemented and on dates of compliance required by this regulation but also internal development not driven by regulation.

In the CLE scenario, reduction technique application rates from 2005 to 2020 have been defined considering the requirement for compliance with the French regulation for this type of industry (Circulaire of November 23<sup>rd</sup>, 2004). NMVOC limits are implemented for this activity. The compliance date for existing installations is October 2005. However at this date, all installations will not be in compliance. This has been taken into account through the low application rate of measures 01 or 02 in 2005.

The application rates for the current legislation scenario are presented in table A.5.

Table A.5: Application rates and applicability for each combination of reduction measures in CLE scenario

RIC PMC SMC	Application rate in 2000 [%]		Appl. [%]	Application rate in 2010 [%]	Appl. [%]	Application rate in 2015 [%]	Appl. [%]	Application rate in 2020 [%]	Appl. [%]
01 00 00	100	50	100	0	100	0	100	0	100
01 01 00	0	50	100	50	100	50	100	0	100
01 02 00	0	0	100	50	100	50	100	100	100
01 03 00	0	0	100	0	100	0	100	0	100
01 04 00	0	0	100	0	100	0	100	0	100
Total RIC 01	100	100	-	100	-	100	-	100	-

#### B. Trends in emissions and total costs of the CLE scenario

Table B.1 presents trends in NMVOC emissions from 2000 to 2020 according to the CLE scenario and associated total annual costs (Data presented in the table B.1 are directly provided by ECODAT and based on input parameters defined in chapter A).

Table B.1: trends in emissions and total annual costs of emission reductions in the CLE scenario

	2000	2005	2010	2015	2020
NMVOC emissions	t COV				
CLE scenario	13689	14790	15270	13863	15823
Total annual costs	k€year	k€year	k€year	k€year	k€year
CLE scenario	0	0	-147	-426	-1000